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Neutrino Masses and Fermion Flavor

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Abstract

Neutrino Masses and Fermion Flavor

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In this dissertation, I discuss the role of neutrino masses and fermion flavor in modern particle physics and present several efforts aimed at exploiting these properties in searches for new physics. In particular, I discuss (1) the effects of neutrino decays on neutrino propagation; (2) the sensitivity of the Deep Underground Neutrino Experiment (DUNE) to new physics scenarios; (3) how the flavor structure of the standard model (SM) might arise from an $SU(2)$ symmetry; (4) the sensitivities of experiments looking for lepton-flavor violation to lepton-number violation; and (5) an algorithm for constructing chiral fermion sectors in nonabelian gauge models.
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B.1 The tree-level (a) and one-loop-level (b) contributions of 0$\nu\beta\beta$ from the model presented in Eq. (B.1.2).
CHAPTER 1

Introduction

1.1. What’s Wrong with the Standard Model?

The standard model of particle physics (SM) has proven to be remarkably successful in describing physical phenomena. In the half century since its formulation \[21\,26\], it has withstood nearly every experimental challenge\(^1\) culminating in the discovery of the Higgs boson \[38\,39\]. However, it is well known that the SM is not the ultimate description of the natural world; there are observed phenomena that lie outside of its purview. These include the following:

(1) Gravity is absent from the SM, and a consistent quantum-mechanical description of gravity remains elusive.

(2) The Universe is, as far as we can tell, comprised of matter with a negligible amount of antimatter (see Ref. \[40\] and references therein). Various mechanisms have been proposed to explain this, but no clear candidate has emerged.

(3) Our Universe contains a substantial amount of nonluminous matter, named dark matter \[41\,42\]. The dark matter is not comprised of SM particles and has not been detected in terrestrial experiments.

(4) The acceleration of the expansion of the Universe \[41\,44\] suggests that there exists a form of energy – dubbed dark energy – that is governed by a negative

\(^1\)Exceptions to this include modest tension with measurements of anomalous magnetic moments \[1\,27\,29\] and of some \(b\)-related processes \[30\,37\].
equation-of-state parameter. The SM cannot make predictions regarding dark energy.

(5) Neutrino oscillations \cite{45,56} have revealed that neutrinos have small masses, but the SM is agnostic regarding these.

(6) The fermions of the SM appear in three otherwise identical copies – known as flavors or generations – except that their masses differ by orders of magnitude.

This dissertation focuses on the last two items – neutrino masses and fermion flavor – and my attempts to address various phenomena associated with them. In the remainder of this section, I will address in more detail why these questions are important.

1.1.1. Neutrino Masses

There are two well-motivated mechanisms for generating neutrino masses. The first is the Dirac mass mechanism, wherein the left-chiral neutrino field $\nu_L$ is paired with a right-chiral field $N_R$, often called a sterile neutrino, to form a massive Dirac field. This is precisely how the other fermions of the SM acquire their masses. For Dirac fields, particles and antiparticles are distinct physical objects.

The other mechanism is the Majorana mass mechanism, wherein the neutrino and the antineutrino are the same object. The existence of a Majorana (component of a) neutrino mass necessarily implies that lepton number – the accidental, global $U(1)$ symmetry of the SM under which charged leptons and neutrinos have charge $+1$ while their antiparticles have charge $-1$ – is not conserved in Nature. I note two consequences of this.

Firstly, Majorana neutrino masses would imply that there must be new physics at some high scale, and that this physics is quite different from the SM. This could be one of
the strongest clues we have regarding the nature of new physics, especially if dark matter experiments continue to yield null results. It would also indicate that any number of other lepton-number-violating processes might occur in Earth-based experiments; more will be said of this in chapter 7.

Secondly, one of the necessary conditions for generating a matter-antimatter asymmetry [57] is that baryon number is violated. In models of leptogenesis [58], violation of lepton number is transferred to baryon number, thus (potentially) allowing for the asymmetry we observe today. I will not discuss this further here, but understanding whether or not lepton number is violated, and how large that violation is, has far-reaching consequences beyond simply understanding neutrino oscillations.

1.1.2. Fermion Flavor – Who Ordered That?

The existence of three flavors of fermions does not, strictly speaking, require new physics in order to be explained. Fermion masses and mixings could be random, lacking any pattern or explanation. While this anarchy hypothesis [59][62] cannot be logically excluded, it is unsatisfactory insofar as it provides no predictions regarding flavor phenomena; it is purely reactive. Acknowledging that this is a matter of theoretical prejudice, the dynamics of flavor will be explained in this dissertation by proposing an underlying structure, as opposed to randomness.

One of the overarching themes of physics in the last century was that the behavior of a physical system is dictated by the symmetries that it possesses. It is natural, then, to apply this philosophy to flavor in the SM. Several historical attempts to explain flavor will be outlined in chapter 6, but each is predicated on the notion that the low-energy flavor
dynamics we observe are the remnant of some (badly broken) high-energy symmetry. If this is the case, then the flavor sector could be our best chance to see new symmetries of Nature beyond those on which the SM is built – $SU(3)_c \times SU(2)_L \times U(1)_Y$, CPT and Lorentz invariance – particularly if supersymmetry continues to elude experiment.

1.2. This Dissertation

This dissertation contains my attempts to address phenomena related to neutrino masses and flavor physics (often at the same time). In chapters 2 and 3, I present analyses in which nonstandard effects – in particular, nonorthonormality of the neutrino mass basis and neutrino decay – are introduced into neutrino oscillations. In chapters 4 and 5, I discuss the sensitivity of the Deep Underground Neutrino Experiment (DUNE) to additional neutrino degrees of freedom in two scenarios of new physics. In chapter 6, I present a proposal for how the flavor structure of the SM may be governed by a single vectorial $SU(2)$ symmetry, and in chapter 7, I discuss the sensitivity of the Mu2e experiment to the scale of lepton-number-violating (LNV) physics. Lastly, in chapter 8, I present an algorithm for generating chiral fermion sectors in models with nonabelian gauge symmetry.

The chapters that follow are based on the following papers:


CHAPTER 2

Nonunitary Neutrino Propagation from Neutrino Decay

2.1. Introduction

Neutrino oscillations, first unambiguously observed towards the end of the twentieth century, have proven to be a powerful tool for fundamental physics research. Their observations revolutionized our understanding of neutrinos, revealing that these have tiny but nonzero masses. Moreover, they can be used to reveal new phenomena including the existence of new, weaker-than-weak interactions involving neutrinos and ordinary matter – which lead to non-standard matter effects [63] – or the existence of light sterile neutrinos or new contributions to the charged-current weak interactions – which lead to different nonunitary $3 \times 3$ leptonic mixing matrices [64–67]. Neutrino oscillations also provide powerful testbeds of some of the most basic assumptions of fundamental physics [68], including tests of whether neutrino propagation is Lorentz invariant [69,70], whether neutrinos obey the $CPT$ theorem [69,71], whether there are exotic sources of decoherence in the time-evolution of the neutrino states [72,73], etc.

In this chapter, we explore the consequences of the hypothesis that the neutrino propagation Hamiltonian is not Hermitian. When applied to the active neutrinos, these include new parameters for neutrino oscillation observables that are not captured by the different scenarios considered in the literature to date. We compute the transition probabilities,
concentrating on the case where the nonunitary effects are small, and discuss the different qualitative aspects of the associated phenomenology.

It is important to stress that nonunitary time evolution need not be an extravagant hypothesis. Neutrino propagation is nonunitary if one takes into account the possibility that neutrinos interact with and decay into other generic light states, a generalization of what is known to occur in the neutral kaon system \cite{74, 75}. A similar version of this phenomenon is also realized in resonant leptogenesis \cite{76}.

### 2.2. Formalism

We start by postulating that the neutrino states involved in the production and detection processes are orthonormal. Generically, we refer to these as flavor eigenstates $|\nu_\alpha\rangle$ and our assumption amounts to imposing

\begin{equation}
\langle \nu_\alpha | \nu_\beta \rangle = \delta_{\alpha\beta},
\end{equation}

where $\alpha, \beta$ are flavor indices. For the case of the light, active neutrinos of the standard model (SM), this assumption certainly holds true if both production and detection occur via the standard charged-current weak interactions and if there are no additional neutrino states. In that case, $\alpha, \beta = e, \mu, \tau$. In practice, this implies that as long as the production and detection processes occur through the weak interactions, there are no flavor-changing phenomena in the limit that the baseline is much shorter than the dimensionful parameters that govern propagation, as will become clear momentarily.

It is important to stress the importance of the assumption that there are no additional neutral fermions that can mix with the three SM flavor states. This assumption sets our
framework apart from the nonunitarity scenario analyzed in [67] where such an assumption
is implicit. In [67], the neutrino state appearing in the left-handed charged current along
with the lepton $\alpha$ is written as the linear combination $|\nu_\alpha\rangle = \sum_i U_{\alpha i}|\nu_i\rangle$ where $i$ runs over
all mass eigenstates, including the heavy ones. Since the production of physical $|\nu_i\rangle$ states
is kinematically forbidden if they are sufficiently heavy, the linear transformation that
rotates from the produced flavor state to the orthogonal mass eigenstates is nonunitary.

On the other hand, we shall see below that in our framework the implicit assumption
is that there is new physics which can mediate neutrino decay into as-of-yet-unknown
states. The neutrino states involved in weak interactions are those of the SM and they
are orthogonal much in the same way as kaon states produced by strong interactions
are orthogonal. In flight, however, new physics can produce an effectively nonunitary
propagation, playing a role analogous to that played by weak interactions in the kaon
system.

Neutrino flavor-evolution in space is governed by the usual Schrödinger-like equation,
valid in the limit of ultra-relativistic neutrinos assuming that the initial states are perfectly
coherent,

\begin{equation}
\frac{id}{dL}|\nu_\alpha(L)\rangle = [\mathcal{H}_{\text{eff}}]_{\alpha\beta}|\nu_\beta(L)\rangle,
\end{equation}

where $L$ is the distance traversed by the neutrino. The effective Hamiltonian $\mathcal{H}_{\text{eff}}$, which
we assume is a generic matrix, can be parameterized as

\begin{equation}
\mathcal{H}_{\text{eff}} = M - i\Gamma,
\end{equation}
where $M$ and $\Gamma$ are Hermitian matrices. For $\Gamma = 0$, we have standard oscillations. The eigenvalues of $M$ are, as usual, $m_i^2/2E$, where $E$ is the neutrino energy and $m_i, i = 1, 2, \ldots$, are real. $\Gamma$ also has real eigenvalues and can be diagonalized by a unitary matrix. We explore the most general case where $M$ and $\Gamma$ cannot be simultaneously diagonalized, i.e., the mass eigenstates need not coincide with the eigenstates of the interaction that induces neutrino decay.

Time evolution governed by a non-Hermitian Hamiltonian is generically expected if there are new interactions that couple the light neutrinos to new, light many-particle states. We provide a quick description of the formalism, which has been developed for the kaon system \cite{[4, 5, 7]} and can be readily adapted to neutrino propagation. The main difference between the two is that in the neutrino case there are no constraints from $CPT$ invariance which, for the kaons, lead to some simplifications.

Consider a system consisting of light neutrino states $|\nu_0i\rangle$ along with new many-particle states $|\phi_0k\rangle$, with the index $k$ understood to run over both discrete and continuous labels required to identify such states. It is convenient for this analysis to work in the mass basis so that $|\nu_0i\rangle$ and $|\phi_0k\rangle$ are eigenstates of a free-particle Hamiltonian $H_0^0$:

\begin{equation}
(2.2.4) \quad H_0^0|\nu_0i\rangle = E_i|\nu_0i\rangle, \quad H_0^0|\phi_0k\rangle = E(k)|\phi_0k\rangle.
\end{equation}

The complete propagation Hamiltonian $H$ of the system is assumed to involve new interactions and can be split into

\begin{equation}
(2.2.5) \quad H = H_0 + H'.
\end{equation}
In the context of neutrino oscillations, $\mathcal{H}_0$ describes the standard propagation Hamiltonian for the neutrino mass eigenstates in the absence of new interactions. On the other hand, the new physics piece $\mathcal{H}'$ is completely general. In particular, it can induce transitions between the $|\nu_{0i}\rangle$ and the $|\phi_{0k}\rangle$.

At any time $t$, the state of the system $|\psi(t)\rangle$ can be written as a linear combination of the light neutrino eigenstates $|\nu_{0i}\rangle$ and the $|\phi_{0k}\rangle$ as

$$|\psi(t)\rangle = \sum_i c_i(t) |\nu_{0i}\rangle + \sum_k C_k(t) |\phi_{0k}\rangle,$$

(2.2.6)

The time evolution of $|\psi(t)\rangle$ is governed by the Schrödinger equation

$$i \frac{d}{dt} \begin{pmatrix} c(t) \\ C(t) \end{pmatrix} = \mathcal{H} \begin{pmatrix} c(t) \\ C(t) \end{pmatrix},$$

(2.2.7)

where $c(t)$ and $C(t)$ are column vectors formed by the coefficients $c_i(t)$ and $C_k(t)$ respectively. Eq. (2.2.7) is exact.

Because $\mathcal{H}$ is Hermitian, the evolution of the complete system is unitary. Any neutrino produced at time zero satisfies $\sum_i |c_i(0)|^2 = 1$, while the probability that it remains a neutrino at some time $t$ is $P_{\nu\rightarrow\nu} = \sum_i |c_i(t)|^2$. It is clear that

$$P_{\nu\rightarrow\nu} = \sum_i |c_i(t)|^2 = 1 - \sum_k |C_k(t)|^2 \leq 1,$$

(2.2.8)

for all $t$\footnote{Note that we make no assumptions about the number of $|\nu_{0i}\rangle$ states. New single-particle states – e.g., sterile neutrinos – would simply imply that there are more $|\nu_{0i}\rangle$ states than active neutrinos.}
For the case in which the processes of production and detection involve only linear combinations of neutrino states $|\nu_{0i}\rangle$, it has proven useful to devise a way to reduce Eq. (2.2.7) to a differential equation only for the vector $c(t)$. This can be accomplished under the *Weisskopf-Wigner approximation* (WW). WW assumes that the spectrum of accessible $|\phi_{0k}\rangle$ modes is broad and that the matrix elements of the Hamiltonian with respect to the new states $\langle \phi_{0j}|\mathcal{H}'|\phi_{0k}\rangle$ can be neglected. Under these conditions, \[ i\frac{d}{dt} c(t) = \mathcal{H}_{\text{eff}} c(t) = (M - i\Gamma) c(t), \] where $M$ and $\Gamma$ are Hermitian matrices with matrix elements given by \[ M_{ij} = (E_i - \bar{E})\delta_{ij} + \langle \nu_{0i}|\mathcal{H}'|\nu_{0j}\rangle \] \[ - \sum_k \frac{\langle \nu_{0i}|\mathcal{H}'|\phi_{0k}\rangle\langle \phi_{0k}|\mathcal{H}'|\nu_{0j}\rangle}{E(k) - \bar{E}}, \] \[ \Gamma_{ij} = \pi \sum_k \langle \nu_{0i}|\mathcal{H}'|\phi_{0k}\rangle\langle \phi_{0k}|\mathcal{H}'|\nu_{0j}\rangle\delta(E(k) - \bar{E}) \] and $\bar{E}$ is the average energy of the neutrino beam. Within WW, Eq. (2.2.3) appears naturally as a result of integrating out the new states, taking into account that the new states may be on-shell. Moreover, it is easy to see that $\Gamma$ is positive definite. That is, WW only yields neutrino states that decay into the new states but never the other way around. Furthermore, off-diagonal $\Gamma_{ij}$ occur when different $\mathcal{H}_0$ eigenstates can access the same $\phi_{0k}$ state, i.e., the different neutrino mass eigenstates can decay into the same final state.

In this work we assume that neutrino evolution is dictated by Eq. (2.2.9), but we are also be interested in violations of WW that may invalidate the constraint that $\Gamma$ is
positive definite. In particular, these could happen if the matrix elements $\langle \phi_0 | \mathcal{H}' | \phi_0 \rangle$ cannot be neglected. In other words, we assume that there are conditions under which Eq. (2.2.9) is a good description of neutrino propagation physics while the restriction that $\Gamma$ is positive definite need not apply. On the other hand, Eq. (2.2.8) is a consequence of the more general hypothesis that the neutrinos mix with new, unidentified degrees of freedom, so we pay special attention to what these constraints imply. Of course, if one wishes to simply explore how well neutrino oscillations are governed by the standard laws of quantum mechanics, no constraints on $\Gamma$, other than those imposed by experimental data, need apply.

Eq. (2.2.9) can be written in the flavor basis, as in Eq. (2.2.2), by performing the unitary transformation that links the two orthonormal sets of states $|\nu_0 \rangle$ and $|\nu_\alpha \rangle$. Solving Eq. (2.2.2) is straightforward. Let $N$ be a generic matrix such that

\begin{equation}
(2.2.12) \quad \tilde{\mathcal{H}} = N \mathcal{H} N^{-1}, \quad \tilde{\mathcal{H}} = \text{diag}\{h_1, h_2, \ldots\},
\end{equation}

where $h_i$ are complex numbers, and define the eigenstates $|\nu_i \rangle$ of the effective Hamiltonian as

\begin{equation}
(2.2.13) \quad |\nu_\alpha \rangle = N_{\alpha i} |\nu_i \rangle.
\end{equation}

The matrix $N$ is not uniquely defined by Eq. (2.2.13); rescalings of the eigenvalues are still possible. In order to define it completely, we further impose

\begin{equation}
(2.2.14) \quad \langle \nu_i | \nu_i \rangle = 1, \forall i.
\end{equation}
In general, the states $|\nu_i\rangle$ and $|\nu_j\rangle$, $i \neq j$, are \textit{not} orthogonal. We define

\begin{equation}
(2.2.15) \quad \langle \nu_i | \nu_j \rangle \equiv H_{ij} = (\mathbb{I} + \delta)_{ij}
\end{equation}

where $\mathbb{I}$ is the identity matrix, $H$ and $\delta$ are Hermitian matrices, and $\delta_{ii} = 0, \forall i$. It is convenient to express $N$ in terms of $\delta$. Eq. \((2.2.1)\) and \((2.2.13)\) imply

\begin{equation}
(2.2.16) \quad N (\mathbb{I} + \delta^T) N^\dagger = \mathbb{I},
\end{equation}

hence

\begin{equation}
(2.2.17) \quad N \left( \mathbb{I} + \delta^T \right)^{1/2} = V,
\end{equation}

\begin{equation}
(2.2.18) \quad N = V \left( \mathbb{I} + \delta^T \right)^{-1/2},
\end{equation}

where $V$ is a unitary matrix. When $\delta = 0$, $N$ is a unitary matrix and the Hamiltonian eigenstates form an orthonormal basis in spite of the fact that the $h_i$ are, in general, complex. This special case is the one usually considered when one addresses neutrino decay (see, for example, \cite{79, 80}; for a detailed discussion see \cite{81}). It is equivalent to postulating that $M$ and $\Gamma$ can be simultaneously diagonalized, and the eigenvalues of $\Gamma$ are proportional to the lifetimes of the neutrino mass eigenstates.

$\Gamma \ll M$ implies $\delta_{ij} \ll 1$ and

\begin{equation}
(2.2.19) \quad N \sim V \left( \mathbb{I} - \delta^T / 2 \right).
\end{equation}

We will restrict our discussions to this case, unless otherwise noted.
The solution to Eq. (2.2.2), assuming that the neutrino is in state $|\nu_\alpha\rangle$ at $L = 0$, is

$$|\nu_\alpha(L)\rangle = \sum_i N_{\alpha i} e^{-ih_i L(N^{-1})_{i\beta}} |\nu_\beta\rangle,$$

and the oscillation amplitudes are

$$A_{\alpha\beta} = \langle \nu_\alpha | \nu_\beta(t) \rangle = Ne^{-i\tilde{\Phi} L N^{-1}},$$

trivially related to the oscillation probabilities, $P_{\alpha\beta} \equiv |A_{\alpha\beta}|^2$, which are the observables directly accessible to neutrino oscillation experiments.

Eq. (2.2.21) leads to unitarity-violating effects that are qualitatively different from postulating the existence of new oscillation lengths (i.e., light sterile neutrinos), or postulating that the weak-interaction eigenstates are not orthogonal [65, 67]. Some of the differences are easy to spot. For instance Eq. (2.2.21) does not allow for any flavor change in the limit $L \to 0$ ($NN^{-1} \equiv I$ even if $N$ is not unitary), unlike the effects discussed in [67]. Also, Eq. (2.2.21) does not contain any new oscillation lengths: the new dimensionful parameters lead to exponential decay (or growth) of $P_{\alpha\beta}$, as will be discussed in more detail in the remainder of this chapter.

2.3. Two-Neutrino Oscillations

It is instructive to discuss the case of two neutrino flavors in detail in order to illustrate the phenomena described by Eq. (2.2.21). In this case, we define

$$\langle \nu_1 | \nu_2 \rangle \equiv e^{i\kappa},$$
where $\epsilon, \zeta$ are real and positive, $\zeta \in [0, 2\pi)$. Further defining $h_{1,2} = a_{1,2} - ib_{1,2}$ and parameterizing the $2 \times 2$ unitary matrix $V$ with the mixing angle $\theta$, in the usual way\footnote{It is straightforward to show that, like in the standard unitary case, potential Majorana phases in $V$ play no role in neutrino oscillations, even for $\delta_{CP} \neq 0$.} we find

$$N \sim \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} 1 & -\frac{1}{2} \epsilon e^{-i\zeta} \\ -\frac{1}{2} \epsilon e^{i\zeta} & 1 \end{pmatrix},$$

keeping in mind that $\epsilon \ll 1$. Setting $\alpha, \beta = e, \mu$ for the sake of definiteness we find the oscillation probabilities

$$P_{ee} = e^{-2b_1 L} \cos^4 \theta + e^{-2b_2 L} \sin^4 \theta$$

$$+ \frac{1}{2} e^{-(b_1 + b_2) L} \sin 2\theta \left[ \sin 2\theta \cos \Delta L - 2\epsilon \sin \zeta \sin \Delta L \right],$$

$$P_{e\mu} = \frac{1}{4} \left( e^{-2b_2 L} + e^{-2b_1 L} - 2e^{-(b_1 + b_2) L} \cos \Delta L \right) \sin 2\theta \left( \sin 2\theta - 2\epsilon \cos \zeta \right),$$

$$P_{\mu e} = \frac{1}{4} \left( e^{-2b_2 L} + e^{-2b_1 L} - 2e^{-(b_1 + b_2) L} \cos \Delta L \right) \sin 2\theta \left( \sin 2\theta + 2\epsilon \cos \zeta \right),$$

$$P_{\mu\mu} = e^{-2b_2 L} \cos^4 \theta + e^{-2b_1 L} \sin^4 \theta$$

$$+ \frac{1}{2} e^{-(b_1 + b_2) L} \sin 2\theta \left[ \sin 2\theta \cos \Delta L + 2\epsilon \sin \zeta \sin \Delta L \right],$$

where $\Delta = a_2 - a_1$ plays the role of $\Delta m^2/2E$ in the standard case and can be chosen positive. The expressions above ignore terms of $\mathcal{O}(\epsilon^2)$, an approximation that is not appropriate in the limit $\theta \to 0$. The two new dimensionful parameters $b_{1,2}$ lead to the exponential decay/growth of all oscillations probabilities. Lorentz invariance dictates that $b_i \propto d_i/E$, where $d_{1,2}$ are constants with dimensions of mass-squared. In the limit $\epsilon \to 0$, we recover the well-known expressions for neutrino oscillations under the assumption that
the neutrino mass eigenstates have a finite lifetime. In the more general case where the mass eigenstates do not coincide with the decay eigenstates, the nonunitarity of the propagation leads to new mixing parameters, $\epsilon$ and $\zeta$.

As discussed earlier, the physics responsible for $\Gamma \neq 0$ imposes constraints on the different parameters. In the two-flavor case, in the basis where $M$ is diagonal with diagonal elements $a_1$ and $a_2$ (chosen positive), $\Gamma_{ii} = b_i$ in the limit $\Gamma_{ij} \ll a_1, a_2, \forall i, j$. In the same basis, defining $\Gamma_{12} = \Gamma_{21}^* = b$,

\[
(2.3.7) \quad \epsilon e^{i\zeta} = -\frac{2ib}{\Delta}
\]

In the context of the Weisskopf-Wigner approximation, $\Gamma$ is constrained to be positive-definite: $b_1, b_2 > 0$, $b_1b_2 \geq |b|^2$. In turn, these imply that $\epsilon \leq 2\sqrt{b_1b_2}/\Delta$.

The less stringent constraint $\sum_\beta P_{\alpha\beta} \leq 1$, for all $\alpha$, translates into $b_1, b_2 \geq 0$ and

\[
(2.3.8) \quad \epsilon \leq C_\zeta \frac{b_1 \cot \theta + b_2 \tan \theta}{\Delta} \cap \epsilon \leq C'_\zeta \frac{b_2 \cot \theta + b_1 \tan \theta}{\Delta},
\]

where $C_\zeta, C'_\zeta$ are $O(1)$ non-illuminating functions of $\zeta$ such that $1 < C_\zeta \lesssim 2$. This constraint allows for $\epsilon \neq 0$ as long as both $b_1, b_2 \neq 0$. Importantly and opposed to the case in which WW is assumed, we find that for small mixing ($\sin 2\theta \ll 1$), $\epsilon$ values larger than $b_{1,2}/\Delta$ are allowed. This is potentially relevant for the $1-3$ sector, as well as for the application of this formalism to sterile neutrinos.

Regardless of the origin of $\Gamma$, it is instructive to consider the case $|b_1L|, |b_2L| \to 0$. Under these circumstances

\[
(2.3.9) \quad P_{ee} = 1 - \sin^2 2\theta \sin^2 (\Delta L/2) - \sin 2\theta (\epsilon \sin \zeta) \sin \Delta L,
\]
\begin{align*}
(2.3.10) \quad P_{e\mu} &= \sin 2\theta (\sin 2\theta - 2\epsilon \cos \zeta) \sin^2(\Delta L/2), \\
(2.3.11) \quad P_{\mu e} &= \sin 2\theta (\sin 2\theta + 2\epsilon \cos \zeta) \sin^2(\Delta L/2), \\
(2.3.12) \quad P_{\mu\mu} &= 1 - \sin^2 2\theta \sin^2(\Delta L/2) + \sin 2\theta (\epsilon \sin \zeta) \sin \Delta L.
\end{align*}

Note that these are only good approximations in scenarios where \( \sum_\beta P_{\alpha\beta} > 1 \), in which case \( P_{\alpha\beta} \) need to be carefully reinterpreted as they cannot stand, mathematically speaking, for probabilities. Nonetheless, the above expressions are easy to explore – only two new dimensionless parameters appear – and are useful in order to illustrate the consequences of \( \epsilon, \zeta \neq 0 \).

Some interesting features are worthy of note. Even when the decay effects are turned off, unitarity is violated – \( P_{ee} + P_{e\mu} \neq 1 \) – along with, in the case \( \zeta \neq \pi/2, 3\pi/2, T \) invariance – \( P_{e\mu} \neq P_{\mu e} \). The oscillation length is the same for all \( P_{\alpha\beta} \), \( L_{\text{osc}} = 2\pi/\Delta \), but the survival probabilities are out of phase, i.e., maxima and minima do not correspond to \( L = nL_{\text{osc}} \), for natural \( n \). The amplitudes of the oscillations, \( A_{\alpha\beta} \) – differences between the smallest and largest \( P_{\alpha\beta} \) – for appearance and disappearance are also different. For example

\begin{align*}
(2.3.13) \quad A_{ee} &= \sin^2 2\theta \sqrt{1 + \left( \frac{2\epsilon \sin \zeta}{\sin 2\theta} \right)^2}, \\
(2.3.14) \quad A_{\mu e} &= \sin^2 2\theta \left( 1 + \frac{2\epsilon \cos \zeta}{\sin 2\theta} \right).
\end{align*}

A measurement of \( \nu_e \) disappearance can report an effective mixing angle \( \sin^2 2\theta_{\text{eff}} \equiv A_{\alpha\beta} \) that is different from that observed in appearance experiments. For example, if \( 2\epsilon \ll \frac{\sin 2\theta_{\text{eff}}}{2} \),
\[ \sin 2\theta, \text{ nonunitarity effects in disappearance are much smaller than those in appearance, unless } \cos \zeta \text{ is small.} \]

Under a \( CP \) transformation \( N \to (N^{-1})^T \), so antineutrinos are governed by the same differential equation except for \( \zeta \to \pi - \zeta \), i.e., \( \sin \zeta \to \sin \zeta, \cos \zeta \to -\cos \zeta \). For example, ignoring terms of \( O(\epsilon^2) \),

\[
P_{\bar{e}\bar{e}} = e^{-2b_1L} \cos^4 \theta + e^{-2b_2L} \sin^4 \theta \\
+ \frac{1}{2} e^{-(b_1+b_2)L} \sin 2\theta \left[ \sin 2\theta \cos \Delta L - 2\epsilon \sin \sin \Delta L \right] ,
\]

\[
(2.3.16) \quad P_{\mu\mu} = \frac{1}{4} \left( e^{-2b_2 L} + e^{-2b_1 L} - 2e^{-(b_1+b_2)L} \cos \Delta L \right) \sin 2\theta \left( \sin 2\theta - 2\epsilon \cos \zeta \right) .
\]

As expected, \( CPT \) invariance is preserved, i.e., \( P_{\alpha\beta} = P_{\bar{\beta}\bar{\alpha}} \), while \( CP \) invariance is not unless \( \zeta = \pi/2, 3\pi/2 \). Nonunitary propagation leads to new \( CP \)-violating phenomena, even in the two-flavor case.

\( CP \) invariance and \( T \) invariance violation are also present, as long as \( \epsilon \cos \zeta \neq 0 \), in the regime where the oscillatory terms average out, i.e., \( \Delta L \gg 1 \). In this case,

\[
(2.3.17) \quad P_{ee} = e^{-2b_1L} \cos^4 \theta + e^{-2b_2L} \sin^4 \theta ,
\]

\[
(2.3.18) \quad P_{\mu\mu} = e^{-2b_1L} \sin^4 \theta + e^{-2b_2L} \cos^4 \theta ,
\]

\[
(2.3.19) \quad P_{e\mu} = \frac{\sin^2 2\theta}{4} \left( e^{-2b_2 L} + e^{-2b_1 L} \right) \left( 1 - \frac{2\epsilon \cos \zeta}{\sin 2\theta} \right) ,
\]

\[
(2.3.20) \quad P_{\mu e} = \frac{\sin^2 2\theta}{4} \left( e^{-2b_2 L} + e^{-2b_1 L} \right) \left( 1 + \frac{2\epsilon \cos \zeta}{\sin 2\theta} \right) .
\]

\( P_{\bar{e}\bar{e}} = P_{ee} \), while \( P_{e\mu} - P_{\mu e} = P_{e\mu} - P_{\bar{e}\bar{\mu}} \propto \epsilon \cos \zeta \).
All expressions above ignore terms of $O(\epsilon^2)$ and are not good approximations in the limit $\sin 2\theta \ll \epsilon$. In the limit $\theta \to 0$, it is easy to compute the oscillation probabilities. Ignoring $O(\epsilon^3)$ terms\(^3\)

\[(2.3.21)\quad P_{ee} = \left(1 + \frac{\epsilon^2}{2}\right) e^{-2b_1L} - \frac{\epsilon^2}{2} e^{-(b_1+b_2)L} \cos \Delta L,\]

\[(2.3.22)\quad P_{\mu\mu} = \left(1 + \frac{\epsilon^2}{2}\right) e^{-2b_2L} - \frac{\epsilon^2}{2} e^{-(b_1+b_2)L} \cos \Delta L,\]

\[(2.3.23)\quad P_{e\mu} = \frac{\epsilon^2}{4} \left(e^{-2b_1L} + e^{-2b_2L} - 2e^{-(b_1+b_2)L} \cos \Delta L\right),\]

while $P_{\mu e} = P_{e\mu}$. CP invariance is preserved – none of the expressions depend of $\zeta$, so $P_{\alpha\beta} = P_{\bar{\alpha}\bar{\beta}}$, $\forall \alpha, \beta$ – but nonzero $\epsilon$ implies flavor change as long as the neutrino masses are different ($\Delta \neq 0$).

In the $\theta \to 0$ limit, the constraint $\sum_{\alpha} P_{\alpha\beta} < 1$ translates into $b_1, b_2 \geq 0$ and

\[(2.3.24)\quad \epsilon \leq \sqrt{\frac{\pi \min(b_1, b_2)}{2\Delta}},\]

where $\min(b_1, b_2)$ indicates the smaller between $b_1$ and $b_2$, so nonzero $\epsilon$ requires both $b_1, b_2$ nonzero. Furthermore, $\sum_{\alpha} P_{\alpha\beta} < 1$ also implies that oscillatory effects cannot dominate over the exponential decay.

### 2.4. Three-Neutrino Oscillations

It is easy to extend the discussion to the three-flavor case. We define

\[(2.4.1)\quad \langle \nu_1 | \nu_2 \rangle = \epsilon_3 e^{i\zeta_3}, \quad \langle \nu_1 | \nu_3 \rangle = \epsilon_2 e^{i\zeta_2}, \quad \langle \nu_2 | \nu_3 \rangle = \epsilon_1 e^{i\zeta_1}\]

\(^3\)Here we include $O(\delta^2)$ contributions to $N$, replacing Eq. (2.2.19) with $N \sim I(1 + 3\epsilon^2/8) - \delta/2$.\]
where $\epsilon_i \geq 0$ and $\zeta_i \in [0, 2\pi)$. Thus, in the limit $\epsilon_i \ll 1$, $N$ is given by Eq. (2.2.19) where

$$\delta = \begin{pmatrix} 0 & e^{-i\zeta_3} \epsilon_3 & e^{-i\zeta_2} \epsilon_2 \\ e^{i\zeta_3} \epsilon_3 & 0 & e^{-i\zeta_1} \epsilon_1 \\ e^{i\zeta_2} \epsilon_2 & e^{i\zeta_1} \epsilon_1 & 0 \end{pmatrix},$$

while the $3 \times 3$ unitary matrix $V$ can be parameterized in the usual way,

$$V = \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-i\delta_{CP}} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta_{CP}} & c_{12}c_{23} - s_{12}s_{23}s_{13}e^{i\delta_{CP}} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta_{CP}} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta_{CP}} & c_{23}c_{13} \end{pmatrix},$$

where $s_{ij} = \sin \theta_{ij}$, $c_{ij} = \cos \theta_{ij}$ and $\delta_{CP}$ is the Dirac $CP$-odd phase. As in the two-flavor case, neutrino oscillations are not sensitive to Majorana phases in $V$.

Using Eq. (2.2.21), the transition probabilities can be written as

$$P_{\alpha\beta} = \frac{1}{|e^{-ih_i t}|^2} (N_{\alpha i}^* N_{\beta i}^{-1}) (N_{\alpha k}^* N_{\beta k}^{-1*}) + \sum_{i \neq k} e^{-ih_i t} e^{ih_k t} (N_{\alpha i}^* N_{\beta i}^{-1}) (N_{\alpha k}^* N_{\beta k}^{-1*}),$$

where $h_i = a_i - ib_i$. As before, $\Delta_{ij} = (a_i - a_j)$ play the role of oscillation frequencies, $\Delta m_{ij}^2/2E$, while the different $b_i \propto d_i/E$, $i = 1, 2, 3$ lead to exponential decay (or growth).

Complete expressions for the different $P_{\alpha\beta}$ are rather cumbersome and not particularly illuminating. They depend on all decay parameters as well as the new mixing parameters $\epsilon_{1,2,3}$ and the new $CP$-odd phases $\zeta_{1,2,3}$. As in the two-flavor case, the transitions for antineutrinos are governed by the same expressions, except for $N \to (N^{-1})^T$, or $V \to V^*$, $\Delta \to -\Delta$. In terms of the parameterization introduced here, this translates into
$\delta_{CP} \rightarrow -\delta_{CP}$, $\zeta_i \rightarrow \pi - \zeta_i$. As expected, $CPT$ invariance is preserved, $P_{\alpha\beta} = P_{\bar{\beta}\bar{\alpha}}$, but $CP$ invariance and $T$ invariance are violated unless $\epsilon_i \cos \zeta_i = 0$ for all $i$. This is true even when three-flavor effects are turned-off (some mixing angles and some mass-squared differences vanish) and persists in the limit $\Delta_{31}L, \Delta_{21}L \gg 1$.

For the case of standard neutrinos, bounds on some of the new physics parameters have been discussed in the literature, mostly in the context of standard neutrino decay ($\delta_{ij} = 0$ in Eq.(2.2.15)). However, the bounds on the $\epsilon_i$ we will discuss are indirect, all of them deriving from the bounds on the $b_i$, and relatively weak if WW is abandoned. Here we summarize qualitatively some of these bounds. A quantitative discussion on how nonunitary neutrino propagation is constrained by current data and the potential reach of next-generation experiments is forthcoming.

In what follows, it will prove convenient to define the Hamiltonian eigenstates as

$$h_i = a_i - ib_i \equiv \frac{1}{2E} (m_i^2 - id_i),$$

where the $d_i$ have dimensions of mass-squared. Below, we assume that $m_i^2$ agree with the results obtained by analyzing the world’s neutrino data under the assumption that neutrino propagation is unitary, and use the standard definition for the ordering of the masses [68].

A finite neutrino lifetime can dramatically impact all the indirect information we have on primordial neutrinos. The nature of the decay products and the interactions, however, plays a role in determining if and how decaying neutrinos impact the cosmic microwave background, structure formation, etc, so bounds on decay parameters are model-dependent (see, for example, [82 [83]), ranging from stringent to non-existent. A future
observation of nonzero neutrino mass effects in cosmic surveys may change the picture dramatically [84].

The recent observation of ultra-high energy neutrinos from potentially extragalactic sources [85] implies that at least one of the $d_i$ is tiny. Much more information can be obtained – especially if the $d_i$ are not zero – with more statistics and flavor information [86] (see also, for example, [87–91]). A similarly stringent bound – at least one of the $d_i$ is zero for most practical purposes – comes from the observation of neutrinos from SN1987A [79].

Closer to home, solar neutrino data place strong constraints on some neutrino decay parameters. Data on $^8$B-neutrinos from Super-Kamiokande and SNO constrain $d_2 \lesssim 10^{-11}$ eV$^2$ [92], assuming $d_1$ is zero. A more detailed analysis, including data from Borexino, should also allow one place bounds on $d_1$. Atmospheric neutrino data constrain $d_3 \lesssim 10^{-5}$ eV$^2$ [93], assuming $d_{1,2}$ are zero.\footnote{As this work was about to be submitted for publication, an analysis of long-baseline neutrino data appeared on the preprint archives [94]. The bound quoted in that analysis is about an order of magnitude stronger than the one quoted here.} Shorter-baseline neutrino experiments (e.g., reactor and beam experiments) constrain $d_i \lesssim 10^{(-7)-(4)}$ eV$^2$ for all $i = 1, 2, 3$.

If $\Gamma$ is positive definite, $\epsilon_i \lesssim \sqrt{d_j d_k} / \Delta m^2$ and the bounds above imply that at least two of the $\epsilon_i$ are tiny given the constraints from solar neutrino data (at least $\epsilon \lesssim 10^{-5}$), while the third one might be of order a few percent ($\lesssim 10^{-5}$ eV$^2/|\Delta m_{13}^2|$). The less stringent requirement $\sum_\alpha P_{\alpha \beta} \leq 1$ allows for more $\epsilon_i$ of order several percent, potentially enhanced by the fact that $\theta_{13}$ is small. If no restriction is imposed on $\Gamma$ or $\sum_\alpha P_{\alpha \beta}$, joint analyses of nonzero $d_i$ and $\epsilon_i$ are required in order to establish the currently allowed values of these phenomenological parameters.
2.5. Conclusions

In summary, nonunitary neutrino propagation can be realized if neutrinos couple to new light states – lighter than the active neutrinos – which can interact among themselves. Here, we study some of the consequences of this hypothesis. This scenario is qualitatively different from the unitarity violation setups that have been previously discussed in the literature and leads to new phenomena – including new sources of CP invariance violation and new mass-scales – that can only be probed in oscillation experiments. A lot of work remains to be done, including a quantitative discussion of current bounds on nonunitary propagation, three-flavor phenomenology and prospects for next-generation oscillation experiments, potential applications to the short-baseline anomalies and other searches for new neutrino oscillation lengths, etc. We also need to address matter effects, especially when it comes to addressing their impact on the nonunitarity parameters – especially the $\epsilon$ parameters – and some of the constraints we have discussed here. These issues will be addressed in future work.
CHAPTER 3

Solar Neutrinos and the Decaying Neutrino Hypothesis

3.1. Introduction

The discovery of distinct nonzero neutrino masses and nontrivial lepton mixing opened the door to several fundamental questions that revolve around the properties of the neutral leptons. Here we concentrate on what, experimentally and model-independently, is known about the neutrino lifetime.

In the absence of interactions and degrees of freedom beyond those of the Standard Model, the two heaviest neutrinos – $\nu_2$ and $\nu_3$ ($\nu_1$ and $\nu_2$) in the case of the so-called normal (inverted) neutrino mass hierarchy [1] – are unstable, decaying into lighter neutrinos and photons ($\nu_i \rightarrow \nu_j \nu_k \nu_l$ or $\nu_i \rightarrow \nu_j + \gamma$, where $i,j,k,l = 1,2,3$). The associated lifetimes, given the tiny neutrino masses, are longer than $10^{37}$ years – much longer than the age of the universe. The presence of new interactions, degrees of freedom, etc., can, of course, change the picture dramatically.

Experimental bounds on the lifetimes of the neutrinos are much shorter than those expected from the Standard Model minimally augmented to include nonzero neutrino masses. Consulting ‘The Review of Particle Physics’ [1], one encounters different bounds that span almost twenty orders of magnitude. Bounds on the neutrino magnetic moment, for example, translate into bounds on radiative neutrino decays [95]. Results from cosmic surveys sensitive to the expansion rate of the universe at different epochs are consistent
with the existence of around three independent neutrino states, naively indicating that
these do not decay within the span of billions of years. In order to translate measurements
of the expansion rate of the universe into a bound on the neutrino lifetime, however, one
must consider the nature of the neutrino decay process, since the daughters of the putative
decay also contribute to the expansion rate of the universe and could, in principle, mimic
the contributions of their parents [82, 83]. The observation of the effects of nonzero
neutrino masses in cosmic surveys might change the picture significantly [84].

Model-independent bounds exist from experiments where the number of neutrinos
produced in the source can be compared to the number of neutrinos detected some distance
away. These include all neutrino oscillation experiments. Given a baseline $L$ and a
neutrino energy $E$, one expects to be sensitive to a neutrino decay width $\Gamma_i$ for $\nu_i$ with
mass $m_i$ such that

$$\Gamma_i m_i \frac{L}{E} \equiv d_i \frac{L}{E} = 5.07 \left( \frac{d_i}{\text{eV}^2} \right) \left( \frac{L}{\text{km}} \right) \left( \frac{\text{GeV}}{E} \right) \gtrsim 1.$$  

Here, for convenience, we define $d_i \equiv \Gamma_i m_i$, which has dimensions of energy-squared,
for two reasons. On one hand, all bounds discussed here are sensitive to $d_i$: it is not
possible to disentangle the neutrino mass from its decay width, both being unknown.
On the other hand, $d_i$, measured in eV$^2$, can be easily and directly compared to the
neutrino mass-squared differences that are measured in neutrino oscillation experiments
and compete’ with the decay effects. For conversion purposes, $d_i = 10^{-11}$ eV$^2$ translates
into a lifetime $\tau_i = 70 \mu s$ for a neutrino with mass $m_i = 1$ eV.

Using Eq. (3.1.1), it is easy to naively estimate that long-baseline accelerator ex-
periments like MINOS, T2K, and NovA, with $L/E \sim 10^3 \text{ km/GeV}$, are sensitive to
$d_i \gtrsim 10^{-4}$ eV$^2$, atmospheric neutrino experiments like SuperKamiokande, with $L/E \lesssim 10^5$ km/GeV, are sensitive to $d_i \gtrsim 10^{-6}$ eV$^2$, and the KamLAND reactor neutrino experiment, with $L/E \lesssim 2 \times 10^4$ km/GeV, is sensitive to $d_i \gtrsim 10^{-5}$ eV$^2$. Detailed analyses of atmospheric and MINOS data, for example, translate into $d_3 \lesssim 10^{-5}$ eV$^2$ and $d_3 < 1.2 \times 10^{-4}$ eV$^2$, respectively, assuming $d_1, d_2 \ll d_3$.

Astrophysical neutrinos, when directly observed in Earth-bound detectors, provide significantly more stringent bounds on some of the $d_i$. The observation of neutrinos from Supernova 1987A implies that at least one of the neutrino mass eigenstates made it from the explosion to the Earth and can be translated into $d_i < 1.2 \times 10^{-21}$ eV$^2$ for at least one $i = 1, 2, 3$. A strong bound on at least one of the $d_i$ can also be derived from the current and future observations of ultra-high-energy neutrinos using the IceCube detector.

Solar neutrinos have $L/E \sim 10^{11}$ km/GeV and hence are sensitive to $d_i \gtrsim 10^{-12}$ eV$^2$. The authors of \cite{92,96} pointed out that the $^8$B solar neutrino data translate into a robust bound on $d_2 \lesssim 10^{-11}$ eV$^2$, mostly independent from $d_1$ and $d_3$. In this chapter, we revisit the impact of decaying neutrinos on solar neutrino data. Since the publication of \cite{92,96}, our understanding of solar neutrinos and neutrino properties has improved significantly. Increasingly precise KamLAND data not only confirmed the neutrino oscillation interpretation of solar neutrino data, but also provided a precision measurement of the solar mass-squared difference, $\Delta m^2_{12} \equiv m_2^2 - m_1^2$, and a good independent measurement of the solar mixing angle $\theta_{12}$ \cite{97}. Borexino data allow a precision measurement of $^7$Be solar neutrinos, and a clean measurement of the $pp$ solar neutrinos \cite{98}. Finally, recent reactor \cite{56,99,100} and accelerator data \cite{101} have measured the reactor angle $\theta_{13}$, revealing
that it is nonzero but quite small, $\sin^2 \theta_{13} \sim 0.02$. We will argue that all this information allows one to place, almost model-independently, bounds on both $d_1$ and $d_2$ from solar neutrino data. These results, when combined with results from atmospheric neutrinos, allow one to unambiguously place bounds on all three $d_i$, $i = 1, 2, 3$, which are robust, mostly model independent, and do not depend on the values of the neutrino masses or the neutrino mass hierarchy.

We will show, \textit{a posteriori}, that decay effects are negligible for the $L/E$ values probed by the KamLAND experiment. This implies that the oscillation results obtained from KamLAND apply even if the neutrinos have a finite lifetime, including the fact that $\Delta m^2_{12} \sim 10^{-4}$ eV$^2$ and $\sin^2 2\theta_{12} \sim 0.8$. This in turn implies that neutrino oscillations from the core to the edge of the Sun, to a good approximation, satisfy the adiabatic approximation. Ignoring the (small) day–night effect but taking into account that the different neutrinos can decay into final states not accessible to the different solar neutrino detectors, the probability $P_{e\alpha}$ that a neutrino with energy $E$ born in the Sun as a $\nu_e$ is detected as a $\nu_\alpha$, $\alpha = e, \mu, \tau$ one astronomical unit $L_\odot$ away from the Sun is

\begin{equation}
(3.1.2) \quad P_{e\alpha}(E) \simeq \sum_{i=1,2,3} p_{ei}(E)|U_{ai}|^2 e^{-d_i L_\odot / E},
\end{equation}

where $U_{ai}$, $i = 1, 2, 3$, are the elements of the neutrino mixing matrix, while $p_{ei}(E)$ are the probabilities that the neutrino exits the Sun as $\nu_i$ neutrino mass eigenstates. Strictly speaking, Eq. (3.1.2) is a good approximation when $d_i R_\odot / E \ll 1$, where $R_\odot$ is the average solar radius. We will show that this is indeed the case for $d_1$ and $d_2$, and we argue in the next section that solar data are not sensitive to $d_3$ effects.
3.2. Experimental Status of Neutrino Decay

Given that $|\Delta m^2_{13}| \sim 2 \times 10^{-3}$ eV$^2$ – even if one includes nonzero neutrino decay widths \cite{53,54} – $p_{e3}(E) \simeq |U_{e3}|^2$ for all relevant solar neutrino energies, $E \in [100 \, \text{keV}, 20 \, \text{MeV}]$. Since $|U_{e3}|^2 = \sin^2 \theta_{13} \simeq 0.02$ is small, given the precision of the solar neutrino data, $d_3$ related effects are irrelevant. In other words, the solar data are consistent with all $d_3$ values. We anticipate that $d_3 \neq 0$ effects impact only modestly the constraints on the other oscillation and decay parameters. Henceforth, we ignore $\theta_{13}$ effects – we formally set it to zero – and treat solar neutrino oscillations as if there were only two neutrinos, $\nu_e$ and $\nu_a$ (a for active).

At high solar neutrino energies, $E \gtrsim 5$ MeV, $p_{e2} \sim 1$, $p_{e1} \sim 0$, such that $P_{ee} \sim \sin^2 \theta_{12} e^{-d_2 L_\odot/E}$ and $P_{ea} \sim \cos^2 \theta_{12} e^{-d_2 L_\odot/E}$. $^8$B solar neutrino data are hence sensitive to $d_2$ but have little sensitivity to $d_1$ \cite{92}. Recent solar data from SNO \cite{102} indicate a $P_{ee}$ that decreases slowly as the neutrino energy decreases (as opposed to increasing, as predicted by the standard scenario, $d_1 = d_2 = 0$), a fact that is consistent with a judicious choice of $d_2$. For illustrative purposes, Fig. 3.1 depicts $P_{ee}$ (black) and $P_{ea}$ (red) as a function of $E$, for $\sin^2 \theta_{12} = 0.29$, $\Delta m^2_{12} = 7.5 \times 10^{-5}$ eV$^2$, $d_1 = 0$, and $d_2 = 0$ (solid) or $d_2 = 2 \times 10^{-12}$ eV$^2$ (dashed).

At low solar neutrino energies, $E \lesssim 1$ MeV, solar neutrino oscillations are well approximated by simple, averaged-out vacuum oscillations such that $p_{e1} \sim \cos^2 \theta_{12}$, $p_{e2} \sim \sin^2 \theta_{12}$, and $P_{ee} \sim \cos^4 \theta_{12} e^{-d_1 L_\odot/E} + \sin^4 \theta_{12} e^{-d_2 L_\odot/E}$ and $P_{ea} \sim \sin^2 \theta_{12} \cos^2 \theta_{12} (e^{-d_1 L_\odot/E} + e^{-d_2 L_\odot/E})$. $^7$Be and $pp$ solar neutrino measurements are hence sensitive to both $d_1$ and $d_2$. In isolation, the low-energy solar neutrino data can be used to place a bound on either $d_1$ or $d_2$, but not both. This is easy to see: the data are consistent with $e^{-d_1 L_\odot/E} \to 0$
or $e^{-d_2 L_\odot/E} \to 0$ as long as one judiciously chooses $\sin^2 \theta_{12}$. For example, in the limit, say, $e^{-d_1 L_\odot/E} \to 0$, $P_{ee} \sim \sin^4 \theta_{12}$ and $P_{ea} \simeq \sin^2 \theta_{12} \cos^2 \theta_{12}$ can be made to fit the data, roughly, $P_{ee} \sim 0.55$ [98], by choosing $\sin^2 \theta_{12} = 0.75$ (in the “dark side” [103]), which is consistent with data from KamLAND [97]. This possibility, however, is ruled out by $^8$B data, which require $\sin^2 \theta_{12} \sim 0.3$.

In summary, combined low and high energy solar neutrino data allow one to place nontrivial bounds on both $d_1$ and $d_2$, i.e., the possibility that either $e^{-d_1 L_\odot/E} \to 0$ or $e^{-d_2 L_\odot/E} \to 0$ is ruled out. While $d_2$ is mostly constrained by the $^8$B data, $d_1$ is mostly constrained by the $^7$Be and $pp$ data. Given the order-of-magnitude difference between
the neutrino energies, we anticipate the $d_1$ bound to be, roughly, an order of magnitude stronger than the $d_2$ bound.

### 3.3. Results

In order to estimate the upper bounds on $d_1$ and $d_2$, we perform a simple $\chi^2$ fit to $\sin^2 \theta_{12}, d_1, d_2$, fixing $\Delta m^2_{12} = 7.5 \times 10^{-5}$ eV$^2$, the best fit from KamLAND, and setting $\sin^2 \theta_{13} = 0$, as discussed earlier. Given that KamLAND provides the dominant contribution to the measurement of $\Delta m^2_{12}$, this is a reasonable approximation. Since in the decaying-neutrinos scenario $P_{ee} + P_{ea} \leq 1$, we need to consider separately the information on the electron and the active neutrino components of the solar neutrino flux. In detail, we include the following experimental information, depicted in Fig. 3.1:

- $P_{ee} = 0.56 \pm 0.06$ for $E = 380$ keV, as extracted from a combined fit to Borexino and low-energy neutrino data [98]. This analysis is performed, effectively, by using Borexino data in order to establish the oscillated $^7$Be neutrino flux and hence extract the $pp$ neutrino flux from other data. This procedure depends only weakly on the hypothesis that $P_{ee} + P_{ea} = 1$. This result is consistent with Borexino’s recent independent measurement of the low energy solar neutrino flux [104].

- $s = P_{ee} + rP_{ea} = 0.62 \pm 0.05$ for $E = 862$ keV from the Borexino data [98].

- $r = 0.22$ is the ratio of the $\nu_e + e$ to the $\nu_a + e$ elastic scattering cross-sections at $^7$Be neutrino energies.

- SNO performed a detailed measurement of $P_{ee}$ as a function of energy [102]. We choose $P_{ee}$ values at $E = 4$ MeV and $E = 10$ MeV, $P_{ee} = 0.26 \pm 0.12$ and
\( P_{ee} = 0.32 \pm 0.02 \), respectively, as representatives of the SNO data. These points are chosen in order to both capture the statistical power of the SNO experiment and to include some of the shape information. A proper treatment of the SNO data, including all different observables, correlations, etc., can only be handled by the Collaboration itself. We verify that, in the case \( d_1 = d_2 = 0 \), our extracted best fit value for \( \sin^2 \theta_{12} \) and the associated one sigma error bar are in good agreement with the most recent global analyses of neutrino data [105].

- The SNO experiment is also sensitive to the presence of a \( \nu_a \) flux from the Sun thanks to its neutral current and \( \nu + e \) elastic scattering measurements. It is, therefore, possible to measure \( P_{ee} \) and \( P_{ea} \) as a function of energy with SNO data (see, for example, [52]). Ref. [102], however, does not discuss the independent extraction of \( P_{ea} \) from the data, replacing it instead by \( 1 - P_{ee} \). Here we estimate the extracted value of \( P_{ea} \) from SNO data as follows. We define the central value using \( P_{ea} = 1 - P_{ee} \) while fixing the one-sigma error bar on \( P_{ea} \) as that on \( P_{ee} \), multiplied by \( \sqrt{5} \). The factor of 5 is close to the ratio of the elastic \( \nu_e + e \) cross-section to that for \( \nu_a + e \) at \( ^{8}\text{B} \) neutrino energies and agrees with the relative uncertainties for the electron and active neutrino fluxes measured by SNO in Ref. [52].

We note that SuperKamiokande also measures the neutrino flux using elastic neutrino–electron scattering (see, e.g., [106]). We do not include data from SuperKamiokande in our simplified fit as they mostly contribute to the measurement of \( P_{ea} \) – which we can only estimate here – and have a higher energy threshold than SNO data.
Fig. 3.2 depicts the result of our fit in the $d_1 - d_2$ plane, obtained after marginalizing over $\sin^2 \theta_{12}$. The best fit point $(d_1, d_2) = (3.4 \times 10^{-19} \text{ eV}^2, 1.6 \times 10^{-13} \text{ eV}^2)$ is indicated by a dot. The hypothesis $d_1 = d_2 = 0$ fits the data quite well. At the 2$\sigma$ confidence level, $d_1 < 1.6 \times 10^{-13} \text{ eV}^2$ and $d_2 < 9.3 \times 10^{-13} \text{ eV}^2$, in agreement with the naive estimates discussed.
above. The constraints above justify the approximations that led to Eq. (3.1.2), especially $d_{1,2}R_\odot/E \ll 1$ for all solar neutrino energies. Our results indicate that the neutrino decay hypothesis does not allow for a fit to the solar data that is significantly better than the standard large mixing angle solution, mostly due to the low energy $^7$Be and $pp$ neutrino measurements. We emphasize, however, that a detailed analysis of all solar neutrino data including the neutrino decay hypothesis is best left to the experimental collaborations, and that a reanalysis of the SNO data – one that treats both $P_{ee}(E)$ and $P_{ea}(E)$ as independent functions – as a function of energy is required. We hope our results encourage the pursuit of such an analysis.

### 3.4. Conclusions

In summary, we have argued that the solar neutrino data, combined with reactor data, allow one to place mostly model-independent bounds on the lifetimes of $\nu_1$ and $\nu_2$. Using a subset of the solar neutrino data and the data from KamLAND, we estimate that $d_1 < 1.6 \times 10^{-13}$ eV$^2$ and $d_2 < 9.3 \times 10^{-13}$ eV$^2$ at the two-sigma confidence level. A complete analysis would reveal exactly where these bounds lie. As a by-product of our analysis, the atmospheric neutrino bound discussed in [93] applies, robustly, to $\nu_3$: $d_3 \lesssim 10^{-5}$ eV$^2$. Along with solar and atmospheric neutrino data, the only other robust bound comes from SN1987A which translates, as discussed earlier, into $d_i < 1.2 \times 10^{-21}$ eV$^2$ for one of the three mass-eigenstates, most likely $\nu_1$ or $\nu_2$.

The bounds are “mostly model-independent” in the following sense. They are independent from the values of the neutrino masses themselves, and apply for both mass hierarchies. No assumption is made regarding the nature of the neutrino – Majorana or
Dirac – or of the daughter particles into which the neutrinos would be decaying. We are assuming, however, that if the decay products were to consist of lighter active neutrinos, these would not leave a significant imprint in the detectors under consideration, i.e., they don’t look like the parent neutrinos. This is a modest assumption. Daughter neutrinos from neutrino decay have, necessarily, less energy than their parents, and only those that decay along the flight-path of the parent make it to the detector. We also do not allow for the possibility, discussed in a more generic context in Ref. [107], that the neutrino decay hypothesis translates into more mixing parameters, i.e., that the neutrino mass and decay eigenstates are not the same.
CHAPTER 4

A Sterile Neutrino at the Deep Underground Neutrino Experiment

4.1. Introduction

It is now established, beyond reasonable doubt, that neutrinos have mass and that leptons mix. In order to further explore the neutrino sector and exploit the oscillation phenomenon, ambitious next-generation, long-baseline neutrino oscillation experiments are under serious consideration, including the Deep Underground Neutrino Experiment (DUNE) proposal in the United States and the HyperKamiokande detector (and accompanying neutrino source in J-PARC) in Japan. The goals of these projects include the search for leptonic CP-invariance violation and testing the limits of the so-called three-massive-neutrinos paradigm (for more see, for example, Ref. [68]).

The hypothesis that there are three neutrinos, at least two of which are massive, and that these interact as prescribed by the standard model of electroweak interactions, accommodates almost all neutrino data. There is, however, plenty of room for new phenomena. The unitarity of the leptonic mixing matrix, for example, has not been thoroughly explored (see, for example, Ref. [109]). In spite of tremendous experimental progress,

\[^{1}\text{Arguably, the data only allow unitarity checks for the first row, } \sum_{i=1,2,3} |U_{ei}|^2 = 1, \text{ and third column, } \sum_{\alpha=e,\mu,\tau} |U_{\alpha3}|^2 = 1.\]
little nontrivial information regarding the appropriateness of the three-massive-neutrinos paradigm has been collected over the past two decades.

Next-generation long-baseline experiments can probe several different new phenomena, including new, weaker-than-weak interactions involving neutrinos and charged fermions [110] that lead to anomalous matter effects, new long-range forces [111] and the existence of light new states [112]. Here, we concentrate on the simple hypothesis that there is a fourth neutrino mass-eigenstate of unknown, but small, mass – less than a few eV – and assume that there is a nonzero probability that the new neutrino state can be measured as one of the active neutrino states, i.e., we assume the leptonic mixing matrix $U$ to be $4 \times 4$ and that $U_{\alpha 4}$, $\alpha = e, \mu, \tau$ are nonzero. Electroweak precision data require the fourth neutrino flavor eigenstate not to interact with the $W$ and $Z$ bosons with standard model strength, so we refer to it as a sterile neutrino.

We concentrate on this hypothesis for several reasons. It is simple, easy to parameterize and familiar [112]. Indeed, certain aspects of the effects of sterile neutrinos on different long-baseline experiments have been studied in the recent past (see, for example, Refs. [113–119]). Sterile neutrinos are also a natural and benign extension of the standard model and could be a side effect of the mechanism responsible for the nonzero neutrino masses (see, for example, Refs. [120, 121]). Furthermore, the so-called short-baseline anomalies [50, 122–125] might be pointing to more new physics in the leptonic sector, though a convincing, robust explanation remains elusive. Sterile neutrino interpretations to the short-baseline anomalies are, arguably, the simplest explanations of these data. Here, we remain agnostic regarding the new-physics origin of the short-baseline anomalies but, on occasion, will highlight the region of mass and mixing space that is preferred
by them. Finally, we would like to explore whether light sterile neutrinos can serve as proxies for other, in principle unknown, phenomena that might manifest themselves in long-baseline neutrino oscillation experiments. This aspect of our analysis will become more clear later.

This chapter is organized as follows. In section 4.2, we review four-flavor neutrino oscillations. Since we are interested in a large range of new mass-squared differences, we pay special attention to the neutrino oscillation probabilities in the limits when the new oscillation frequency is much larger or much smaller than the known oscillation frequencies. In section 4.3, we discuss in detail the capabilities of DUNE to (a) rule out the sterile neutrino hypothesis assuming the data are consistent with the three-massive-neutrinos paradigm; (b) determine the new mixing parameters assuming there is one sterile neutrino, where we assume the new mass-squared difference ranges from $10^{-5} \, \text{eV}^2$ to $1 \, \text{eV}^2$; and (c) diagnose that there is physics beyond the three-massive-neutrinos paradigm assuming there is a fourth mass eigenstate. In section 4.4, we offer some concluding remarks.

4.2. Oscillations With Four Neutrinos

We consider a fourth neutrino $\nu_s$ that does not participate in the weak interactions but that can mix with the other three neutrinos of the standard model. The misalignment between the mass eigenstates $\nu_i$ ($i = 1, 2, 3, 4$) and flavor eigenstates $\nu_\alpha$ ($\alpha = e, \mu, \tau, s$) can be described by a general $4 \times 4$ unitary matrix parameterized by six angles $\phi_{ij}$ ($i, j = 1, 2, 3, 4; i < j$) and three phases $\eta_1, \eta_2, \eta_3$. We choose the matrix elements $U_{\alpha i}$ to
be:

\[
\begin{align*}
U_{e2} &= s_{12}c_{13}c_{14}, \quad (4.2.1) \\
U_{e3} &= e^{-i\eta_1} s_{13}c_{14}, \quad (4.2.2) \\
U_{e4} &= e^{-i\eta_2} s_{14}, \quad (4.2.3) \\
U_{\mu 2} &= c_{24} \left( c_{12}c_{23} - e^{i\eta_1} s_{12}s_{13}s_{23} \right) - e^{i(\eta_2 - \eta_1)} s_{12}s_{14}s_{24}c_{13}, \quad (4.2.4) \\
U_{\mu 3} &= s_{23}c_{13}c_{24} - e^{i(\eta_2 - \eta_3 - \eta_1)} s_{13}s_{14}s_{24}, \quad (4.2.5) \\
U_{\mu 4} &= e^{-i\eta_3} s_{24}c_{14}, \quad (4.2.6) \\
U_{\tau 2} &= c_{34} \left( -c_{12}s_{23} - e^{i\eta_1} s_{12}s_{13}c_{23} \right) - e^{i\eta_2} c_{13}c_{24}s_{12}s_{14}s_{34} \left( -e^{i\eta_3} \left( c_{12}c_{23} - e^{i\eta_1} s_{12}s_{13}s_{23} \right) \right) s_{24}s_{34}, \quad (4.2.7) \\
U_{\tau 3} &= c_{13}c_{23}c_{34} - e^{i(\eta_2 - \eta_3)} s_{13}s_{14}s_{34}c_{13}c_{24} - e^{i\eta_3} s_{23}s_{24}s_{34}c_{13}, \quad (4.2.8) \\
U_{\tau 4} &= s_{34}c_{14}c_{24}, \quad (4.2.9)
\end{align*}
\]

where \( s_{ij} \equiv \sin \phi_{ij}, c_{ij} \equiv \cos \phi_{ij} \). The matrix elements not listed here can be determined through the unitarity conditions of \( U \).

When the new mixing angles \( \phi_{14}, \phi_{24}, \) and \( \phi_{34} \) vanish, one encounters oscillations among only three neutrinos, and we can map the remaining parameters \( \{ \phi_{12}, \phi_{13}, \phi_{23}, \eta_1 \} \rightarrow \{ \theta_{12}, \theta_{13}, \theta_{23}, \delta_{CP} \} \), the well-known mixing parameters that define the standard \( 3 \times 3 \) leptonic mixing matrix in the three-massive-neutrinos paradigm (using the Particle Data Group convention \[\text{II}\]). In the limit where \( \phi_{14}, \phi_{24}, \) and \( \phi_{34} \) are small, the angles \( \phi_{12}, \phi_{13} \) and \( \phi_{23} \) play roles similar to those of \( \theta_{12}, \theta_{13} \) and \( \theta_{23} \), respectively. We discuss this in

\[\text{We ignore potential Majorana phases because they do not affect oscillations.}\]
more detail in section 4.3. The best-fit values from Ref. [1] for a three-flavor fit to existing
data are $\sin^2 \theta_{12} = 0.308 \pm 0.017$, $\sin^2 \theta_{13} = 0.0234^{+0.0020}_{-0.0019}$, and $\sin^2 \theta_{23} = 0.437^{+0.033}_{-0.023}$; the
$CP$-odd phase $\delta_{CP}$ is virtually unconstrained.

The amplitude for $\nu_\alpha$ to be detected as $\nu_\beta$ after propagating a distance $L$ in vacuum
is

\begin{equation}
A_{\alpha\beta} = \delta_{\alpha\beta} + U_{\alpha 2} U_{\beta 2}^* \left( e^{-i\Delta_{12}} - 1 \right) + U_{\alpha 3} U_{\beta 3}^* \left( e^{-i\Delta_{13}} - 1 \right) + U_{\alpha 4} U_{\beta 4}^* \left( e^{-i\Delta_{14}} - 1 \right),
\end{equation}

where $\Delta_{ij} \equiv 2.54 \left( \Delta m^2_{ij} / 1 \text{eV}^2 \right) (L/1 \text{km}) (1 \text{GeV}/E_\nu)$, $E_\nu$ is the neutrino energy, $\Delta m^2_{ij} \equiv m_j^2 - m_i^2$, and $m_i$ is the mass of $\nu_i$. The corresponding probability is $P_{\alpha\beta} = |A_{\alpha\beta}|^2$.

Eq. (4.2.10) assumes that the four mass eigenstates remain coherent over the neutrino’s
evolution. The amplitude $A_{\alpha\beta}^{\overline{\nu}}$ for $\overline{\nu}_\alpha$ to be detected as $\overline{\nu}_\beta$ is equal to $A_{\alpha\beta}$ in Eq. (4.2.10)
with the exchange $U_{\alpha i} U_{\beta i}^* \leftrightarrow U_{\beta i} U_{\alpha i}^*$, for all $i = 2, 3, 4$. Unless otherwise noted, we will
assume that the values of the mass-squared splittings $\Delta m^2_{12}$ and $\Delta m^2_{13}$ are close to the
ones that fit the neutrino data assuming there are only three neutrino species (explicitly,
$\Delta m^2_{12} = 7.54 \times 10^{-5} \text{eV}^2$, $\Delta m^2_{13} = 2.43 \times 10^{-3} \text{eV}^2$, assuming the neutrino mass hierarchy
is normal [1]), as we will discuss in Sec. 4.3. The value of $m_4$ is mostly unconstrained,
so $\Delta m^2_{14}$ can be larger or smaller than $\Delta m^2_{12}$ and $\Delta m^2_{13}$. We do, however, restrict our
analyses to positive $\Delta m^2_{14}$, i.e., $m_4 > m_1$. In summary, including the fact that we will
always assume the normal neutrino mass hierarchy for the mostly active states, our masses
are ordered as follows: $m_1 < m_2 < m_3$, and $m_4 > m_1$. As we vary $\Delta m^2_{14}$, we allow for all
different mass orderings: $m_4 \leq m_2 < m_3$; $m_2 < m_4 < m_3$; and $m_2 < m_3 \leq m_4$.

\[\text{If } \nu_4 \text{ decoheres from the other three neutrinos, then the expression for } P_{\alpha\beta} \text{ is modified by neglecting the}\]
\[\text{interference of the oscillations related to } \Delta_{14} \text{ with those of } \Delta_{12} \text{ and } \Delta_{13}, \text{ cf. Eq. (4.2.12). Decoherence}\]
\[\text{occurs if, for example, } \nu_4 \text{ is produced incoherently, or, during propagation, the } \nu_4 \text{ wavepacket becomes}\]
\[\text{well-separated from the wavepacket containing } \nu_1, \nu_2 \text{ and } \nu_3.\]
The amplitude simplifies considerably when $\Delta_{14} \ll 1$. In this limit, the last term in Eq. (4.2.10) is small compared to the others, so

$$P_{\alpha\beta} \simeq \left| \delta_{\alpha\beta} + U_{\alpha 2} U_{\beta 2}^* \left( e^{-i\Delta_{12}} - 1 \right) + U_{\alpha 3} U_{\beta 3}^* \left( e^{-i\Delta_{13}} - 1 \right) \right|^2.$$  

Because the experimental normalization uncertainties we will consider are $\mathcal{O}(1\%)$, the oscillations associated with $\Delta m_{14}^2$ will not be discernible if $\Delta_{14} \lesssim 10^{-2}$ over the entire range of reconstructed neutrino energies. For long-baseline oscillation experiments with $L \sim \mathcal{O}(10^3 \text{ km})$ and $E_\nu \sim \mathcal{O}(1 - 10 \text{ GeV})$, this condition translates into $\Delta m_{14}^2 \lesssim 10^{-4} \text{ eV}^2$. Nonetheless, in this scenario, oscillations can be distinct from those among only three neutrinos. Here, the elements $U_{\alpha i}$, $\alpha = e, \mu, \tau$; $i = 1, 2, 3$ do not form a unitary matrix and the number of independent parameters is larger than four, including sources of $CP$-invariance violation beyond the phase $\eta_1 \[^{118, 119}\]$. We return to this in Sec. 4.3.

When $\Delta_{14} \gg 1$ but $\nu_4$ is light enough to be produced coherently in the initial neutrino state, the oscillations of $\Delta m_{14}^2$ can be too rapid to be resolved by the finite energy resolution employed by the experiment. The oscillations of $\Delta m_{14}^2$ average out if $\Delta_{14} \times (\delta E/E_\nu)$ is, roughly, larger than $2\pi$, where the energy bin width is $\delta E$ and the bin’s central energy is $E_\nu$. For $L \sim \mathcal{O}(10^3 \text{ km})$, $E_\nu \sim \mathcal{O}(1 - 10 \text{ GeV})$, and $\delta E \sim 0.25 \text{ GeV}$, this will occur if $\Delta m_{14}^2 \gtrsim 1 \text{ eV}^2$. In this case,

$$P_{\alpha\beta} \simeq \left| \delta_{\alpha\beta} - U_{\alpha 4} U_{\beta 4}^* \left( e^{-i\Delta_{12}} - 1 \right) + U_{\alpha 2} U_{\beta 2}^* \left( e^{-i\Delta_{13}} - 1 \right) \right|^2 + \left| U_{\alpha 4} U_{\beta 4}^* \right|^2.$$  

\(^{4}\)Note that $\Delta m_{12}^2$ is close to this limit, i.e., the wavelengths of its associated oscillations are too long to significantly impact oscillations at such an experiment. Nonetheless, sensitivity to the oscillations associated with $\Delta m_{12}^2$ comes from the interference with the oscillations due to $\Delta m_{13}^2$. As we discuss in Appendix A.1, long-baseline experiments rely on information regarding $\Delta m_{12}^2$ and $\theta_{12}$ from other sources, including solar and reactor neutrinos, in order to precisely measure all oscillation parameters.
This limit is, as far as measurements of the oscillation probabilities are concerned, equivalent to the decoherence of $\nu_4$ from the other neutrinos. As in the $\Delta_{14} \ll 1$ limit, oscillations are in general distinct from those among only three neutrinos. For example, one is, in principle, also sensitive to sources of $CP$-invariance violation beyond the phase $\eta_1$ \[118, 119\].

When neutrinos propagate through matter, elastic, coherent, forward scattering modifies the oscillation probabilities in a well-known way. This can be parameterized via an effective potential generated by the background of electrons, protons and neutrons. The Hamiltonian $\delta H_{\alpha\beta}$ that describes neutrino oscillations, in the flavor basis, is \[126\]

\[
\left( \frac{\delta H_{\alpha\beta}}{1 \text{ km}^{-1}} \right) = \left( \frac{A}{1 \text{ eV}^2} \right) \delta_{\alpha e} \delta_{\beta e} + \left( \frac{A'}{1 \text{ eV}^2} \right) \delta_{\alpha s} \delta_{\beta s},
\]

where $(A/1 \text{ eV}^2) = (3.85 \times 10^{-4}) Y_e (\rho/1 \text{ g cm}^{-3})$ characterizes the charged-current interactions, $(A'/1 \text{ eV}^2) = (1.92 \times 10^{-4})(1 - Y_e)(\rho/1 \text{ g cm}^{-3})$ characterizes the neutral-current interactions, $Y_e$ is the electron fraction for the matter background, and $\rho$ is the density of the background.\[5\] The signs of $A$ and $A'$ are flipped for antineutrinos. The Earth’s crust typically has $Y_e \simeq 0.5$ and $\rho \simeq 3 \text{ g cm}^{-3}$ \[126\]. In the presence of matter, the Hamiltonian is no longer diagonal in the mass basis and the exact expressions for the oscillation probabilities are much more cumbersome. In our analyses, we treat the flavor evolution of the neutrino states numerically.

Our analysis makes use of initially muon-type neutrinos produced in pion decay to study $P_{\mu\mu}$ and $P_{\mu e}$. Because of experimental challenges involved in working with $\tau$ leptons,
we do not consider oscillations into $\nu_\tau$. Consequently, we do not expect to learn much about $\phi_{34}$, which only appears in the matrix elements $U_{\tau i}$. For long-baseline oscillation experiments with $L \sim \mathcal{O}(10^3 \text{ km})$ and $E_\nu \sim \mathcal{O}(1 - 10 \text{ GeV})$, $P_{\mu\mu}$ is mostly sensitive to $\phi_{24}$, while $P_{\mu\tau}$ is sensitive to both $\phi_{24}$ and $\phi_{14}$, mostly via the product $\sin \phi_{24} \sin \phi_{14}$. Therefore, we expect DUNE to have greater sensitivity to $\phi_{24}$ than to $\phi_{14}$. Furthermore, these two channels both depend on the $CP$-odd phase $\eta_1$, as well as the combination

$$(4.2.14) \quad \eta_s \equiv \eta_2 - \eta_3.$$ 

In order to distinguish the effects of $\eta_2$ from $\eta_3$, one requires information regarding $U_{\tau i}$, which, as just argued above, is unavailable in the absence of searches for $\tau$ appearance or disappearance.

4.3. Experimental Sensitivity to a Fourth Neutrino at DUNE

We investigate the sensitivity of the proposed Deep Underground Neutrino Experiment (DUNE) $^8$ to a fourth neutrino. We consider that DUNE consists of a 34 kiloton liquid argon detector and utilizes a 1.2 MW neutrino and antineutrino beams originating 1300 km upstream at Fermilab, consistent with the proposal in Ref. $^8$. The neutrino energy ranges between 0.5 and 20 GeV and the flux is largest around 3.0 GeV. In the following analyses, we simulate six years of data collection: 3 years each with the neutrino and antineutrino beams.

$^8$The study of tau appearance requires neutrino energies above the tau-production threshold for neutrino–nucleon scattering, around 3.4 GeV. Hence, for the energies under consideration here, tau appearance is severely phase-space suppressed. Furthermore, detectors must be able to identify taus with nonzero efficiency, an issue that is actively under investigation.
We use the neutrino fluxes and signal reconstruction efficiencies projected in Ref. [8] and the neutrino–nucleon cross-sections reported in Ref. [127] to calculate expected yields. For a three-neutrino scenario, we use input values consistent with the best-fit results compiled in Ref. [1]: $\sin^2 \theta_{12} = 0.308$, $\sin^2 \theta_{13} = 0.0235$, $\sin^2 \theta_{23} = 0.437$, $\Delta m^2_{12} = 7.54 \times 10^{-5}$ eV$^2$, $\Delta m^2_{13} = +2.43 \times 10^{-3}$ eV$^2$ (namely, a normal hierarchy), and $\delta_{CP} = 0$. The four dominant backgrounds are consequences of muon-type neutrino neutral-current scattering ("$\nu_\mu$ NC"), tau-type neutrino charged-current scattering ("$\nu_\mu \rightarrow \nu_\tau$ CC"), muon-type neutrino charged-current scattering ("$\nu_\mu \rightarrow \nu_\mu$ CC"), and beam electron-type neutrino charged-current scattering ("$\nu_e \rightarrow \nu_e$ beam CC"), depicted in Figs. 5.2(a)-(d). The rates associated with these backgrounds are taken from Ref. [8]. We reproduce the signal and background yields in Ref. [8] for the appearance ($P_{\mu e}$) and disappearance ($P_{\mu \mu}$) channels, shown as dashed lines in Figs. 5.2(a)-(d), i.e., "$\nu_\mu \rightarrow \nu_e$ signal 3$\nu$" and "$\nu_\mu \rightarrow \nu_\mu$ signal 3$\nu$," respectively. In Appendix A.1, we demonstrate comparable sensitivity to those computed in Ref. [8].

In order to illustrate the effects of a fourth neutrino, the expected yields along with the three-neutrino yields in Fig. 5.2 are depicted for $\sin^2 \phi_{14} = 0.023$, $\sin^2 \phi_{24} = 0.030$, $\sin^2 \phi_{34} = 0$, $\Delta m^2_{14} = 10^{-2}$ eV$^2$, and $\eta_s = 0$ ("$\nu_\mu \rightarrow \nu_e$ signal 4$\nu$" and "$\nu_\mu \rightarrow \nu_\mu$ signal 4$\nu$"). We choose the value of $\Delta m^2_{14}$ such that several oscillations due to the fourth neutrino occur within the energy window of the experiment. Here, the input values of $\phi_{12}$, $\phi_{13}$, and $\phi_{23}$ are slightly different from the values mentioned above for $\theta_{12}$, $\theta_{13}$, and $\theta_{23}$, and are chosen so that the values of $|U_{e2}|^2$, $|U_{e3}|^2$, and $|U_{\mu 3}|^2$ are consistent with three-flavor fits to the neutrino data [1].

\footnote{We do not have the freedom to set all nine matrix elements $U_{\alpha i}$ ($\alpha = e, \mu, \tau; i = 1, 2, 3$) equal to their three-neutrino best-fit values. Explicitly, we choose $|U_{e2}|^2 = 0.301$, $|U_{e3}|^2 = 0.023$, and $|U_{\mu 3}|^2 = 0.427$.}
Figure 4.1. Expected signal and background yields for six years (3y $\nu + 3y \bar{\nu}$) of data collection at DUNE, using fluxes projected by Ref. [8], for a 34 kiloton detector, and a 1.2 MW beam. (a) and (b) show appearance channel yields for neutrino and antineutrino beams, respectively, while (c) and (d) show disappearance channel yields. The 3$\nu$ signal corresponds to the standard three-neutrino hypothesis, where $\sin^2 \theta_{12} = 0.308$, $\sin^2 \theta_{13} = 0.0235$, $\sin^2 \theta_{23} = 0.437$, $\Delta m_{12}^2 = 7.54 \times 10^{-5}$ eV$^2$, $\Delta m_{13}^2 = 2.43 \times 10^{-3}$ eV$^2$, $\delta_{CP} = 0$, while the 4$\nu$ signal corresponds to $\sin^2 \phi_{12} = 0.315$, $\sin^2 \phi_{13} = 0.024$, $\sin^2 \phi_{23} = 0.456$, $\sin^2 \phi_{14} = 0.023$, $\sin^2 \phi_{24} = 0.030$, $\Delta m_{14}^2 = 10^{-2}$ eV$^2$, $\eta_1 = 0$, and $\eta_s = 0$. Statistical uncertainties are shown as vertical bars in each bin. Backgrounds are defined in the text and are assumed to be identical for the three- and four-neutrino scenarios: any discrepancy is negligible after accounting for a 5% normalization uncertainty.
Figure 4.2. Expected exclusion limits for $\sin^2 \phi_{14}$ (a) and $\sin^2 \phi_{24}$ (b) vs. $\Delta m^2_{14}$ at DUNE (blue), assuming a 34 kiloton detector and a 1.2 MW beam with six years ($3\nu + 3\bar{\nu}$) of data collection. The exclusion limits become independent of $\Delta m^2_{14}$ when the mass-squared difference is large ($\gtrsim 10^{-1}$ eV$^2$) or small ($\lesssim 10^{-4}$ eV$^2$). Results from the Daya Bay [9] (red) and Bugey [10] (orange) are shown in (a), and results from MINOS [11] (maroon) are shown in (b). The four-neutrino parameters we consider in section 4.3.2 listed in Table 4.1 are denoted by black stars above.

4.3.1. Constraining the Four-Neutrino Hypothesis

If the data are consistent with the three-neutrino scenario outlined above, one can place upper bounds on the values of $\phi_{14}$ and $\phi_{24}$ for given values of $\Delta m^2_{14}$. We calculate 95% confidence level (CL) exclusion limits for a fourth neutrino in the $\sin^2 \phi_{14} - \Delta m^2_{14}$ and $\sin^2 \phi_{24} - \Delta m^2_{14}$ planes, depicted in Fig. 4.2, using the appearance and disappearance channels and assuming running for three years each with the neutrino and antineutrino beams. We
include normalization uncertainties of 1% and 5% for the signal and background yields, respectively.

Fig. 4.2(a) also depicts the results from the Daya Bay [9] and Bugey [10] experiments in the $\sin^2 \phi_{14} - \Delta m_{14}^2$ plane. The existing experiments have greater sensitivity to $\sin^2 \phi_{14}$ for values of $\Delta m_{14}^2 \gtrsim 10^{-4} \text{eV}^2$. For smaller values of $\Delta m_{14}^2 \lesssim 10^{-4} \text{eV}^2$, none of the experimental probes, including DUNE, can resolve the long new oscillation length. Nonetheless, since DUNE measures both appearance and disappearance, we can constrain large values of $\sin^2 \phi_{14}$ as these render the upper-left $3 \times 3$ mixing submatrix unacceptably nonunitary. The same phenomenon can be observed in the $\sin^2 \phi_{24} - \Delta m_{14}^2$ plane (Fig. 4.2(b)). Large values of $\sin^2 \phi_{24}$ are ruled out, even for small values of $\Delta m_{14}^2$.

In the $\sin^2 \phi_{24} - \Delta m_{14}^2$ plane (Fig. 4.2(b)), we also show results from the MINOS [11] experiment and note that DUNE will be sensitive to lower values of the mixing angle and the mass-squared difference, due to DUNE having greater expected yield and a broader range of $L/E_{\nu}$ values. Because the disappearance channels depend strongly on $|U_{\mu 4}|^2$, and have higher yields than the appearance channels, DUNE has greater sensitivity to $\phi_{24}$ than $\phi_{14}$. We also note that, as expected and discussed in the previous section, if the mass-squared difference is either small, $\Delta m_{14}^2 \lesssim 10^{-4} \text{eV}^2$, or large, $\Delta m_{14}^2 \gtrsim 1 \text{eV}^2$, the limits are independent of the new mass-squared difference. Finally, the sensitivity in the $\sin^2 \phi_{24} - \Delta m_{14}^2$ plane extends to lower values of $\Delta m_{14}^2$ than that in the $\sin^2 \phi_{24} - \Delta m_{14}^2$ plane due to the higher yield of the disappearance channel.
Additionally, we calculate exclusion limits at 95% CL in the $4|U_{e4}|^2|U_{\mu 4}|^2 - \Delta m_{14}^2$ plane\(^8\) in order to compare the DUNE sensitivity to the proposed short-baseline experiment $\nu$STORM \(^9\), and the current long-baseline experiments MINOS, OPERA, and ICARUS \(^{11,13,14}\). Additionally, we include the results of the global fit to all neutrino data assuming a four-neutrino scenario, reported in Ref. \(^{15}\). This fit includes data from short-baseline experiments, including the short-baseline anomalies discussed earlier. In Fig. 4.3 we see that DUNE is sensitive to lower values of $\Delta m_{14}^2$ than any existing or proposed experiment due to its access to a wider range of $L/E_\nu$ values.

4.3.2. Measuring the New Mixing Parameters

Assuming the existence of a fourth neutrino, we explore the capability of DUNE to measure the new mixing angles and mass-squared difference. We choose three sets of parameters, listed in Tables 4.1 and 4.2 and denoted by black stars in Figs. 4.2 and 4.3 and calculate expected yields for the appearance and disappearance channels. Case 1 is consistent with the global four-neutrino fit performed in Ref. \(^{15}\) (the red ellipse in Fig. 4.3). Here, $\Delta m_{14}^2$ is large enough that we expect the oscillations associated to the new oscillation length to average out at DUNE. Case 2 uses the same mixing angles as case 1, but with a lower value of $\Delta m_{14}^2$. The parameters are within the the reach of DUNE, but outside the reach of current and proposed short-baseline experiments\(^9\). Here, $\Delta m_{14}^2$ is in the limit when oscillations due to the new mass-squared difference are dominant, the appearance channel oscillation probability takes the simple form

\[
P_{\mu e} \simeq 4|U_{e4}|^2|U_{\mu 4}|^2 \sin^2 \left( \frac{\Delta m_{14}^2 L}{4E_\nu} \right) \equiv \sin^2 (2\theta_{e\mu}) \sin^2 \left( \frac{\Delta m_{14}^2 L}{4E_\nu} \right).
\]

The effective mixing angle $\theta_{e\mu}$ is commonly used in the literature for $\nu_\mu \rightarrow \nu_e$ short-baseline appearance searches (see, for example, \(^{11,13,14,128,129}\)).

\(^8\)Note, however, that case 2 is in slight disagreements with existing bounds from Daya Bay and MINOS, see Fig. 4.2.
Figure 4.3. Exclusion limits in the $4|U_{e4}|^2|U_{\mu4}|^4 - \Delta m^2_{14}$ plane for various existing and proposed neutrino experiments. Expected exclusion limits are shown at 95% CL for the proposed DUNE (blue) and $\nu$STORM [12] (purple) experiments. Results are shown at 90% CL for the MINOS and Bugey [11] (orange), OPERA [13] (teal), and the ICARUS [14] (dark blue) experiments. Additionally, the fit to the 3+1 scenario including the short-baseline anomalies, reported in Ref. [15], is shown. The three sets of four-neutrino parameters we consider in section 4.3.2 listed in Table 4.1 are denoted by black stars above.
Table 4.1. Input values of the parameters for the three scenarios considered for the four-neutrino hypothesis. Values of $\phi_{12}$, $\phi_{13}$, and $\phi_{23}$ are chosen to be consistent with the best-fit values of $|U_{e2}|^2$, $|U_{e3}|^2$, and $|U_{\mu 3}|^2$, given choices of $\phi_{14}$ and $\phi_{24}$. Here, $\eta_s \equiv \eta_2 - \eta_3$. Note that $\Delta m^2_{14}$ is explicitly assumed to be positive, i.e., $m_4^2 > m_1^2$.

<table>
<thead>
<tr>
<th>Case</th>
<th>$\sin^2 \phi_{14}$</th>
<th>$\sin^2 \phi_{24}$</th>
<th>$\Delta m^2_{14}$ (eV$^2$)</th>
<th>$\eta_s$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>0.023</td>
<td>0.030</td>
<td>0.93</td>
<td>$-\pi/4$</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.023</td>
<td>0.030</td>
<td>$1.0 \times 10^{-2}$</td>
<td>$-\pi/4$</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.040</td>
<td>0.320</td>
<td>$1.0 \times 10^{-5}$</td>
<td>$-\pi/4$</td>
</tr>
</tbody>
</table>

Table 4.2. A continuation of Table 4.1.

is small enough that we expect the oscillations associated to the new oscillation length to be visible at DUNE. Case 3 has a much lower mass-squared difference, $\Delta m^2_{14} = 10^{-5}$ eV$^2$, but has large values of $\phi_{14}$ and $\phi_{24}$\footnote{A recent analysis of solar and reactor data constrain $\sin^2 \phi_{14} \lesssim 0.04$\cite{130}. This bound is not depicted in Fig. 4.2.} Here, $\Delta m^2_{14}$ is too small to be seen at DUNE. Nonetheless, as discussed earlier, the new mixing angles are large enough that nontrivial information on $\phi_{14}$ and $\phi_{24}$ can be extracted.

In all three cases, we assume that the neutrino mass hierarchy for the mostly active states is normal, i.e. $\Delta m^2_{13} = +2.43 \times 10^{-3}$ eV$^2$, and in all cases we assume $\eta_1 = \pi/3$ and $\eta_s = -\pi/4$, typical of scenarios where $CP$-invariance violating effects are large\footnote{We explored several other sets of input values for $\eta_1$ and $\eta_s$. This particular choice leads to generically large effects without extraordinary cancellations, enhancements, or ambiguities.}. For completeness, we also assume, in all cases, $\sin^2 \phi_{34} = 0$. Gaussian priors are adopted, mostly from solar neutrino data and data from KamLAND, on the solar parameters, $|U_{e2}|^2 = 0.301 \pm 0.015$ and $\Delta m^2_{12} = (7.54 \pm 0.24) \times 10^{-5}$ eV$^2$\cite{11}. Without these priors,
DUNE is mostly insensitive to either $\Delta m^2_{12}$ or $\phi_{12}$. We make use of the Markov Chain Monte Carlo package emcee [131], which estimates a probability distribution for each fitting parameter. Figs. A.4, A.5, and A.6 in Appendix A.2 depict sensitivity contours (68.3%, 95%, and 99% CL) and one-dimensional $\chi^2$ distributions for the ten parameters for cases 1, 2, and 3, respectively. Input values from Table 4.1 are shown as stars in the two-dimensional plots. Given that the amount of information in Figs. A.4, A.5, and A.6 is somewhat overwhelming, the 68.3%, 95%, and 99% CL sensitivity contours are depicted in Figs. 4.4, 4.5, and 4.6 for a subset of the parameters of interest for cases 1, 2, and 3, respectively, in order to guide the following discussions.

Fig. 4.4 depicts the fit results for a subset of the parameters ($\sin^2 \phi_{24}$, $\sin^2 \phi_{14}$, $\eta_1$, $\eta_s$ and $\Delta m^2_{14}$), assuming case 1. Here, the values of $\sin^2 \phi_{24}$ and $\Delta m^2_{14}$ can be excluded from 0 at the 99% CL, while the value of $\sin^2 \phi_{14}$ is consistent with 0 at 68.3% and $\eta_s$ cannot be constrained at the 95% CL. Nonetheless, the CP-odd phase $\eta_1$, which can be more or less trivially associated with the CP-odd phase $\delta_{CP}$ in the three-neutrino scenario, is constrained to be nonzero at the 99% CL. As expected, there is little sensitivity to $\Delta m^2_{14}$, except for establishing that it is large ($\Delta m^2_{14} > 7.9 \times 10^{-2} \text{ eV}^2$ at the 99% CL).

Fig. 4.5 depicts the fit results for a subset of the parameters ($\sin^2 \phi_{24}$, $\sin^2 \phi_{14}$, $\eta_1$, and $\eta_s$), assuming case 2. Here, the values of $\sin^2 \phi_{14}$, $\sin^2 \phi_{24}$, $\Delta m^2_{14}$ (cf. Fig. A.5), and $\eta_s$ are observed at at least the 95% CL, i.e., the fit establishes that none of the new physics parameters vanish. In particular, the values of $\sin^2 \phi_{14}$, $\sin^2 \phi_{24}$, and $\Delta m^2_{14}$ are excluded from zero at the 99% CL. In this case, there is enough sensitivity to the two independent CP-odd phases to establish that not only there are new neutrino degrees of freedom but that there is more than one new CP-invariance violating parameter in the theory. In
summary, one can establish that there is new physics beyond the standard paradigm, and that the new physics is *CP*-invariance violating.

Fig. 4.6 depicts the fit results for a subset of the parameters \((\sin^2 \phi_{24}, \sin^2 \phi_{14}, \Delta m_{14}^2)\), assuming case 3. The results here are somewhat similar to (but less constraining than) those from case 1. The measurement of \(\Delta m_{14}^2\) is consistent with 0 at 68.3% CL. but, as expected, the data reveal that it is small \((\Delta m_{14}^2 < 1.6 \times 10^{-4} \text{ eV}^2\) at the 99% CL). The
new $CP$-odd phase cannot be measured significantly (cf. Fig. A.6). On the other hand, one can exclude the hypothesis that the $CP$-odd phase $\eta_1$ is zero, but the sensitivity is worse than what one can achieve if the data were consistent with the three-flavor scenario.

If there is a fourth neutrino mass-eigenstate, the parameters of the fourth neutrino may significantly affect DUNE’s ability to measure the mixing angles naively associated with three-neutrino oscillation. For example, as shown in Appendix A.1 and in Ref. [8], the expected measurement precision for $\theta_{13}$ assuming a three-neutrino scenario is $\delta \theta_{13}/\theta_{13} \simeq 3\%$. In cases 1 and 3, this precision is much worse, $\delta \phi_{13}/\phi_{13} \simeq 10\%$. In case 2, however, the precision with which $\phi_{13}$ can be measured is $\delta \phi_{13}/\phi_{13} \simeq 4\%$, i.e., similar to the precision obtained in the three-neutrino scenario. This happens because, in case 2, one can mostly disentangle effects due to the different oscillation frequencies.
4.3.3. Testing the Three-Massive-Neutrinos Paradigm

In Sec. 4.3.1, we simulated data assuming a three-neutrino scenario and, by analyzing it assuming the four-neutrino hypothesis, were able to constrain the values of the new mixing parameters. In Sec. 4.3.2, we simulated data assuming different four-neutrino scenarios and, by analyzing it assuming the four-neutrino hypothesis, were able to constrain or measure, sometimes quite precisely, the new mixing parameters. Here we address a
different question: if we were to simulate data consistent with a four-neutrino scenario, would we be able to tell that there are more than three neutrinos? More concretely, would the analysis of the data assuming the three-massive-neutrinos paradigm reveal that the paradigm is incorrect?

To address this question, we fit the expected yields from case 2, introduced in Sec. 4.3.2 (see Table 4.1) assuming the three-neutrino hypothesis. We obtain best-fit values of $\theta_{12}$, $\theta_{13}$, $\theta_{23}$, $\Delta m_{12}^2$, $\Delta m_{13}^2$, and $\delta_{CP}$, along with associated uncertainties. The precision with which the parameters can be measured is comparable to what would be expected of DUNE if the data were consistent with the three-neutrino hypothesis. We also find, however, that the overall quality of the fit is poor: $\chi^2_{\text{min}}/\text{degrees of freedom (dof)} \simeq 180/114$, or a discrepancy of roughly 4$\sigma$. Hence, the three-neutrino hypothesis cannot mimic the additional oscillations associated with $\Delta m_{14}^2 = 10^{-2}$ eV$^2$, for any set of values of the three-neutrino parameters.$^{12}$

Once a bad goodness-of-fit is established, it becomes crucial to identify in which way the three-neutrino hypothesis fails. This can be done in a variety of ways. Here, for illustrative purposes, we try to diagnose the poor goodness-of-fit by splitting the data set into two subsets: the appearance data and the disappearance data, and analyze both subsets separately (combining neutrino and antineutrino data in each case). In both subchannels, the extraction of $\theta_{12}$ and $\Delta m_{12}^2$ is mostly driven by the priors from solar neutrino data, while the disappearance data are mostly insensitive to the $CP$-odd parameter $\delta_{CP}$. For these two reasons, it is most illuminating to examine the measurements obtained from

$^{12}$While we concentrate on case 2 here, we obtain poor fits also by assuming data consistent with cases 1 and 3, where the new oscillation frequency cannot be explicitly observed. The discrepancy is most significant for case 2, however.
these two fits in the $\sin^2 \theta_{13} - \sin^2 \theta_{23}$ plane, depicted in Fig. 4.7. Fig. 4.7 reveals that the appearance and disappearance channels favor different values of $\sin^2 \theta_{13}$ and $\sin^2 \theta_{23}$, with no overlap of the preferred regions at the 68.3% CL. For the appearance channels, the fit has $\chi^2_{\text{min}}/\text{dof} \simeq 78/54$ (roughly 2$\sigma$), and for the disappearance channels, $\chi^2_{\text{min}}/\text{dof} \simeq 91/54$ (roughly 3$\sigma$). The overall four-sigma (highly significant) discrepancy, therefore, is, in some sense, the product of a mediocre fit in the appearance channel, a poor fit in the disappearance channel, and the fact that the two subsets of data point to different regions of the parameter space.

Figure 4.7. Expected sensitivity contours at 68.3%, 95%, and 99% for neutrino and antineutrino appearance channels (blue, orange, red), and neutrino and antineutrino disappearance channels (green, teal, blue) in the $\sin^2 \theta_{13} - \sin^2 \theta_{23}$ plane, assuming the data are consistent with case 2 and analyzing it assuming the three-massive neutrinos paradigm.

The shapes observed in Fig. 4.7 are easy to understand. In a three-neutrino scheme, the disappearance probability $P_{\mu \mu}$ depends mostly on the $|U_{e3}|^2(1 - |U_{\mu 3}|^2)$. The best fit values translates into the relations $\sin^2 \theta_{23} \sim 0.43(1 + \sin^2 \theta_{13})$ or $\sin^2 \theta_{23} \sim 0.57(1 + \sin^2 \theta_{13})$,
which explains the approximately linear shapes in Fig. 4.7. The appearance channels, on the other hand, are mostly sensitive to the product $\sin^2 \theta_{13} \sin^2 \theta_{23}$, which explains the hyperbolic shape in Fig. 4.7. Hence, in order to fit the four-neutrino data, the two different data sets wander towards different best-fit values for $\sin^2 \theta_{13}$ and $\sin^2 \theta_{23}$ as they strive to maintain the different combinations of these parameters constant. In Appendix A.1 we repeat this analysis, this time simulating data consistent with the three-neutrino scenario. The results are depicted in Fig. A.3. The shapes obtained from the two subsets are similar to those in Fig. 4.7, but in this case the two analyses point to the same values of $\sin^2 \theta_{13}$ and $\sin^2 \theta_{23}$.

In summary, not only is the goodness-of-fit poor, it is also possible to ascertain that different measurements of the mixing parameters are inconsistent with one another if one assumes that the three-massive-neutrinos paradigm is correct. There are several other “inconsistency checks” one would perform in order to reveal that new physics is affecting the long-baseline oscillations, including comparing data obtained with the neutrino beam and the antineutrino beam, comparing DUNE data with those from HyperKamiokande (same $L/E_\nu$ values, but different neutrino energies and baselines), comparing DUNE data with data from “$\theta_{13}$” reactor neutrino experiments [55, 56, 100], medium baseline reactor experiments [132, 133], atmospheric neutrino experiments (for example, PINGU [134]), etc.

### 4.4. Summary and Conclusions

Ambitious next-generation long-baseline neutrino oscillation experiments are currently under serious consideration, especially the superbeam experiments Fermilab to DUNE in
the United States and J-PARC to HyperKamiokande in Japan. Among the goals of these projects are searching for \(CP\)-invariance violation in the lepton sector and testing the limits of the three-massive-neutrinos paradigm. Here, we addressed the capabilities of the DUNE experiment to discover a fourth neutrino mass-eigenstate or, instead, constrain its existence, either falsifying or strengthening the three-massive-neutrinos paradigm. While several different new phenomena could manifest themselves at long-baseline neutrino experiments, we chose one new neutrino mass-eigenstate for a few reasons. First, oscillation effects due to a new light neutrino mass-eigenstate are easy to parameterize, and familiar. Second, light sterile neutrinos are a natural and benign extension of the standard model and could, for example, be a side effect of the mechanism responsible for the nonzero neutrino masses. Finally, the so-called short-baseline anomalies may be interpreted as evidence for new neutrino degrees of freedom, so it is possible, even though the evidence is not particularly robust, that new neutrino states have already been found.

Assuming coherent oscillations, we discuss the oscillation probabilities involving a fourth neutrino for a wide range of values for the new mass-squared difference, including \(|\Delta m^2_{14}| \gg |\Delta m^2_{13}|\), when the new oscillation length is short and expected to lead to averaged-out effects at DUNE; \(|\Delta m^2_{14}| \ll |\Delta m^2_{13}|\), when the new oscillation length is too long to be observed at DUNE, or \(|\Delta m^2_{14}| \sim |\Delta m^2_{13}|\), when DUNE is sensitive to the new oscillation frequency. We highlight the fact that, in all three cases, the values of the active elements of the fourth column of the mixing matrix, \(U_{\alpha 4}, \alpha = e, \mu, \tau\), have a nontrivial impact on the experiment as long as these are large enough. We also discuss the extra sources of \(CP\)-invariance violation that arise from phases in the new mixing matrix elements. Given access to the \(\nu_e\)-appearance and \(\nu_\mu\)-disappearance channels, we
find that DUNE is, in principle, sensitive to two of the three $CP$-odd phases in the mixing matrix.

We simulate data in the DUNE experiment assuming a 34 kt detector, a 1.2 MW proton beam, and 3 years each of neutrino and antineutrino data collection, exploring different scenarios. If the data are consistent with three-neutrinos (i.e., there are no accessible new light neutrinos) we find that DUNE is less sensitive than, for instance, the Daya Bay experiment when it comes to constraining $|U_{e4}|^2$ if $|\Delta m^2_{14}| \gtrsim |\Delta m^2_{13}|$, while DUNE can outperform current long-baseline experiments when it comes to constraining $|U_{\mu 4}|^2$ if $|\Delta m^2_{14}| \gtrsim |\Delta m^2_{13}|$. On the other hand, if $|\Delta m^2_{14}| \lesssim |\Delta m^2_{13}|$, DUNE outperforms all current experiments when it comes to constraining new, light neutrino mass eigenstates thanks, in part, to the broad-band-beam nature of experiment and the fact that it measures both $\nu_\mu$ disappearance and $\nu_e$ appearance.

If the data are consistent with the existence of a fourth neutrino, DUNE has the capability to measure the new mixing parameters. This capability, however, depends strongly on the values of the parameters associated with the fourth neutrino, particularly $\Delta m^2_{14}$. We find that there are circumstances under which DUNE can not only discover new physics but also establish that there are new sources of $CP$-invariance violation. We emphasize that, if there is a new neutrino mass-eigenstate, the $\nu_e$ and $\nu_\mu$ data at DUNE can only explore a subset of the existing parameter space. One of the new mixing angles, and one of the two new sources of $CP$-invariance violation can only be accessed if one could also study $\nu_\tau$ appearance (or construct a $\nu_\tau$ beam, a much more challenging proposition).
We also briefly addressed whether DUNE data could reveal the existence of physics beyond the three-massive-neutrinos paradigm if the data were consistent with the existence of a fourth neutrino. We find that DUNE data are precise enough to reveal that a three-neutrino fit to data consistent with four neutrinos is poor (assuming the new mixing parameters are accessible). We also show that, in this scenario, fits to disjoint subsets of DUNE data point to different regions of the three-neutrino parameter space, another sign of new physics beyond three active neutrinos with nonzero mass. In order to properly diagnose that (a) there is physics beyond the three-massive-neutrinos paradigm, and (b) determine the nature of the new physics, it is likely that one will need more and better data. We hope to return to these important issues in a future study of long-baseline neutrino oscillations and new phenomena.
CHAPTER 5

Large, Extra Dimensions at the Deep Underground Neutrino Experiment

5.1. Introduction

Neutrino oscillation experiments have revolutionized our understanding of the neutrino sector of the standard model (SM). It is now established that at least two of the three known neutrinos are massive, and that the mass and flavor eigenstates are distinct. There are still several unanswered questions in neutrino physics, including the neutrino mass hierarchy, the potential existence of new neutrino states, and the status of $CP$ invariance in the lepton sector. To address these questions and further investigate the neutrino oscillation phenomenon, we need a new generation of neutrino oscillation experiments. The long-baseline Deep Underground Neutrino Experiment (DUNE) in the U.S. and the Hyper-Kamiokande (HyperK) experiment in Japan are proposed to answer these and several other questions, and are poised to provide qualitatively better and more precise tests of the current three-massive-neutrinos paradigm.

Although the absolute neutrino masses are not yet determined, we can indirectly infer from cosmic surveys that the known neutrino masses are below the eV-scale. More direct, albeit weaker bounds come from kinematical probes of nonzero neutrino masses. The fact that neutrino masses are much smaller than all known fermion masses in the SM is widely interpreted as evidence that the mechanism behind neutrino masses
is different from that of all other known particles. The hypothesis that there are more, compactified dimensions of space, and that these are large (i.e., much larger than the inverse of the Planck mass) was introduced in order to address the infamous SM hierarchy problem \[140\,\,142\], and also provides a mechanism for understanding why neutrino masses are parametrically smaller than charged-fermion masses. In these large-extra-dimension (LED) models, it is natural to assume that singlets of the SM gauge group, such as the graviton or the right-handed neutrino states, can propagate unconstrained in all dimensions, while the SM-charged objects are confined to a four-dimensional spacetime. If there are right-handed neutrino fields that propagate in (some submanifold of) the bulk), the equivalent four-dimensional neutrino Yukawa couplings are suppressed relative to charged-fermion Yukawa couplings by a factor proportional to the volume of the extra dimensions \[143\,\,144\]. In these scenarios, neutrinos are light for the same reason gravity appears to be weakly coupled.

The Kaluza-Klein (KK) modes of the higher-dimensional right-handed neutrino fields behave as an infinite tower of sterile neutrinos. If these are light enough, one expects deviations from the three-massive-neutrinos paradigm in neutrino oscillation experiments. The neutrino oscillation phenomenology of LED models has been extensively studied in the literature (see, for example, Refs. \[17\,\,18\,\,145\,\,149\]). It has also been proposed \[19\] that the reactor anomaly can be explained within the LED framework. More generically, the equivalence between the LED model and a framework with several sterile neutrinos was discussed in \[16\]. Other phenomenological aspects of LED models and their application to nonzero neutrino masses have also been explored in depth in the literature (see for example, Refs. \[150\,\,151\]).
We study the potential of the Deep Underground Neutrino Experiment (DUNE) to exclude or observe the effects of the LED model, and investigate how well DUNE can constrain the LED parameters. Highlights include the discussion of $CP$-invariance violation phenomena in the LED model using the DUNE experiment. Several other new physics scenarios can be studied using the precise measurements of the DUNE experiment. The capability of DUNE to test the one-sterile-neutrino hypothesis was recently explored in detail in Ref. [2, 152] while the effects of nonstandard interactions (NSI) of neutrinos were investigated in [153–156]. Here, we also explore the ability of DUNE to differentiate the LED hypothesis from the three-neutrino and the four-neutrino hypotheses.

The chapter is organized as follows: We discuss the LED formalism and the related neutrino oscillation probabilities in Section 5.2. The sensitivity of DUNE to the LED hypothesis is studied in Section 5.3, and we demonstrate the capability of DUNE to measure nonzero LED parameters in Section 5.4. Section 5.5 is devoted to studying the ability of DUNE to differentiate qualitatively distinct scenarios. We summarize our results and offer some conclusions in Section 5.6.

5.2. Formalism and Oscillation Probabilities

In this section we discuss the neutrino oscillation probabilities in LED models, and restrict our discussion to models with one relevant extra-dimension. We extend the SM with three massless five-dimensional gauge-singlet fermions $\Psi^\alpha \equiv (\psi^\alpha_L, \psi^\alpha_R)$ associated to the three active neutrinos $\nu^\alpha_L$. The indices $\alpha$ correspond to $e, \mu, \tau$, in spite of the fact that there are no charged leptons associated to $\Psi^\alpha$. The fifth dimension is compactified with periodic boundary conditions in such a way that, from a four-dimensional point of view, $\Psi^\alpha$
can be decomposed into a tower of Kaluza-Klein (KK) states $\psi_{L,R}^{(n)}$ ($n = 0, \pm 1, \cdots, \pm \infty$). Redefining the new fields as $\nu_{R}^{(0)} \equiv \psi_{R}^{(0)}$ and $\nu_{L,R}^{(n)} \equiv \left( \psi_{L,R}^{(n)} + \psi_{L,R}^{(-n)} \right) / \sqrt{2}$, ($n = 1, \ldots, \infty$), the mass terms of the Lagrangian, after electroweak symmetry breaking, are [143, 144, 157]:

$$L_{\text{mass}} = m_{D}^{\alpha\beta} \bar{\nu}_{R}^{\alpha} \nu_{L}^{\beta} + \sqrt{2} \sum_{n=1}^{\infty} \bar{\nu}_{R}^{(n)} \nu_{L}^{(n)} + \sum_{n=1}^{\infty} \frac{n}{R_{ED}} \bar{\nu}_{R}^{(n)} \nu_{L}^{(n)} + \text{h.c.},$$

(5.2.1)

$$\equiv \sum_{i=1}^{3} \mathcal{N}_{L(R)}^{i} M^{i} \mathcal{N}_{L}^{i} + \text{h.c.},$$

where $m^{D}$ is the Dirac mass matrix proportional to the neutrino Yukawa couplings and $R_{ED}$ is the radius of compactification. Note that all massive fermions are Dirac fermions. It is convenient to define mass pseudoeigenstates $\mathcal{N}_{L(R)}^{i}$ by rotating the neutrino states to a basis in which $m^{D}$ is diagonal:

$$\mathcal{N}_{L(R)}^{i} = \left( \nu^{(0)}_{i}, \nu^{(1)}_{i}, \nu^{(2)}_{i}, \cdots \right)^{T}_{L(R)}.$$

(5.2.2)

In this basis, the mass matrix is given by

$$M^{i} = \begin{pmatrix} m_{i}^{D} & 0 & 0 & 0 & \cdots \\ \sqrt{2}m_{i}^{D} & 1/R_{ED} & 0 & 0 & \cdots \\ \sqrt{2}m_{i}^{D} & 0 & 2/R_{ED} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

(5.2.3)
where $m^D_i$ are the elements of the diagonalized Dirac mass matrix $(m^D)_d = \text{diag}(m^D_1, m^D_2, m^D_3)$.

The relation between the active neutrinos in the SM and the corresponding mass pseudo-eigenstates is given by

$$\nu^\alpha_L = \sum_{i=1}^3 U^{\alpha i} \nu^{(0)}_i, \quad (\alpha = e, \mu, \tau),$$

where the $3 \times 3$ unitary matrix $U$ describes the mismatch between the flavor and mass (pseudo)eigenstates of neutrinos. This matrix is parametrized by three mixing angles $(\theta_{12}, \theta_{13}, \theta_{23})$ and one $CP$-violating Dirac phase $\delta_{13}$. In the limit $m^D \times R_{\text{ED}} \to 0$, the KK modes and the active neutrinos decouple, and $U$ is the standard neutrino mixing matrix.

We are interested in values of $R_{\text{ED}}$ such that $R_{\text{ED}}^{-1}$ is larger than $m^D_i$, but small enough that nontrivial effects might be observed in long-baseline oscillation experiments.

The true neutrino masses are found by diagonalizing the $n \times n$ matrix $M_i^d M_i$ with an $n \times n$ unitary matrix $S$ as: $S_i^T M_i^d M_i S_i$. Therefore, the true mass eigenstates are $\mathcal{N}_{iL} = \left(\nu^{(0)}_i, \nu^{(1)}_i, \nu^{(2)}_i, \ldots\right)^T = S_i^T \mathcal{N}_i L$. Using Eq. (5.2.4) we can obtain a relation between the active neutrinos of the SM and the mass eigenstates of the KK neutrinos,

$$\nu^{\alpha L} = \sum_{i=1}^3 U^{\alpha i} \nu^{(0)}_i = \sum_{i=1}^3 U^{\alpha i} \sum_{n=0}^{\infty} S_i^{0n} \nu^{(n)}_i L, \quad (\alpha = e, \mu, \tau),$$

where

$$(S_i^{0n})^2 = \frac{2}{1 + \pi^2 (m_i^D R_{\text{ED}})^2 + \left(\lambda_i^{(n)}\right)^2 / (m_i^D R_{\text{ED}})^2}.$$
Above, \((\lambda_i^{(n)})^2\) are the eigenvalues of the matrices \(R_{ED}^2 M_i^\dagger M_i\), and are obtained by solving the following transcendental equation \[143, 145, 157\]:

\[
(5.2.7) \quad \lambda_i^{(n)} - \pi (m_i^D R_{ED})^2 \cot \left( \pi \lambda_i^{(n)} \right) = 0.
\]

The roots of this transcendental equation satisfy the relation \(n \leq \lambda_i^{(n)} \leq (n + 1/2)\), so the masses of the neutrino states in the LED model are

\[
(5.2.8) \quad m_i^{(n)} = \frac{\lambda_i^{(n)}}{R_{ED}} \simeq \frac{n}{R_{ED}}, \quad (n = 0, 1, \ldots),
\]

where \(n = 0\) and \(n \geq 1\) correspond to the mostly active and mostly sterile neutrinos, respectively. As mentioned earlier, we are interested in \(R_{ED}^{-1} \gg m^D\).

The Dirac masses \((m_1^D, m_2^D, m_3^D)\) which appear in the Hamiltonian are not the masses of the mostly active neutrinos. They are, however, related to the mostly active neutrino masses and are hence constrained by neutrino oscillation data, along with \(R_{ED}\). The solar and atmospheric mass-squared differences are

\[
(5.2.9) \quad \Delta m^2_{\text{sol}} \equiv \Delta m^2_{21} = \frac{\left(\lambda_2^{(0)}\right)^2 - \left(\lambda_1^{(0)}\right)^2}{R_{ED}^2},
\]

\[
\Delta m^2_{\text{atm}} \equiv |\Delta m^2_{31}| = \left| \frac{\left(\lambda_3^{(0)}\right)^2 - \left(\lambda_1^{(0)}\right)^2}{R_{ED}^2} \right|.
\]

We can solve the equations above and replace two among \((m_1^D, m_2^D, m_3^D, R_{ED})\) with \(\Delta m^2_{21}\) and \(\Delta m^2_{31}\), which are constrained by experiment\(^1\). Hence, the LED framework can be

\(^1\)We follow the discussion in [18]. Explicitly, for the normal hierarchy (NH) case \((\lambda_1^{(0)} < \lambda_2^{(0)} < \lambda_3^{(0)})\), we use Eq. (5.2.7) to find \(\lambda_1^{(0)}\) as a function of \((m_1^D, R_{ED})\) while Eq. (5.2.9) is used to express \(\lambda_{2(3)}^{(0)}\) as a function of \(\lambda_1^{(0)}\). Eq. (5.2.7) then provides a relation between \(m_{2(3)}^D\) and \((m_1^D, R_{ED})\). For the inverted
characterized by the standard oscillation parameters – $\theta_{12}, \theta_{13}, \theta_{23}, \delta_{13}, \Delta m^2_{21},$ and $\Delta m^2_{31}$ – and two new free parameters, which we choose to be $m_0 \equiv m^D_1(3)$ and $R_{ED}$, for the NH (IH) case.

Neutrino flavor evolution in the LED model is governed by the following equation [16]:

$$i \frac{d}{dr} N_{iL} = \left[ \frac{1}{2E_\nu} M_i^T M_i N_{iL} + \sum_{j=1}^{3} \left( \begin{array}{cc} \nu_{ij} & 0_{1 \times n} \\ 0_{n \times 1} & 0_{n \times n} \end{array} \right) \right]_{n \to \infty} \mathcal{N}_{iL},$$

$$V_{ij} = \sum_{\alpha=e,\mu,\tau} U_{\alpha i}^* U_{\alpha j} \left( \delta_{\alpha e} V_{CC} + V_{NC} \right)$$

where $V_{CC} = \sqrt{2}G_FN_e$ and $V_{NC} = -\sqrt{2}/2G_FN_n$ are the charged- and neutral-current matter potentials, $G_F$ is the Fermi constant and $N_{e(n)}$ is the electron (neutron) number density along the trajectory of the neutrinos. For the purposes of this work, we assume the electron and neutron number densities to be the same and constant. As usual, $U_{\alpha i} \leftrightarrow U_{\alpha i}^*$ and the sign of the matter potentials are reversed when one considers the flavor evolution of antineutrinos.

The equivalence between the LED model and a $(3+3N)$ sterile framework with $N$ KK modes was explored in detail in Ref. [16]. The flavor and mass eigenstates in a $(3 + 3N)$ framework are related by a $(3 + 3N) \times (3 + 3N)$ unitary matrix $W$,

$$\mathcal{N}_{\alpha L} = \sum_{l=1}^{3+3N} W_{\alpha l} \mathcal{N}_{lL}^\prime,$$

hierarchy (IH) case ($\lambda^{(0)}_3 < \lambda^{(0)}_2 < \lambda^{(0)}_1$) we follow the same procedure to express $m^{D}_{1(2)}$ as a function of $(m^{D}_3, R_{ED})$. Note that the equations above only have solutions for $0 \leq \lambda^{(0)}_i \leq 0.5$. 


where \( N_{\alpha L} = \left( \nu_e, \nu_\mu, \nu_\tau, \nu_{s_1}, \nu_{s_2}, \nu_{s_3}, \cdots \right)_L^T \), in which \( \nu_{s_i} \) are the sterile eigenstates. Comparing Eqs. \( (5.2.5) \) and \( (5.2.11) \),

\[
(5.2.12) \quad \nu_{\alpha L} = \sum_{i=1}^{3} U_{\alpha i} \sum_{n=0}^{N} S_{i}^{0n} \nu_{iL}^{(n)} = \sum_{i=1}^{3} \sum_{n=0}^{N} W_{\alpha(i+3n)}^{(n)} \nu_{iL}^{(n)}, \quad (\alpha = e, \mu, \tau),
\]

so

\[
(5.2.13) \quad W_{\alpha(i+3n)} = U_{\alpha i} S_{i}^{0n}, \quad (i = 1, 2, 3; \alpha = e, \mu, \tau; \ n = 0, 1, \cdots, N).
\]

For \( R_{ED}^{-1} \gg m^D \) we have \(|S_{i}^{0n}|^2 \propto n^{-2}\), so KK modes slowly decouple as they get heavier. This implies that there is a finite value of \( N \) above which the \( 3 + 3N \) model is indistinguishable from the LED model. We have considered 2 KK modes in our calculations and have verified that the inclusion of more KK modes does not change our results. In fact, we have verified that, for the simulations performed here, 1 KK mode is sufficient. We further justify this approximation below.

When matter effects can be ignored, the oscillation probabilities are

\[
P(\nu_\alpha \to \nu_\beta) = \delta_{\alpha\beta} - 4 \sum_{l>m}^{3} \Re \left[ W_{\alpha l} W_{\beta l}^* W_{\alpha m} W_{\beta m} \right] \sin^2 \left( \frac{\Delta m^2_{lm} L}{4E_\nu} \right)
\]

\[
(5.2.14) + 2 \sum_{l>m}^{3} \Im \left[ W_{\alpha l} W_{\beta l}^* W_{\alpha m} W_{\beta m} \right] \sin \left( \frac{\Delta m^2_{lm} L}{2E_\nu} \right), \quad (l, m = 1, \cdots, 3 + 3N),
\]
where $L$ is the oscillation baseline, $E_\nu$ is the neutrino energy, and $\Delta m^2_{lm} \equiv m_l^2 - m_m^2$ with $m_{l=i+3n} \equiv m_i^{(n)} = \frac{\lambda_i^{(n)}}{R_{ED}}$. Matter effects will modify the oscillation probabilities in a well-known way.\footnote{Matter effects can lead to resonant flavor-conversion. For the effective two-neutrino system $\nu_i^{(n)} - \nu_i^{(0)}$ in the LED model, the resonance condition occurs for high neutrino energies \cite{158}:}

$E_{\nu}^{\text{res}} = \left(\frac{\lambda_i^{(n)}}{2 V_{NC} R_{ED}^2}\right)^2 - \left(\frac{\lambda_i^{(0)}}{2 V_{NC} R_{ED}^2}\right)^2 \approx \frac{n^2}{2 V_{NC} 2 \text{eV}} \frac{R_{ED}^{-1}}{2 \text{eV}} \approx n^2 \text{ TeV}.$

We are interested in the DUNE experiment, where neutrino energies are of order 1 GeV, and hence do not need to worry about the the resonant conversion of the active states into sterile KK modes.
matrix $W$ is, for the NH and IH, respectively,

\[(5.2.16)\]

\[
W^\text{(NH)}_{\alpha i} \approx \begin{pmatrix}
0.97 U_{e1} & 0.97 U_{e2} & 0.9 U_{e3} & 0.2 U_{e1} & 0.2 U_{e2} & 0.3 U_{e3} & 0.1 U_{e1} & 0.1 U_{e2} & 0.1 U_{e3} & \ldots \\
0.97 U_{\mu 1} & 0.97 U_{\mu 2} & 0.9 U_{\mu 3} & 0.2 U_{\mu 1} & 0.2 U_{\mu 2} & 0.3 U_{\mu 3} & 0.1 U_{\mu 1} & 0.1 U_{\mu 2} & 0.1 U_{\mu 3} & \ldots \\
0.97 U_{\tau 1} & 0.97 U_{\tau 2} & 0.9 U_{\tau 3} & 0.2 U_{\tau 1} & 0.2 U_{\tau 2} & 0.3 U_{\tau 3} & 0.1 U_{\tau 1} & 0.1 U_{\tau 2} & 0.1 U_{\tau 3} & \ldots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix},
\]

\[
W^\text{(IH)}_{\alpha i} \approx \begin{pmatrix}
0.95 U_{e1} & 0.9 U_{e2} & 0.97 U_{e3} & 0.3 U_{e1} & 0.3 U_{e2} & 0.2 U_{e3} & 0.1 U_{e1} & 0.1 U_{e2} & 0.1 U_{e3} & \ldots \\
0.95 U_{\mu 1} & 0.9 U_{\mu 2} & 0.97 U_{\mu 3} & 0.3 U_{\mu 1} & 0.3 U_{\mu 2} & 0.2 U_{\mu 3} & 0.1 U_{\mu 1} & 0.1 U_{\mu 2} & 0.1 U_{\mu 3} & \ldots \\
0.95 U_{\tau 1} & 0.9 U_{\tau 2} & 0.97 U_{\tau 3} & 0.3 U_{\tau 1} & 0.3 U_{\tau 2} & 0.2 U_{\tau 3} & 0.1 U_{\tau 1} & 0.1 U_{\tau 2} & 0.1 U_{\tau 3} & \ldots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix},
\]

where $U_{\alpha i}$ are parameterized by $\theta_{ij}$, $i, j = 1, 2, 3, i < j$, in the usual way \[1\]. From Eq. \[(5.2.16)\], it is easy to see that $W_{\alpha i} \sim U_{\alpha i}$ for the mostly active states ($i = 1, 2, 3$), while the top-left ($3 \times 3$)-submatrix of $W$ is not quite unitary. The slow decrease of $S$ as the KK-number increases can be readily observed. It is also easy to see that the effects of the mass eigenstates 7, 8, 9, proportional to $|U|^2$ are suppressed relative to those of states 4, 5, 6 by a factor of four. One can quickly check that all are significantly smaller than $|U_{e3}|^2$ ($|0.14 U_{e1}|^2 \sim 0.01$ is the largest $|U_{\alpha i}|$ for $i = 7, 8, 9$ in Eq. \[(5.2.16)\]). Furthermore, the oscillation frequencies associated to these states are also four times larger than those.
from the first KK mode and, for the $R_{\text{ED}}$ values of interest, their effects always average out at long-baseline experiments like DUNE. For all these reasons, one set of KK modes is, for DUNE neutrino energies and LED parameters of interest, a good proxy for the LED scenario. As mentioned earlier, all results discussed henceforth were computed including the effects of two KK modes (hence a 3+6 model).

When simulating data consistent with the LED hypothesis, we have to include input values for the $\theta_{ij}$ parameters. When doing that, we try to emulate as well as possible the current best-fit values, which we take to represent the existing neutrino data. In order to do that, we assume that the information that the current data provide for the three-neutrino mixing matrix elements $U_{\alpha i}$ applies to $W_{\alpha i}$ for $i = 1, 2, 3$. Hence, the best-fit value for the LED parameter $\sin^2 \theta_{13}$, for example, is not identical to that of the three-neutrino parameter $\sin^2 \theta_{13} = 0.0219$ [1]. They are, however, similar and related. For $R_{\text{ED}}^{-1} = 0.38$ eV, $m_0 = 5 \times 10^{-2}$ eV, and the NH, the best fit value for $(\sin^2 \theta_{13})_{\text{LED}} = 0.0219/0.94^2 = 0.025$ (see Eq. (5.2.16)). This recipe cannot be followed exactly, so we decide on the best-fit, input values for the LED $\theta_{ij}$ parameters by equating the $|W_{e2}|, |W_{e3}|, |W_{\mu 3}|$ to the best-fit values of $|U_{e2}|, |U_{e3}|, |U_{\mu 3}|$ obtained in the three-neutrino framework.

To understand the effect of the LED parameters on the oscillation of neutrinos, we show in Fig. 5.1 the probabilities of $\nu_\mu \to \nu_e$ (top-left) and $\bar{\nu}_\mu \to \bar{\nu}_e$ (top-right) as well as the survival probabilities of $\nu_\mu$ (bottom-left) and $\bar{\nu}_\mu$ (bottom-right) in the energy range of DUNE for the three-neutrino scheme and the LED formalism with dashed and solid curves, respectively. In all the panels we have fixed the parameters $\Delta m^2_{j1}$, $j = 2, 3$ and $\theta_{ij}$, $i, j = 1, 2, 3, i < j$, to the best-fit values reported in Ref. [1] (see also Table 5.1), for
3 different values of $\delta_{13}$. For the LED hypothesis, we further choose $m_0 = 5 \times 10^{-2}$ eV and $R_{\text{ED}}^{-1} = (5 \times 10^{-5} \text{ cm})^{-1} = 0.38$ eV. We see that for fixed values of $\theta_{ij}$, the oscillation probabilities in the LED case are suppressed with respect to the three-flavor scenario, as discussed above. This effect can be partially remedied by increasing the values of the LED $\theta_{ij}$ parameters. Fig. 5.1 also clearly depicts the fast oscillations associated to the presence of the KK modes.

5.3. Excluding the LED Hypothesis

In this section we investigate the sensitivity of DUNE to the model described in Sec. 5.2. We assume, as laid out in [135, 136], that DUNE is comprised of a 34-kiloton liquid argon detector located 1300 km from the neutrino source at Fermilab. The neutrino or antineutrino beam is produced by directing a 1.2 MW beam of protons onto a fixed target. We use the neutrino fluxes and reconstruction efficiencies reported in Ref. [8] to calculate event yields, as well as the neutrino-nucleon cross-sections reported in Ref. [127]. The neutrino energies range from 0.5 GeV to 20.0 GeV with maximum flux at around 3.0 GeV. Events are binned in 0.25 GeV bins from 0.5 GeV to 8.0 GeV, resulting in 30 independent counting measurements for each of the four data samples discussed below. Our analysis thus contains 120 degrees of freedom before subtracting the number of parameters describing any particular hypothesis. We simulate a detector resolution of $\sigma_{\text{GeV}} = 0.15/\sqrt{E_{\text{GeV}}}$ for electrons and $\sigma_{\text{GeV}} = 0.20/\sqrt{E_{\text{GeV}}}$ for muons, and assume three years of operation each for the neutrino beam and the antineutrino beam.

These are similar but not identical to the ones discussed in Ref. [136]. Ref. [136] reports updated reconstruction efficiencies which lead to reduced neutral current backgrounds for the appearance channels. In this light, our results can be viewed as somewhat conservative.
Figure 5.1. Oscillation probabilities assuming a three-neutrino framework (dashed) and an LED hypothesis with $m_0 = 5 \times 10^{-2}$ eV and $R_{ED}^{-1} = 0.38$ eV ($R_{ED} = 5 \times 10^{-5}$ cm), for the normal neutrino mass hierarchy, $\Delta m^2_{13} > 0$. The values of the other oscillation parameters are tabulated in Table 5.1, see text for details. The top row displays appearance probabilities $P(\nu_\mu \rightarrow \nu_e)$ (left) and $P(\bar{\nu}_\mu \rightarrow \bar{\nu}_e)$ (right), and has curves shown for $\delta_{13} = -\pi/2$ (green), $\delta_{13} = 0$ (gray), and $\delta_{13} = \pi/2$ (purple). The bottom row displays disappearance probabilities $P(\nu_\mu \rightarrow \nu_\mu)$ (left) and $P(\bar{\nu}_\mu \rightarrow \bar{\nu}_\mu)$ (right).

When generating data assuming the standard three-neutrino framework, we assume the best-fit values for the oscillation parameters from Ref. [1], summarized in Table 5.1. Since the neutrino mass hierarchy is unknown, we simulate data using either the normal hierarchy (NH) or inverted hierarchy (IH). We assume, however, that the hierarchy will
be known by the time DUNE collects data and therefore analyze the simulated data with the correct hierarchy hypothesis.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Normal Hierarchy</th>
<th>Inverted Hierarchy</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sin^2 \theta_{12}$</td>
<td>$0.304 \pm 0.014$</td>
<td>$0.304 \pm 0.014$</td>
</tr>
<tr>
<td>$\sin^2 \theta_{13}$</td>
<td>$(2.19 \pm 0.12) \times 10^{-2}$</td>
<td>$(2.19 \pm 0.12) \times 10^{-2}$</td>
</tr>
<tr>
<td>$\sin^2 \theta_{23}$</td>
<td>0.514$^{+0.055}_{-0.056}$</td>
<td>0.511$^{+0.055}_{-0.055}$</td>
</tr>
<tr>
<td>$\Delta m^2_{21}$</td>
<td>$(7.53 \pm 0.18) \times 10^{-5}$ eV$^2$</td>
<td>$(7.53 \pm 0.18) \times 10^{-5}$ eV$^2$</td>
</tr>
<tr>
<td>$\Delta m^2_{31}$</td>
<td>$(2.51 \pm 0.06) \times 10^{-3}$ eV$^2$</td>
<td>$-(2.41 \pm 0.06) \times 10^{-3}$ eV$^2$</td>
</tr>
<tr>
<td>$</td>
<td>U_{e2}</td>
<td>^2$</td>
</tr>
</tbody>
</table>

Table 5.1. Best-fit values of three-neutrino mixing parameters assuming the normal or inverted mass hierarchy. Values come from the 2015 update to Ref. [1], and the parameter $|U_{e2}|^2$, which is used later in our analysis, is derived from the fits to $\sin^2 \theta_{12}$ and $\sin^2 \theta_{13}$. While there exist, currently, weak constraints on the $CP$-odd parameter $\delta_{13}$, we work under the assumption that it is unconstrained.

Fig. 5.2 displays expected event yields for neutrino appearance $(P(\nu_\mu \rightarrow \nu_e)$, top-left), antineutrino appearance $(P(\bar{\nu}_\mu \rightarrow \bar{\nu}_e)$, top-right), neutrino disappearance $(P(\nu_\mu \rightarrow \nu_\mu)$, bottom-left), and antineutrino disappearance $(P(\bar{\nu}_\mu \rightarrow \bar{\nu}_\mu)$, bottom-right). In each panel, the expected event yield at DUNE is displayed for a three-neutrino hypothesis with parameters from Table 5.1 for the normal hierarchy, $\delta_{13} = 0$, and for a nonzero LED hypothesis with all homonymous parameters the same plus $m_0 = 5 \times 10^{-2}$ eV and $(R_{ED})^{-1} = 0.38$ eV$^4$. The dominant backgrounds are neutral-current scattering of muon-neutrinos ("$\nu_\mu$ NC"); charged-current scattering of tau-neutrinos ("$\nu_\mu \rightarrow \nu_\tau$ CC"); neutral-current scattering of unoscillated muon-type neutrinos ("$\nu_\mu \rightarrow \nu_\mu$ NC"); and charged-current scattering of unoscillated, contaminant electron-type neutrinos ("$\nu_e \rightarrow \nu_e$ CC"). The rates of these processes are estimated from Ref. [8], and are not recalculated.

\footnote{This is done for illustrative purposes only. The set of LED parameters that best mimics the three-flavor paradigm will have best-fit values of, for example, $\theta_{ij}$, $i,j = 1,2,3, i < j$, that are different from the input three-flavor values for $\theta_{ij}$, as discussed earlier.}
Figure 5.2. Expected event yields at DUNE assuming three years of either neutrino-beam mode (left) or antineutrino-beam mode (right). The top row displays $\nu_e$ and $\bar{\nu}_e$ appearance yields and the bottom row displays $\nu_\mu$ and $\bar{\nu}_\mu$ disappearance yields. In each panel, we show the expected yield assuming a three-neutrino hypothesis with parameters from Table 5.1 for the normal hierarchy in blue, with error bars representing statistical uncertainties, and assuming a nonzero LED hypothesis with $m_0 = 5 \times 10^{-2}$ eV and $R_{\text{ED}}^{-1} = 0.38$ eV in black. The contribution of events associated to opposite-sign muons and electrons is included in the signal. Backgrounds are discussed in the text and shown under the expected signals.
in our analyses for different hypotheses, as 1% signal and 5% background normalization uncertainties overwhelm any noticeable effects.

We analyze pseudodata simulated under the standard three-neutrino framework and $\delta_{13} = 0$ with the LED hypothesis. The resulting 95% confidence level (CL) limit in the $R_{ED}^{-1}m_0$ plane is shown in black in Fig. 5.3(a) for the NH and in Fig. 5.3(b) for the IH. In the analysis, following Refs. [2,155], we include priors on the solar parameters in order to take constraints from solar and KamLAND data into account. More concretely, we add Gaussian priors on $\Delta m^2_{21}$ using the information in Table 5.1 and on $|W_{e2}|^2$ using the information for $|U_{e2}|^2$ tabulated in Table 5.1. In the analysis, we marginalize over all parameters not made explicit in the figures. We have repeated the analysis for several nontrivial input values of $\delta_{13}$ and find the corresponding exclusion limits to be similar to the ones depicted in Fig. 5.3.

The dashed mauve and blue curves in Fig. 5.3 show the exclusion limits at 95% CL from IceCube-40 data and IceCube-79 data, respectively, as calculated in Ref. [16]. The dashed gold curves are the same for a combined analysis of T2K and Daya Bay performed in Ref. [17]. The green regions are preferred at 95% CL by short-baseline oscillation experiments according to analysis published in Ref. [19]. All these curves have, to zeroth order, the same shape as the exclusion curve we obtain for DUNE. This happens because the ratio of $m_0$ and $R_{ED}^{-1}$, when small, can be mapped into an effective mixing angle which governs most oscillation phenomena, as discussed in Ref. [16].

The dot-dashed burgundy curves in Fig. 5.3 show the expected 90% CL exclusion limit of the $\beta$-decay experiment KATRIN, estimated in Ref. [18]. The dependence on $m_0$ and
Figure 5.3. Exclusion limits in the $R_{ED}^{-1}$–$m_0$ plane, assuming either (a) a normal hierarchy or (b) an inverted hierarchy of neutrino masses. The exclusion regions are to the top-left of the relevant curves. Shown are the 95% CL lines from DUNE (black), IceCube-40 (mauve) and Ice-Cube79 (blue) [16], and a combined analysis of T2K and Daya Bay (gold) [17]. We also include the 90% CL line from sensitivity analysis of KATRIN (burgundy) [18]. The shaded green regions are preferred at 95% CL by the reactor anomaly seen in reactor and Gallium experiments [19]. The gray shaded regions are excluded by the measurements of $\Delta m^2_{11}$, as explained in the text. The dotted gray lines are curves along which $\sum_i m_i^{(0)} = 0.25$ eV. Higher values of $\sum_i m_i^{(0)}$ correspond to the regions above and to the right of the dotted gray lines.

on $R_{ED}^{-1}$ is more complicated for $\beta$-decay experiments than for oscillation experiments as the former rely on kinematic information from the electrons emitted in the decay.

The gray shaded regions are excluded on the basis of the mass-squared differences $\Delta m^2_{21}$ and $\Delta m^2_{31}$. As discussed in Sec. 5.2, $\Delta m^2_{i1}$, $i = 2, 3$ characterize the differences
between the lowest-lying physical masses-squared differences, \((\lambda_i^{(0)})^2 - (\lambda_1^{(0)})^2)/R_{ED}^2\). The transcendental equation Eq. (5.2.7) can only be satisfied if \(0 < \lambda_i^{(0)} < 0.5\). Therefore, a point in the \(R_{ED}^{-1} - m_0\) plane is only physical if all \(\lambda_i^{(0)}\) implied by \(\Delta m_{21}^2\) and \(\Delta m_{31}^2\) meet this requirement; the unphysical points define the gray shaded regions \([18]\).

The dotted gray lines are curves along which the sum of the masses of the three mostly active eigenstates, \(\sum_i m_i^{(0)}\), is 0.25 eV. This value is roughly the same as the current upper bound on the sum of the neutrino masses from PLANCK \([42]\). A proper analysis of the cosmology of the LED framework is outside the scope of this work. However, we believe the dotted gray lines capture the spirit of potential cosmological bounds in the \(R_{ED}^{-1} - m_0\) plane, especially if one allows for possible extensions of the LED scenario under consideration here.

### 5.4. Measuring LED Parameters

In this section we simulate data consistent with the LED hypothesis and investigate how well DUNE may measure the new-physics parameters \(m_0\) and \(R_{ED}^{-1}\) along with the other oscillation parameters. As input, we use the values for \(\Delta m_{ij}^2, i = 2, 3\) tabulated in Table 5.1, for the normal and inverted hierarchies, and choose \(\delta_{13} = \pi/3, m_0 = 5 \times 10^{-2}\) eV, and \(R_{ED}^{-1} = 0.38\) eV. We choose these values to be in the region excluded by DUNE shown in Fig. 5.3. As discussed earlier, we choose \(\theta_{ij}, i, j = 1, 2, 3, i < j\), such that \(|W_{e2}|, |W_{e3}|, |W_{\mu 3}|\) agree with the best-fit values of \(|U_{e2}|, |U_{e3}|, |U_{\mu 3}|\) under the three-flavor hypothesis. As in Sec. 5.3, we add Gaussian priors for the solar parameters, identified.

---

5Observed oscillations cannot be due to mixing among mass states from different KK modes. The mixing with the other low-lying state(s) would be large enough to produce a deviation from the three-standard-paradigm that is inconsistent with existing neutrino oscillation data.
Figure 5.4. Expected sensitivity to a nonzero set of LED parameters as measured by DUNE, assuming three years each of neutrino and antineutrino data collection. Fig. 5.4(a) assumes the normal mass hierarchy (NH) and Fig. 5.4(b) assumes the inverted mass hierarchy (IH). The LED parameters assumed here are $m_0 = 5 \times 10^{-2}$ eV and $R_{ED}^{-1} = 0.38$ eV, while $\delta_{13} = \pi/3$. The input values of $\Delta m^2_{ij}$, $i = 1, 2$ are in Table 5.1. The input values for the mixing angles are, for the NH, $\sin^2 \theta_{12} = 0.322$, $\sin^2 \theta_{13} = 0.0247$, $\sin^2 \theta_{23} = 0.581$, and, for the IH, $\sin^2 \theta_{12} = 0.343$, $\sin^2 \theta_{13} = 0.0231$, $\sin^2 \theta_{23} = 0.541$. Here as $\Delta m^2_{21}$ and $|W_{e2}|^2$. The results of these fits are depicted in Fig. 5.4. We marginalize over all parameters not made explicit in the figures.

Fig. 5.4 reveals that, at least at 99% CL, a lower bound on $R_{ED}^{-1}$ can be obtained in both the normal and inverted hierarchy scenarios, while a lower bound on $m_0$ can be set at least at 95% CL for both mass hierarchies. Additionally, if one were to place an independent bound on different combinations of neutrino masses (from, e.g., precision measurements of beta-decay spectra), a 99% CL upper bound on $R_{ED}^{-1}$ (or a lower bound on $R_{ED}$) could be obtained.
Finally, we have verified that the presence of the LED parameters $m_0, R_{ED}^{-1}$ does not significantly impact the sensitivity with which the standard oscillation parameters are measured (see, e.g., Refs. [2, 8] for more details). This includes the $CP$-odd parameter $\delta_{13}$. We have also checked that this result does not depend strongly on the input value of $\delta_{13}$.

### 5.5. Differentiating New Physics Scenarios

In this section we address the capabilities of DUNE to identify whether there is physics beyond the three-flavor paradigm and identify the nature of the new physics, assuming new physics is indeed present. In Sec. 5.5.1, we simulate data consistent with the LED hypothesis, as we did in Sec. 5.4, and try to fit the data with the three-neutrino hypothesis. We then ask whether it is possible to differentiate the LED hypothesis from other new physics scenarios. In particular, we compare the LED hypothesis with that of a fourth neutrino mass eigenstate. In Sec. 5.5.2, we address whether a four-neutrino model can mimic the LED hypothesis, while in Sec. 5.5.3 we ask if the LED hypothesis can mimic a generic four-neutrino model.

#### 5.5.1. Three-Neutrino Fit to the LED Scenario

In order to gauge whether DUNE can rule out the standard paradigm, we simulate data assuming the LED hypothesis is correct, as described in Sec. 5.4, and fit the data assuming the standard three-neutrino paradigm. The fit is performed for two simulated data sets, one assuming a normal hierarchy and the other, an inverted hierarchy. We calculate the minimum of the $\chi^2$ function, $\chi^2_{\text{min}}$, and compare it to the number of degrees of freedom,
dof. We define an equivalent $n\sigma$ discrepancy between the data and hypothesis assuming a $\chi^2$ distribution function with dof degrees of freedom. We include the Gaussian priors on $|U_{e2}|^2$ and $\Delta m_{21}^2$, as discussed in the previous sections (see also [2, 155]).

For the normal hierarchy, the result of the fit is $\chi^2_{\text{min}}/\text{dof} = 210/114$, or a $5.3\sigma$ discrepancy – a poor fit. For the inverted hierarchy, the fit is $\chi^2_{\text{min}}/\text{dof} = 208/114$, or a $5.2\sigma$ discrepancy – also a poor fit. These results are, of course, not surprising. According to Fig. 5.3, the input values of $R_{\text{ED}}^{-1}$ and $m_0$ are far inside the region of LED parameter space DUNE can exclude at 95% CL.

5.5.2. Four-Neutrino Fit to the LED Scenario

If data are consistent with the LED hypothesis so the standard paradigm is ruled out, it is not obvious that DUNE can establish that there are extra dimensions. The LED hypothesis is identical to a $3 + 3N$ active-plus-sterile-neutrinos scenario for large enough $N$. In fact, we argued in the Sec. 5.2 that, for the values of the parameters of relevance here, $N = 1$ is already a good approximation to the LED model. Here, we attempt to fit the simulated LED model to a four-neutrino hypothesis, using the framework described in Ref. [2].

While four neutrinos is less than the six neutrinos that are known to be a good approximation to the LED hypothesis, there is reason to suspect that, at DUNE and given the values of $m_0$ and $R_{\text{ED}}^{-1}$ of interest, the four-neutrino hypothesis is also a good approximation to the LED model. The reasoning is as follows. At the DUNE baseline and given DUNE neutrino energies, oscillation effects associated to the KK modes average

---

6We denote the six mixing angles in a four-neutrino hypothesis as $\phi_{ij}$ ($i, j = 1, 2, 3, 4, i < j$) to emphasize that they are not equivalent to the $\theta_{ij}$ of a three-neutrino hypothesis. The $CP$-violating phase $\eta_1$ is equivalent to $\delta_{13}$, and the new phases $\eta_2$ and $\eta_3$ contribute in the appearance channel in the combination $\eta_s \equiv \eta_2 - \eta_3$. 
out. The same effect can be mimicked by a 3+1 scenario in the limit where the new mass-squared difference is large. The map between the 3+1 and the LED scenario is not completely straightforward, but there are enough relevant degrees of freedom in the 3+1 model to accommodate all LED effects assuming there are no new resolvable mass-squared differences.

For both the NH and IH, we find a good fit (i.e., $\chi^2_{\text{min}} \simeq \text{dof}$). The results of these fits, one for each hierarchy hypothesis, are summarized in Table 5.2. For both hierarchies, the four-neutrino hypothesis favors $\Delta m_{41}^2 > 0.1 \text{ eV}^2$, the range in which oscillations associated with the extra neutrino average out for the energies of interest at DUNE. For this reason, we expect little sensitivity to the new, potentially observable, $CP$-violating phase $\eta_s \equiv \eta_2 - \eta_3$.

Fig. 5.5 displays the result of the fit performed assuming the normal hierarchy in the $\sin^2 \phi_{14} - \Delta m_{41}^2$ and $\sin^2 \phi_{24} - \Delta m_{41}^2$ planes. We find a qualitatively similar result when performing the fit assuming the neutrino mass hierarchy is inverted. Note that the data are consistent with $\sin^2 \phi_{14} = 0$ at 68.3% CL, but $\sin^2 \phi_{24} = 0$ is excluded at more than 99% CL. On the other hand, while it is possible to establish that the new oscillation frequency is large ($\Delta m_{41}^2 > 0.1 \text{ eV}^2$ at a high confidence level), it is not possible to place an upper bound on the new mass-squared difference.

5.5.3. LED Fit to Four-Neutrino Scenarios

Here, we generate data assuming four neutrinos exist, and attempt to fit this simulated data under the LED hypothesis. While it is easy to show that the LED hypothesis, under

\footnote{Seven, $\phi_{12}, \phi_{13}, \phi_{23}, \phi_{14}, \phi_{24}, \eta_1, \eta_s$ in the 3+1 case, compared to six, $\theta_{12}, \theta_{13}, \theta_{23}, \delta_1, m_0, R_{\text{ED}}$, in the LED case.}
### Table 5.2. Results of four-neutrino fits to data generated according to the LED Hypotheses discussed in Sec. 5.4. Best-fit values are the result of a 10-dimensional minimization, while quoted 95% CL ranges are from the marginalized one-dimensional resulting $\chi^2$ distributions for each parameter. The star on $\sin^2 \phi_{34}$ is a reminder that we are not including $\nu_\tau$-appearance information and hence have no sensitivity to $\sin^2 \phi_{34}$. For this reason, we fix it to zero. See Ref. [2] for more information.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Normal Hierarchy (NH)</th>
<th>Inverted Hierarchy (IH)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sin^2 \phi_{12}$</td>
<td>$0.311^{+0.028}_{-0.033}$</td>
<td>$0.287^{+0.003}_{-0.010}$</td>
</tr>
<tr>
<td>$\sin^2 \phi_{13}$</td>
<td>$(2.28^{+0.06}_{-0.04}) \times 10^{-2}$</td>
<td>$(1.95^{+0.33}_{-0.31}) \times 10^{-2}$</td>
</tr>
<tr>
<td>$\sin^2 \phi_{23}$</td>
<td>$0.525^{+0.030}_{-0.042}$</td>
<td>$0.532^{+0.027}_{-0.056}$</td>
</tr>
<tr>
<td>$\sin^2 \phi_{14}$</td>
<td>$(6.20^{+16.43}_{-6.60}) \times 10^{-3}$</td>
<td>$(9.06^{+13.67}_{-9.06}) \times 10^{-3}$</td>
</tr>
<tr>
<td>$\sin^2 \phi_{24}$</td>
<td>$(5.65^{+1.46}_{-1.31}) \times 10^{-2}$</td>
<td>$(6.76^{+0.36}_{-2.41}) \times 10^{-2}$</td>
</tr>
<tr>
<td>$\sin^2 \phi_{34}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$\Delta m_{21}^2$</td>
<td>$(7.50^{+0.35}_{-0.33}) \times 10^{-5} \text{ eV}^2$</td>
<td>$(7.68^{+0.27}_{-0.51}) \times 10^{-5} \text{ eV}^2$</td>
</tr>
<tr>
<td>$\Delta m_{31}^2$</td>
<td>$(2.69^{+0.02}_{-0.03}) \times 10^{-3} \text{ eV}^2$</td>
<td>$(-2.58^{+0.04}_{-0.04}) \times 10^{-3} \text{ eV}^2$</td>
</tr>
<tr>
<td>$\Delta m_{41}^2$</td>
<td>$(0.57^{+0.14}_{-0.37}) \text{ eV}^2$</td>
<td>$(0.56^{+0.14}_{-0.36}) \text{ eV}^2$</td>
</tr>
<tr>
<td>$\eta_1$</td>
<td>$(0.54^{+0.04}_{-0.04}) \pi$</td>
<td>$(0.38^{+0.16}_{-0.1320}) \pi$</td>
</tr>
<tr>
<td>$\eta_s \equiv \eta_2 - \eta_3$</td>
<td>$(-0.03^{+1.03}_{-0.97}) \pi$</td>
<td>$(-0.04^{+1.01}_{-0.96}) \pi$</td>
</tr>
</tbody>
</table>

The circumstances of interest, can be mimicked by a four-neutrino scenario, the converse is by no means obvious. In the LED hypothesis, the elements of the (infinitely large) neutrino mixing matrix are all related and can be uniquely determined once a handful of parameters are fixed, as described in Sec. 5.2. This means that the LED hypothesis can only perfectly mimic a four-neutrino scenario if the mixing angles and $CP$-odd parameters are related in nontrivial ways. In summary, at least at the oscillation probability level, a generic four-neutrino scenario cannot be mimicked by the LED hypothesis.

We pursue the issue by perturbing around the best-fit solutions discussed in the previous subsection and tabulated in Table 5.2. First, we generate data assuming the four-neutrino parameters listed in Table 5.2. In this case, for both the normal and inverted hierarchies, we find that the LED hypothesis generates a good fit ($\chi^2_{\text{min}} \simeq \text{dof}$), with
Figure 5.5. Results of a four-neutrino fit to data generated assuming an LED hypothesis with \( m_0 = 5 \times 10^{-2} \text{ eV} \) and \( R_{\text{ED}}^{-1} = 0.38 \text{ eV} \) assuming the normal hierarchy. Contours shown are 68.3\% (blue), 95\% (orange), and 99\% (red) CL. All unseen parameters are marginalized over.

\[
\frac{m_0}{(R_{\text{ED}})^{-1}} \approx 0.13, \text{ which is what we expect given the original LED hypothesis we assumed in Sec. 5.4.}
\]

Next, we generate data assuming the four-neutrino parameters listed in Table 5.2 with \( \Delta m_{41}^2 = 10^{-2} \text{ eV}^2 \), a value studied more in-depth in Ref. [2]. For this value of \( \Delta m_{41}^2 \), we expect the new oscillations due to the fourth neutrino to be relevant for the energies of interest at DUNE. In this case, for the normal hierarchy, we obtain a fit that has \( \chi^2_{\text{min}}/\text{dof} = 349/112 \), which corresponds to a discrepancy larger than 8\( \sigma \) – a poor fit. For the inverted hierarchy, the fit has \( \chi^2_{\text{min}}/\text{dof} = 402/112 \), corresponding to a larger than 8\( \sigma \) discrepancy – also a poor fit. In either case, DUNE would be able to rule out both the
three-flavor hypothesis and the LED hypothesis, while the four-neutrino hypothesis would provide an excellent fit to the data.

We repeat the exercise, this time assuming the input values of all the four-neutrino parameters are those listed in Table 5.2 except for the new mixing angles. If the input values of $\sin^2 \phi_{14}$ and $\sin^2 \phi_{24}$ are 0.1 and 0.01, respectively, the LED hypothesis also fails to fit the 3+1 scenario, for either mass hierarchy: $\chi^2_{\text{min}}/\text{dof} = 213/112$ ($6.0\sigma$) for the NH, $\chi^2_{\text{min}}/\text{dof} = 241/112$ ($6.7\sigma$) for the IH. In summary, at DUNE, the LED hypothesis can always be mimicked by the 3+1 scenario, but the converse is, by no means, generically true.

5.6. Conclusions

The long-baseline Deep Underground Neutrino Experiment (DUNE) [8] has been proposed to address several outstanding issues in neutrino physics, including the search for new sources of $CP$-invariance violation and precision tests of the validity of the standard three-massive-neutrinos paradigm. In this work, we addressed the ability of DUNE to probe large-extra-dimension (LED) models. These are scenarios where the smallness of neutrino masses is, at least partially, attributed to the existence of one extra compactified dimension of space which is accessible to the right-handed neutrino fields but inaccessible to all fields which are charged under the standard model gauge group. From a four-dimensional point of view, the Kaluza-Klein (KK) expansion of the right-handed neutrinos translates into towers of massive sterile neutrino states, with masses inversely proportional to the size $R_{\text{ED}}$ of the extra dimension.
We discussed in some detail the phenomenon of neutrino oscillations at long-baseline experiments in a five-dimensional LED model. We argued that the LED model, for all practical purposes, maps into a $3 + 3N$-neutrino scenario, and that modest values of $N - N = 1$ or $N = 2$ – capture the details of the LED effects at long-baseline oscillation experiments. Nonetheless, we emphasized that the LED model does not map into a generic $3 + 3N$ model. Instead, the number of new independent mixing parameters is small – six, including four that can be interpreted, to leading order, as the familiar three-neutrino mixing parameters $\theta_{12}, \theta_{23}, \theta_{13}, \delta_{13}$. Furthermore, we highlighted the fact that in LED models, there are no new $CP$-invariance violating parameters; the only source is the $CP$-odd phase $\delta_{13}$, which, to zeroth order, plays the same role in the three-neutrino scenario.

We investigated the sensitivity of DUNE to the LED framework. Assuming that the future DUNE data will be consistent with the three-neutrino paradigm (assuming three years of operation each in neutrino and antineutrino modes), the LED paradigm can be excluded at 95% CL if $R^{-1}_{ED} \leq 0.54 \text{ eV}$ ($R^{-1}_{ED} \leq 0.48 \text{ eV}$) assuming a normal (inverted) hierarchy for the mostly active neutrinos. More stringent limits are obtained if $m_0$, related to the mass of the mostly active states, turns out to be large ($m_0 \gtrsim 0.01 \text{ eV}$). The reach of DUNE is compared to that of existing and future probes in Fig. 5.3.

We also investigated whether DUNE can measure the new physics parameters if its data turn out to be consistent with the LED model. We found that there are values of $m_0$ and $R^{-1}_{ED}$ for which DUNE can establish, at least at the 68% CL, that $m_0$ is not zero and that the extra dimension has a finite size. One concrete example is depicted in Fig. 5.4.
Finally, assuming DUNE data are inconsistent with the three-neutrino paradigm, we explored whether they can reveal the nature of the new physics. We found that data consistent with LED models are inconsistent with the three-neutrino model if the new physics effects are strong enough. Nonetheless, we also found that, as far as DUNE is concerned, there are four-neutrino scenarios which mimic the LED model effectively. We showed, however, that the converse is not true. If DUNE data are consistent with a four-neutrino scenario, it is likely that the data cannot be explained by an LED scenario. In a nutshell, the LED model, in spite of the fact that it contains an infinite number of new neutrino states, has fewer relevant free parameters than a generic four-neutrino model.

The key distinguishing features of LED models are the existence of several sterile neutrinos with hierarchical masses (the new masses are, roughly, $R^{-1}_{ED}, 2R^{-1}_{ED}, 3R^{-1}_{ED}, \ldots$) and strongly correlated elements of the infinite mixing matrix ($U_{\alpha 4} \propto U_{\alpha 1}, U_{\alpha 5} \propto U_{\alpha 2}$, etc, for all $\alpha = e, \mu, \tau$). Both are difficult to establish experimentally in long-baseline experiments because, in those experiments, the effects of the new oscillation frequencies average out. On the other hand, once new physics effects in $\nu_\mu$ disappearance and $\nu_\mu \rightarrow \nu_e$ appearance are established, the LED hypothesis translates into concrete predictions for all other oscillation channels, including $\nu_\mu \rightarrow \nu_\tau$ appearance. This is not the case for a generic 3 + 1 scenario, where the new-physics effects in the $\nu_\tau$-appearance channel cannot be constrained by precision measurements of $\nu_\mu$-disappearance and $\nu_e$-appearance.


CHAPTER 6

Standard Model Flavor from an $SU(2)$ Symmetry

6.1. Introduction

The standard model (SM) matter fields organize into three generations of quarks and leptons with a mass spectrum, with the possible exception of the neutrinos, that is distinctly hierarchical. Moreover, generations mix with large angles in the lepton sector while relatively small angles are observed for the quarks. In the SM, the information about these physical parameters is encoded in the Yukawa couplings. Unobservable in themselves, an explanation for the structure in the Yukawas that gives rise to these masses and mixings has remained elusive. This is the so-called flavor puzzle.

Ever since the SM was proposed, several ideas have been put forward to resolve the flavor puzzle. Of note is the proposal of Froggatt and Nielsen [159] that the origin of the fermionic mass hierarchies is dynamical. This was achieved by positing the existence of a $U(1)$ symmetry under which fermions and a new scalar field were charged. Upon symmetry breaking, masses appeared proportional to powers of the vacuum expectation value of the $U(1)$ scalar.

However, typical Froggatt-Nielsen models struggle to explain the suppression of flavor-changing neutral currents (FCNCs) that the SM elegantly accounts for via the GIM mechanism [160]. In the past decades, experimental measurements have been pushing the limits of FCNCs measurement. Generic arguments now indicate that for nonstandard
FCNCs to exist, new physics related to flavor should appear at least at the PeV scale. In view of this, a different approach to flavor, the minimal flavor violation (MFV) ansatz, has been formulated [161–169].

Within MFV, a prominent role is played by the flavor symmetry the SM would have if the Yukawa couplings were removed. MFV hypothesizes that this flavor symmetry is only broken by the Yukawa matrices at low energies. The SM can then be rephrased as a flavor-invariant theory if one introduces a formal transformation rule for the Yukawas under this flavor group. MFV goes on to posit that any nonrenormalizable operator made of SM fields should be flavor-invariant as well. In particular, the coefficients of flavorful operators, possibly contributing to exotic processes, must be functions of the Yukawa matrices such that the flavor charges of the fields composing the operator are cancelled.

In this way, MFV has two main consequences. First and foremost, it provides a way out of the ever-looming FCNC problem. The structure forced by the SM Yukawa couplings onto the coefficients of the nonrenormalizable operators is enough to lower the smallest possible scale of new flavor physics down to a few TeV. Secondly, it provides predictability, to some extent, since the same Yukawa couplings link the SM masses and mixings with the rates for exotic flavor processes.

In contrast, MFV does not explain, nor is it designed to explain, how the SM Yukawa structure comes about. In this regard, an old idea of Cabibbo [170] has been recently resurrected. The proposal is to take the MFV hypothesis seriously and promote the Yukawa couplings to flavor-charged scalar fields. It is now possible to try to reproduce the SM observables by extremizing a flavor-invariant Yukawa potential. This approach has achieved partial success. In particular, it naturally produces no mixing in the quark
sector while in the lepton sector, it can explain at least one large angle if neutrinos are Majorana in character. On the other hand, other features pertaining to the flavor puzzle are harder to account for, such as the hierarchy of masses and the observed values of the mixing angles, both in the quark and in the lepton sector 168–169, 171–173.

In this chapter, we put forward an alternative hypothesis to MFV. We keep the assumption that the SM is formally invariant under some flavor symmetry, but we abandon the requirement that the Yukawas are fundamental fields under it. We focus on a scenario in which the flavor symmetry of the SM is a single $SU(2)$ group, which we dub flavorspin, that is the same for all fermions. Continuous flavor symmetries have been previously discussed in, for instance, Refs. 174–184. Under flavorspin, quarks and leptons transform as triplets and Yukawa matrices are upgraded to composite spurions, formed by linear combinations of fundamental ones that transform as symmetric or antisymmetric real matrices under flavor $SU(2)$. The ansatz proposed in this chapter shares with MFV the capacity to suppress FCNCs. At the same time, it can account for several features that a solution to the flavor puzzle should target. Moreover, as we shall discuss in detail below, this simple case provides a way to link the flavor features of the quark and lepton sectors, by using the same fundamental spurions everywhere.

The chapter is organized as follows. In the first three sections, our framework is presented in detail and theoretical and analytical results are described. In the later sections, we perform an extensive numerical exploration of the framework and delve into phenomenological features such as the absence of FCNCs. In the final section, we discuss the results and comment on several ways this work could be extended.
6.2. Flavorspin

We consider a theory $\mathcal{L}$ that can generically be written as:

(6.2.1) \[ \mathcal{L} = \mathcal{L}_{SM} + \mathcal{L}_\nu + \mathcal{L}_{NR} . \]

where $\mathcal{L}_{SM}$ is the SM Lagrangian, $\mathcal{L}_\nu$ are renormalizable terms that account for neutrino masses and $\mathcal{L}_{NR}$ are possible nonrenormalizable operators composed of SM fields. The SM piece $\mathcal{L}_{SM}$ can be split into flavorful and flavorless terms as

(6.2.2) \[ \mathcal{L}_{SM} = \mathcal{L}_0 + \mathcal{L}_{Yuk} , \]

where $\mathcal{L}_0$ contains the standard kinetic terms, Higgs potential and gauge interactions. Here, we are mostly interested in the flavorful Yukawa terms, contained in $\mathcal{L}_{Yuk}$. These have the form

(6.2.3) \[ -\mathcal{L}_{Yuk} = \bar{Q}_L Y_u U_R \cdot \tilde{H} + \bar{Q}_L Y_d D_R \cdot H + \bar{L}_L Y_l E_R \cdot H + \text{h.c.} . \]

It is well known that in order to account for neutrino masses, the SM has to be extended. There are many possibilities for doing so consistently; in this work, we will focus on three of them, namely, Dirac neutrinos and the type I and type II seesaw Majorana neutrinos.

- **Dirac neutrinos**: This possibility involves the introduction of a set of right-handed neutrinos $N_R$. Neutrinos acquire a mass exactly the other fermions do,

(6.2.4) \[ \mathcal{L}_\nu = -\bar{L}_L Y_\nu N_R \cdot \tilde{H} + \text{h.c.} . \]
In the purely Dirac neutrino scenario, the SM preserves lepton number (LN) symmetry, the $U(1)$ global symmetry under which both $L_L$ and $N_R$ have charge +1.

- **Type I Seesaw:** Right-handed neutrinos are introduced, in this case with a heavy Majorana mass, profiting from the fact that they are SM singlets,

$$\mathcal{L}_\nu = -\overline{L_L} Y_\nu N_R \cdot \tilde{H} - \frac{1}{2} M N_R N_R^c + \text{h.c.}$$

(6.2.5)

This Lagrangian violates LN. With the charge assignment above, the Yukawa term preserves LN; only the Majorana mass breaks it. In this work, it will be assumed for simplicity that $M$ is proportional to the identity,

$$M \propto \mathbb{I},$$

(6.2.6)

though the results of this work do not depend strongly on this assumption. In addition, the type I seesaw is able to explain the low scale of the neutrino masses. Below the electroweak symmetry breaking (EWSB) scale and after integrating out $N_R$, the light neutrinos acquire Majorana masses given by the matrix

$$m_\nu = \frac{v^2 Y_L Y_\nu^T}{M}.$$

(6.2.7)

which yields the right order of magnitude for the neutrino masses if $M/Y_\nu^2 \sim 10^{15}$ GeV.
• **Type II Seesaw**: The SM is augmented with an $SU(2)_W$ triplet $\Delta$ that couples to the leptons and the Higgs boson as

\[ \mathcal{L}_\nu = -\mu_\Delta HH\Delta - Y_\Delta \bar{L}_L L'^c_\nu \Delta + \text{h.c.} + \ldots \]  

(6.2.8)

where $\mu_\Delta$ has energy dimensions and $Y_\Delta$ is flavor-charged. In this case, after integrating out the triplet and EWSB, the Majorana mass matrix for active neutrinos appears again, given by

\[ m_\nu = \frac{\mu_\Delta v^2 Y_\Delta}{M_\Delta^2}. \]  

(6.2.9)

In all of the above, summation over flavor indices is implicit.

The nonrenormalizable term in Eq. (6.2.1), $\mathcal{L}_{NR}$, consists of all the gauge-invariant operators of dimension higher than 4 that can be constructed out of SM fields [185–187],

\[ \mathcal{L}_{NR} = \sum_{d>4, \alpha} c_\alpha^{(d)} \frac{\Lambda^{d-4}}{\Lambda^{d-4}} O_\alpha^{(d)}, \]  

(6.2.10)

where $d$ is the energy dimension of the operator and $\alpha$ runs over all operators of a given dimension. We will consider here the phenomenologically-relevant $d = 5, 6$ flavorful operators that include one or more fermionic bilinear so that we can decompose $O_\alpha^{(d)}$,

\[ c_\alpha^{(d)} O_\alpha^{(d)} = c_\alpha^{(d)} F_i F_j \cdot Q_\alpha^{(d)}. \]  

(6.2.11)

where $F$ stands for any fermion or antifermion and $i, j$ are flavor indices. The Lorentz structure of such operators is not relevant here.
To define our scenario, the Yukawa couplings are upgraded to spurions, i.e., couplings that formally transform under a flavor symmetry $G_{fl}$. The Lagrangian $\mathcal{L}$ in Eq. (6.2.1) must be $G_{fl}$-invariant under simultaneous transformations of the spurions and the SM fields. The departure from MFV comes in the choice of the flavor group. In standard MFV, one factor of $SU(3)$ is introduced for each type of fermion. We hypothesize instead that the flavor group is

\begin{equation}
G_{fl} = SU(2),
\end{equation}

under which fermions transform as triplets,

\begin{equation}
F \rightarrow OF, \quad F = Q_L, L_L, D_R, U_R, E_R, N_R.
\end{equation}

Here, $O$ is an orthogonal $3 \times 3$ matrix and it is the same for all fermionic fields. This group is the only flavor symmetry we impose. In particular, the SM global $SU(3)^5$ flavor symmetry, apparent when the Yukawa couplings are set to zero, is understood to be mostly accidental. We refer to this flavor $SU(2)$ as flavorspin$^1$.

Demanding that the Yukawa terms are flavorspin-invariant restricts the possible transformation laws for the Yukawa couplings. In this case, they must formally belong in the

\begin{equation}
3 \times 3 = 5 \oplus 3 \oplus 1
\end{equation}

representations of $G_{fl}$. Of these, the singlet term is flavorless, corresponding to a Yukawa matrix proportional to the identity. The possible fundamental Yukawa spurions with

$^1$We will use the name “flavorspin” to refer to the $SU(2)$ of flavor proposed here and, more generally, to the framework constructed using this group; its meaning will be clear from context.
nontrivial flavor structure can therefore be represented by a $3 \times 3$, traceless, symmetric, real Yukawa tensor, corresponding to the 5, and a $3 \times 3$ antisymmetric real one, corresponding to the 3.

The main hypothesis of this work is that all of the SM flavor can be understood from a minimalistic set of $SU(2)$ spurions. Specifically, we assume flavor is determined by two unique spurions in the 3 and 5 representations of $SU(2)$\(^2\). These are denoted by $Y_3$ and $Y_5$ respectively. Under $G_{fl}$, $Y_3$ and $Y_5$ transform as

\[(6.2.15)\quad Y_3 \rightarrow OY_3O^T, \quad Y_5 \rightarrow OY_5O^T.\]

where $O$ is an orthogonal $3 \times 3$ matrix. This rule guarantees that the Lagrangian $\mathcal{L}$ is $G_{fl}$-invariant as long as $Y_X$, $Y_\Delta$ and the $c^{(d)}_{a,ij}$ are polynomial functions of $Y_3$, $Y_5$. Thus, a first approximation to the SM flavor structure is given by

\[(6.2.16)\quad Y_X \equiv f_X(Y_3, Y_5) + \delta_X I, \quad Y_\Delta \equiv f_\Delta(Y_3, Y_5) + \delta_\Delta I, \quad c^{(d)}_{a,ij} \equiv f^{(d)}_{a,ij}(Y_3, Y_5) + \delta^{(d)}_{a,ij}.\]

with $X = u, d, l, \nu$, where the $f$ are polynomial functions of $Y_3$ and $Y_5$, and the $\delta$ coefficients are arbitrary complex numbers.

However, as it stands, Eq. (6.2.16) does not include an evident parameter on which to perform a perturbative expansion. Indeed, one can explicitly check that masses and mixing angles derived from it can be arbitrarily large. On the other hand, several SM observables pertaining flavor are parametrically small. These include the mixing angles in the quark sector and the masses of the first and second generations relative to the

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\(^2\)One could equally well formulate flavorspin as an $SO(3)$ theory of flavor; the 3 and 5 are the vector and tensor representations of $SO(3)$, respectively. The local isomorphism between $SU(2)$ and $SO(3)$ renders the distinction between these two groups irrelevant for our purposes here.
third. We thus restrict the parameter space allowed by Eq. (6.2.16) by making some of the couplings above perturbative. In particular, we will assume a hierarchy between the contributions from the symmetric and antisymmetric spurions to flavor. More specifically, we demand

\[ Y_X \equiv f_X(Y_3, \varepsilon_X Y_5) + \delta_X \mathbb{I}, \quad c_{a, ij}^{(6)} \equiv f^{(6)}_{a, ij}(Y_3, \varepsilon^{(6)}_a Y_5) + \delta^{(6)}_a \mathbb{I}. \]

where \(|\varepsilon_X|, |\delta_X|, |\varepsilon^{(6)}_a|, |\delta^{(6)}_a| \ll 1\). Note that no such assumptions are made for \(Y_\Delta\), nor for the coefficient of the \(d = 5\) Weinberg operator. We will provide a possible argument to justify this apparently arbitrary distinction in a later section based on the fact that these operators violate \(B - L\).

In the remainder of this section, we analyze the features of flavor to be expected at zeroth order from Eq. (6.2.17). Consider the LN-conserving Yukawa coefficients \(Y_X\). Explicitly, Eq. (6.2.17) amounts to the Yukawa matrices taking the form

\[ Y_X = \mu_X (Y^0_X + Y_{\varepsilon X}) \]

with

\[ Y^0_X = iY_3 + A_X e^{ia_X \cdot Y_3^2}, \quad Y_{\varepsilon X} = \varepsilon_X Y_5 + \delta_X \cdot \mathbb{I} + \ldots . \]

The normalization factor \(\mu_X\) sets the overall mass scale of each fermion type and it is fixed so that

\[ \frac{1}{2} \text{Tr}[Y_3 Y_3^T] = 1. \]
The real antisymmetric flavor spurion $Y_3$ is assumed to be $O(1)$ and it is universal, i.e., the zeroth-order terms in $Y_X^0$ are formed by linear combinations of the same $Y_3$ and $Y_3^2$ for all fermion types. The real constants $A_X$ and $\alpha_X$ specify the relative phase and weight of the two terms composing $Y_X^0$. Notice the relative factor of $i$ in Eq. (6.2.19); this amounts to a phase redefinition of the quark fields and is a useful convention, as we will make clear.

By means of $G_{fl}$ transformations, it is always possible to choose a basis in which the $Y_3$ spurion takes the form

$$Y_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}.$$  

(6.2.21)

In this basis, it is evident why the truncation of the series at the quadratic order in $Y_3$ in Eq. (6.2.19) is justified. Higher powers of $Y_3$ need not be introduced since $Y_3^3 = -Y_3$, as can be readily verified. For the remainder of this work, we work in this basis.

The term $Y_{\epsilon X}$ represents the perturbation term and it is formed by a linear combination of the universal, real, symmetric and traceless spurion $Y_5$,

$$Y_5 = \begin{pmatrix} y_{11} & y_{12} & y_{13} \\ y_{12} & y_{22} & y_{23} \\ y_{13} & y_{23} & -(y_{11} + y_{22}) \end{pmatrix},$$

(6.2.22)

and the singlet term, see Eq. (6.2.19). It is assumed that $|\epsilon_X|, |\delta_X| \ll 1$.

Any $Y_X^0$ of the form in Eq. (6.2.19) has one null eigenvalue. Setting aside the neutrinos for the time being – the possibility of Majorana masses changes this picture – it is clear
that, in the unperturbed setup, the lightest charged fermions have vanishing masses. Hence, our scenario automatically leads to a spectrum in which the first generation is much lighter than the other two.

Let us introduce the parameter

\[(6.2.23) \quad \xi_X \equiv 1 - A_X e^{i\alpha_X} \]

It can be easily shown that the two remaining eigenvalues are generically nonzero, their values given by

\[(6.2.24) \quad m_2^2 = (\mu_X v)^2 |\xi_X|^2 \]
\[(6.2.25) \quad m_3^2 = (\mu_X v)^2 |2 - \xi_X|^2 \]

From Eq. (6.2.24), it is possible for \(m_2\) to vanish as well, if \(\xi_X = 0\). It follows that a large hierarchy between the second- and third-generation masses is obtained for \(|\xi_X| \ll 1\).

Since such a hierarchy is observed for both quarks and charged leptons, we will assume

\[(6.2.26) \quad |\xi_X| \ll 1. \]

This assumption is equivalent to assuming that there is a strong hierarchy between \(m_2^2\) and \(m_3^2\). In other words, in order to explain the SM spectrum in flavorspin, aside from \(\{\varepsilon_X, \delta_X\}\), another set of perturbative parameters, the \(\xi_X\), must exist.
The zeroth-order quark mixing can be quickly computed as well. The Yukawa matrices are generically diagonalized by biunitary transformations,

\[ \tilde{Y}_X = V_{XL} Y_X V_{XR}^\dagger, \quad \tilde{Y}_X = \text{diag}\{y_{X1}, y_{X2}, y_{X3}\}, \]

and zeroth order in \(\{\varepsilon_X, \delta_X\}\), we find

\[ V_{uL} = V_{dL} = V_{\ell L} = V_{\nu L} = V_{uR} = V_{dR} = V_{\ell R} = V_{\nu R}. \]

This is because \(Y_3\), being fully antisymmetric, is diagonalized by a similarity transformation \(V^0\). Thus, we have

\[ \tilde{Y}_X^0 = V^0 Y_X^0 V^{0\dagger} \]

where \(\tilde{Y}_X^0\) is diagonal. \(V^0\) is found to be

\[
V^0 \equiv V_{XL}(\varepsilon_X = 0) = V_{XR}(\varepsilon_X = 0) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & -i & 0 \\ 0 & 0 & 1 \end{pmatrix}.
\]

The quark mixing matrix \(V_{CKM}\) is defined as

\[ V_{CKM} = V_{uL}^\dagger V_{dL}. \]

Hence, from Eq. (6.2.30), it follows that there is no mixing in the quark sector at zeroth order in \(\{\varepsilon_X, \delta_X\}\),

\[ V_{CKM} = I + \mathcal{O}(\varepsilon). \]
In the spirit of the ansatz proposed above, the coefficients $c^{(d)}_{\alpha}$ accompanying LN-conserving operators are also assumed to be linear combinations of $Y_3$, $Y_5$ and $I$. With respect to perturbativity, however, the LN-violating couplings $Y_{\Delta}$ of the type II seesaw and $c^{(5)}_W$ are treated differently. In particular, no hierarchy is assumed between the coefficients of the linear combination of fundamental spurions from which $Y_{\Delta}$ is formed. We have, for instance,

$$Y_{\Delta} = \eta_{33} Y_3 Y_3^T + \eta_5 Y_5 + \eta_I I + \cdots$$  \hspace{1cm} (6.2.33)

with all the coefficients being, in principle, of $O(1)$.

Summarizing, we have introduced a framework that posits an $SU(2)$ horizontal flavor group, flavorspin, under which SM fermions transform as triplets. Based on phenomenological considerations, we will focus on a specific scenario in which the following hold:

1. The Lagrangian $\mathcal{L}$ including the SM and possible flavor-charged higher-dimensional operators is invariant under $G_{fl}$.
2. Only two spurions, $Y_3$ and $Y_5$, transforming according to the 3 and 5 representations of $G_{fl}$, respectively, are introduced.
3. The symmetric contribution to the Yukawa couplings, represented by $Y_5$ and the singlet term, is small compared to that of $Y_3$ for $B-L$-conserving, flavor-charged operators. That is, we impose $|\varepsilon_X|, |\delta_X| \ll 1$ in Eq. (6.2.17).
4. The parameters $\xi_X$ parametrizing the hierarchy between the second and third generation satisfy $|\xi_X| \ll 1$.

No hierarchy is assumed between the perturbative parameters $\varepsilon_X$ and $\xi_X$. 
Although the large mass difference between the second- and third-generation fermions is imposed by hand via $|\xi_X| \ll 1$, this feature is intrinsically connected to the large relative phase between the $Y_3$ and $Y_3^2$ contributions to $Y_X$. In particular, the $CP$-invariant possibility $\alpha_X = \pi/2$ would have led to phenomenologically unrealistic degeneracy of the masses of the second- and third-generation states. This will generically lead to large $CP$ violation once nonvanishing mixings emerge due to the $Y_5$ perturbations.

### 6.3. Perturbations in the Quark Sector

There are two main effects of introducing the perturbation $Y_{\varepsilon X}$ in Eq. (6.2.18): (1) To lift the lightest quark masses from zero, and (2) to give rise to small mixing angles. Using $Y_5$ from Eq. (6.2.22), the perturbations induced by $Y_{\varepsilon X}$ to Eq. (6.2.24) can be computed up to the most relevant order. We obtain the following expressions for the perturbed eigenvalues:

\begin{align}
  m_{1X}^2 &= \mu_X^2 v^2 (F_X - G_X) \\
  m_{2X}^2 &= \mu_X^2 v^2 (F_X + G_X) \\
  m_{3X}^2 &= 2\mu_X^2 v^2 (2 + y_{11}\varepsilon_X - 2\delta_X + 2\xi_X)
\end{align}

where

\begin{align}
  F_X &= \frac{1}{8} \left[ (5y_{11}^3 + 4y_{12}^2 + 4y_{13}^2) \varepsilon_X^2 + 8\delta_X^2 + 4\xi_X^2 + 4y_{11}(\varepsilon_X \delta_X + \varepsilon_X \xi_X) + 8\delta_X \xi_X \right] , \\
  G_X &= \frac{1}{8} \left( 4\delta_X + 2\xi_X - y_{11}\varepsilon_X \right) \sqrt{(9y_{11}^2 + 8y_{12}^2 + 8y_{13}^2) \varepsilon_X^2 - 12y_{11}\varepsilon_X \xi_X + 4\xi_X^2} .
\end{align}

\textsuperscript{3}Technically, there is no $CP$ violation at this stage. All the phases in the Lagrangian can be reabsorbed by unitary redefinitions of the quark and lepton fields. However, once perturbations are introduced, the large phase difference between the two terms in $Y_X^2$ will indeed lead to large values for $CP$ violation.
In Eq. (6.3.1), terms have been kept up to the lowest relevant order for the first two eigenvalues, \( m^2_{1,2} \). The mass of the third eigenvalue is corrected at order \( \mathcal{O}(|\varepsilon_X|, |\delta_X|, |\xi_X|) \) and its order of magnitude is determined by the EWSB scale and by the dimensionless coupling \( \mu_X \). It is straightforward to check that for \(|\varepsilon_X|, |\delta_X| \to 0\), the perturbed spectrum reduces to Eq. (6.2.24). Thus, the simplest way to implement the hierarchy between the first- and second-generation masses without imposing any artificial tuning is to assume a hierarchy between the perturbative parameters,

\[(6.3.3) \quad |\varepsilon_X|, |\delta_X| \lesssim |\xi_X| \ll 1.\]

In this case, the second-to-third-generation mass ratio can be approximated by:

\[(6.3.4) \quad \frac{m^2_{2X}}{m^2_{3X}} \sim |\xi_X|^2.\]

Replacing in all of what follows \( X \to u, d \), we obtain \( \xi_{u,d} \sim \mathcal{O}(10^{-2}) \).

A crude, yet useful estimation for the first-to-second-generation mass ratio can also be obtained by keeping only the highest order terms in \( \xi_{u,d} \) in the ratio

\[(6.3.5) \quad \frac{m^2_{1X}}{m^2_{2X}} \sim \frac{3\varepsilon_X}{\xi_X} \cdot y_{11} \sim \varepsilon_X y_{11} \cdot 10^2\]

For the quarks we have: \( m^2_u/m^2_c \sim 10^{-6} \), \( m^2_d/m^2_s \sim 10^{-4} \). Thus, generically we obtain

\[(6.3.6) \quad \frac{\varepsilon_u}{\xi_u} < \frac{\varepsilon_d}{\xi_d}.\]

This result will be validated by our numerical analysis in Sec. (6.5). The latter also shows that the mass ratios and the relatively large size of the Cabibbo angle cannot both be
accounted simply by setting $|\varepsilon_X/\xi_X|$ small. Thus, it is necessary that

$$y_{11}, |\delta_X| \ll 1.$$  \hspace{1cm} (6.3.7)

Finally note that the ratio between the $\mu_X$ determines the scales of the up and down sectors

$$\frac{m_b}{m_t} \sim \frac{\mu_u}{\mu_d}.$$  \hspace{1cm} (6.3.8)

The small $\varepsilon$-parameters also give rise to small mixing angles. The sines of these mixing angles, to leading order in $\varepsilon_X$, are given by

$$\sin \theta_{q12} \simeq \frac{1}{\sqrt{2}} \left| (y_{12} - iy_{13}) \frac{\varepsilon_d}{\xi_d} \frac{\varepsilon_u}{\xi_u} \right|,$$  \hspace{1cm} (6.3.9)

$$\sin \theta_{q13} \simeq \frac{1}{\sqrt{2}} \left| (y_{12} + iy_{13})(\varepsilon_d - \varepsilon_u) \right|,$$  \hspace{1cm} (6.3.10)

$$\sin \theta_{q23} \simeq \frac{1}{4} \left| (y_{11} + 2y_{22} + 2iy_{23})(\varepsilon_d - \varepsilon_u) \right| \sim \frac{1}{2} \left| (y_{22} + iy_{23})(\varepsilon_d - \varepsilon_u) \right|.$$  \hspace{1cm} (6.3.11)

Hence, approximately,

$$\frac{\sin \theta_{q13}}{\sin \theta_{q23}} \sim \left| \frac{y_{12} + iy_{13}}{y_{22} + iy_{23}} \right| \sim 10^{-1}.$$  \hspace{1cm} (6.3.12)

Thus, a mild hierarchy between the values of $\{y_{12}, y_{13}\}$ and those of $\{y_{22}, y_{23}\}$ is expected. Also, from Eq. (6.3.6), we can roughly approximate:

$$\sin \theta_{q12} = \frac{1}{\sqrt{2}} \left| (y_{12} - iy_{13}) \frac{\varepsilon_d}{\xi_d} \right| \sim \frac{m_d}{\sqrt{2}m_s} \left| (y_{12} - iy_{13}) \right|. $$  \hspace{1cm} (6.3.13)
Eqs. (6.3.9)-(6.3.11) illustrate an important consequence of flavorspin: the enhancement of \( \sin \theta_{12} \) with respect to \( \sin \theta_{13} \) and \( \sin \theta_{23} \). A rough order of magnitude estimate of this enhancement is

\[
\frac{\sin \theta_{12}}{\sin \theta_{13}} \approx \frac{1}{|\xi_d|} \sim \frac{m_3}{m_2} \sim 10^2.
\]

We stress that this enhancement is a consequence of the \( SU(2) \) structure coupled to the intergenerational mass hierarchy.

The \( CP \)-violating phase \( \delta_{CP}^q \) in the quark sector can be computed via the Jarlskog invariant \( J \):

\[
J = \left( \sum_{m,n} \epsilon_{ikm} \epsilon_{jn} \right) \Im \left[ V_{ij} V_{kl} V_{i}^{*} V_{k}^{*} \right] = c_{12}^2 c_{13}^2 s_{12} s_{13} s_{23} \sin \delta_{CP}^q,
\]

defining \( s_{ij} \equiv \sin \theta_{ij}^q \) and \( c_{ij} \equiv \cos \theta_{ij}^q \). The leading-order contribution to \( J \) is \( \mathcal{O}(|\varepsilon_X|^3) \). In order to compute it, it is enough to consider the CKM matrix to \( \mathcal{O}(|\varepsilon_X|) \), use \( \{i,j,k,l\} = \{1,2,2,3\} \) in Eq. (6.3.15) and replace the mixing angles using in Eqs. (6.3.9)-(6.3.11).

### 6.4. Leptons

The formalism of the last two sections generalizes straightforwardly to the charged leptons. Neutrinos, however, are a different story since the character of the neutrino masses is not known. We consider both the Dirac and Majorana options.

#### Pure Dirac Masses

For purely Dirac neutrinos, the zeroth-order neutrino masses are given by Eq. (6.2.24) and the effects resulting from the perturbations are given by Eq. (6.3.1). The leptonic mixing
angles are given by the same expressions as in Eqs. (6.3.9)-(6.3.11) with the replacements $d \to \ell$, $u \to \nu$:

\begin{align*}
\sin \theta_{12}^\ell &= \frac{1}{\sqrt{2}} \left| (y_{12} - iy_{13}) \left( \frac{\varepsilon_{\ell}}{\xi_{\ell}} - \frac{\varepsilon_{\nu}}{\xi_{\nu}} \right) \right|, \\
\sin \theta_{13}^\ell &= \frac{1}{\sqrt{2}} \left| (y_{12} + iy_{13}) (\varepsilon_{\ell} - \varepsilon_{\nu}) \right|, \\
\sin \theta_{23}^\ell &= \frac{1}{4} \left| (y_{11} + 2y_{22} + 2iy_{23})(\varepsilon_{\ell} - \varepsilon_{\nu}) \right|.
\end{align*}

Following the analysis of the previous section, it is clear that these formulae cannot reproduce the observed mixing properties of the leptons. In particular, in the lepton sector, all three observable angles are sizable. While the enhancement of $\theta_{12}^\ell$ shown in Eq. (6.4.1) is still relevant and desirable, $\theta_{23}^\ell$ is still predicted to be perturbatively small in Eq. (6.4.3). This angle is known to be close to 45° and cannot be explained in the perturbative framework we have introduced.

**Majorana Masses**

For the case of Majorana neutrinos, several possibilities can be investigated for the structure of the Yukawa matrices. Let us consider, then, a general Majorana mass term for the light neutrino states. It can be written as

\begin{equation}
\mu_{\nu} \nu \nu \mathcal{M}_{\nu} \nu^c,
\end{equation}

where $\mathcal{M}_{\nu}$ is a flavor-charged, symmetric matrix, $\mathcal{M}_{\nu} \equiv \mathcal{M}_{\nu}(Y_3, Y_5)$, and $\mu_{\nu}$ is a dimensionless, possibly small parameter. This mass term is not invariant under the gauge symmetry of the SM and extra fields should be added in order to compensate the $SU(2)_W$...
and hypercharge charges of the neutrino states. This leads to nonrenormalizable neutrino mass operators. The simplest such possibility is to add two Higgs fields to form the dimension-five Weinberg operator,

\[
\frac{c_W^{(5)}}{\Lambda_{LN}} \bar{LL}^c HH, \quad \frac{\nu c_W^{(5)}}{\Lambda_{LN}} = \mu_\nu \mathcal{M}_\nu.
\]

As is well known, there are three ways to generate the Weinberg operator at tree level, the so-called type I, II and III seesaw mechanisms.

In flavorspin, \( M_\nu \) should be considered a polynomial function of the spurions \( Y_3 \) and \( Y_5 \) with complex coefficients. We are interested in truncations of this polynomial inspired by the seesaw mechanisms. They can all be parametrized by an \( M_\nu \) of the form:

\[
M_\nu = \eta_{33} Y_3 Y_3^T + \eta_5 Y_5 + \eta_1 + \eta_{35} (Y_3 Y_5^T + Y_5 Y_3^T) + \eta_{55} Y_5 Y_5^T + \eta_{335} (Y_3 Y_5 Y_3^T + Y_5 Y_3 Y_3^T) + \eta_{353} Y_3 Y_5 Y_3^T,
\]

where for simplicity we have kept terms of at most third-order in \( Y_3, Y_5 \) and that are at most second-order in \( Y_5 \).

A naive consideration and a driving idea of this work is the fact that in the limit

\[
\{\eta_5, \eta_1, \eta_{35}, \eta_{55}, \eta_{335}, \eta_{353}\} \to 0,
\]

one obtains

\[
M_\nu \to M_\nu^0 \equiv \eta_{33} Y_3 Y_3^T = \begin{pmatrix}
0 & 0 & 0 \\
0 & \eta_{33} & 0 \\
0 & 0 & \eta_{33}
\end{pmatrix}.
\]
The mass matrix for Majorana neutrinos is already diagonal in the basis employed here. Eq. (6.4.8) suggests an inverted hierarchy of neutrino masses with two nonzero eigenvalues while the third vanishes. Since the flavor and the mass bases for the neutrinos coincide in this limit, the leptonic mixing matrix, analogous to $V_{CKM}$ in Eq. (6.2.31), is given by:

$$V_{PMNS} = V_{\ell L} = V^0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & -i & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{6.4.9}$$

In particular, contrary to the quark case, flavorspin predicts one large mixing angle $-45^\circ$, at zeroth order -- in the lepton sector with Majorana neutrinos.

However, it is wrong to associate the angle in Eq. (6.4.9) with $\theta_{l_{23}}$. Since the favored pattern in this case is an inverted hierarchy and Eq. (6.4.9) mixes the two states with nonzero masses, this mixing angle should be identified with $\theta_{l_{12}}$. Therefore, presumably large deviations from the zeroth-order structure are required to generate a large $\theta_{l_{23}}$.

 Nonetheless, the fact that one mixing angle automatically comes out large is encouraging. Coming back to Eq. (6.4.6), we explore the following cases in detail:

- **Type I Seesaw:** $\mathcal{M}_\nu$ is assumed to be given by

$$\mathcal{M}_\nu = Y_\nu Y^T_\nu \tag{6.4.10}$$

with $Y_\nu$ defined in Eqs. (6.2.18) and (6.2.19). The coefficients in Eq. (6.4.6) are given by:

$$\eta_{33} = 1 + 2\delta_\nu - (1 - \xi_\nu)^2, \quad \eta_5 = \varepsilon_\nu \delta_\nu, \quad \eta_1 = \delta_\nu^2, \tag{6.4.11}$$
\[ \begin{align*} 
\eta_{35} &= \varepsilon_\nu, \\
\eta_{55} &= \varepsilon_\nu^2, \\
\eta_{335} &= (1 - \xi_\nu)\varepsilon_\nu, \\
\eta_{353} &= 0, 
\end{align*} \]

where we have used \((Y_3^T Y_3)^2 = -Y_3 Y_3^T\). Importantly, the coefficients in \(M_\nu\) are correlated and depend only on the complex numbers \(\xi_\nu, \varepsilon_\nu\) and \(\delta_\nu\), where \(|\xi_\nu|, |\varepsilon_\nu|, |\delta_\nu| \ll 1\).

- **Type II Seesaw**: In this scenario, \(M_\nu\) is identified with \(Y_\nu + Y_\nu^T\). There is no term proportional to \(Y_3\) because \(M_\nu\) is symmetric and, moreover, we set

\[ \eta_{35} = \eta_{55} = \eta_{335} = \eta_{353} = 0. \]

For the other parameters, only \(|\eta_{33}|, |\eta_5|, |\eta_1| \lesssim 1\) is assumed.

Although we are referring to these two scenarios as type I and type II seesaws, these naming conventions should not be taken too literally. In particular, there is no strong argument for the conditions imposed in Eq. (6.4.13) other than simplicity. We will briefly comment on the most general case, as defined in Eq. (6.4.6), in Sec. 6.5.

**Type I Seesaw.** The explicit form of the type I seesaw mass matrix in Eq. (6.4.10) is

\[ \begin{align*} 
M_\nu &= \frac{\mu_\nu^2 v^2}{\Lambda_{LN}} \times \\
&= \begin{pmatrix} 
0 & \varepsilon_\nu (iy_{13} - y_{12}) & -\varepsilon_\nu (iy_{12} + y_{13}) \\
\varepsilon_\nu (iy_{13} - y_{12}) & -2(y_{22}\varepsilon_\nu - iy_{23}\varepsilon_\nu + \delta_\nu + \xi_\nu) & -\varepsilon_\nu (iy_{11} + 2iy_{22} + 2y_{23}) \\
-\varepsilon_\nu (iy_{12} + y_{13}) & -\varepsilon_\nu (iy_{11} + 2iy_{22} + 2y_{23}) & 2(y_{11}\varepsilon_\nu + y_{22}\varepsilon_\nu - iy_{23}\varepsilon_\nu - \delta_\nu - \xi_\nu) 
\end{pmatrix} + \mathcal{O}(\{|\xi_\nu|, |\varepsilon_\nu|, |\delta_\nu|\}^2), 
\end{align*} \]
where $\Lambda_{LN}$ is the scale of LN-violating physics. We consider the masses in the limit $y_{11}, y_{12}, y_{13}, |\xi_\nu|, |\varepsilon_\nu|, |\delta_\nu| \ll 1$; we will justify these limits of $y_{11}, y_{22}$ and $y_{23}$. The neutrino masses become

\begin{align*}
(6.4.15) \quad m_1^2 &= \mathcal{O}(\{y_{12}, y_{13}\}^2), \\
(6.4.16) \quad m_2^2 &= \frac{\mu_{\nu}^4}{\Lambda_{LN}^2} (F_\nu - G_\nu) + \mathcal{O}(\{y_{11}, y_{12}, y_{13}\}^2; \{|\xi_\nu|, |\varepsilon_\nu|, |\delta_\nu|\}^3), \\
(6.4.17) \quad m_3^2 &= \frac{\mu_{\nu}^4}{\Lambda_{LN}^2} (F_\nu + G_\nu) + \mathcal{O}(\{y_{11}, y_{12}, y_{13}\}^2; \{|\xi_\nu|, |\varepsilon_\nu|, |\delta_\nu|\}^3),
\end{align*}

where we have introduced the quantities

\begin{align*}
(6.4.18) \quad F_\nu &= 8|\varepsilon_\nu|^2(y_{22}^2 + y_{23}^2) + 4|\xi_\nu + \delta_\nu^*|^2, \\
(6.4.19) \quad G_\nu &= 8|\varepsilon_\nu|\sqrt{(y_{22}^2 + y_{23}^2)\{|\varepsilon_\nu|^2(y_{22}^2 + y_{23}^2) + |\xi_\nu + \delta_\nu^*|^2\}.}
\end{align*}

The ordering of the neutrino mass eigenstates here differs slightly from that used in analyses of neutrino oscillations. Here, the masses are strictly ordered from least to greatest: $m_1^2 < m_2^2 < m_3^2$. For the latter, however, the ordering depends on the hierarchy; for the normal hierarchy (NH), the ordering is the same as the one used here, but for the inverted hierarchy (IH) the masses are ordered $m_3^2 < m_1^2 < m_2^2$. It will be important to establish, for the rest of this work, the conditions for the NH and IH in the ordering scheme we employ:

\[ m_3^2 - m_2^2 > m_2^2 - m_1^2 \quad \Rightarrow \quad \text{NH}, \]

\footnote{We remind the reader that for neutrino oscillations, the two closest values of $m^2$ are defined to be $m_1^2$ and $m_2^2$, with $m_1^2$ being the lighter of the two. The third is then defined to be $m_3^2$, which may be heavier or lighter than the other two.}
\begin{align*}
(6.4.20) \quad m_3^2 - m_2^2 &< m_2^2 - m_1^2 \quad \Rightarrow \quad \text{IH}.
\end{align*}

For the masses in Eq. (6.4.15) to constitute a NH, the condition $3G_\nu > F_\nu$ must be satisfied; otherwise, neutrinos are organized in an IH. When $|\xi_\nu + \delta^*_\nu| \ll |\varepsilon_\nu|$, then $G_\nu \sim F_\nu$, and the masses may constitute a NH. In the opposite limit,

\begin{align*}
(6.4.21) \quad G_\nu/F_\nu &\rightarrow 2|\varepsilon_\nu| \cdot (y_{22}^2 + y_{23}^2)/|\xi_\nu + \delta^*_\nu| \ll 1,
\end{align*}

and the masses organize in an IH.

**Type II Seesaw.** The explicit form of the type II seesaw mass matrix, from Eqs. (6.4.6) and (6.4.13), is

\begin{align*}
(6.4.22) \quad M_\nu &= \begin{pmatrix}
\eta_1 + \eta_5 y_{11} & \eta_5 y_{12} & \eta_5 y_{13} \\
\eta_5 y_{12} & \eta_1 + \eta_5 y_{22} + \eta_{33} & \eta_5 y_{23} \\
\eta_5 y_{13} & \eta_5 y_{23} & \eta_1 - \eta_5 (y_{11} + y_{22}) + \eta_{33}
\end{pmatrix}.
\end{align*}

For $y_{11}, y_{12}, y_{13} \ll 1$, as well as $|\eta_{33}|, |\eta_5|, |\eta_1| \lesssim 1$, the neutrino masses become

\begin{align*}
(6.4.23) \quad m_1^2 &= \frac{\mu^4 v^4}{\Lambda_{2/LN}^2} \times \eta_1^2 + \mathcal{O}(y_{11}, y_{12}, y_{13}), \\
(6.4.24) \quad m_2^2 &= \frac{\mu^4 v^4}{\Lambda_{2/LN}^2} (H_\nu - K_\nu) + \mathcal{O}(y_{11}, y_{12}, y_{13}; \{|\eta_{33}|, |\eta_5|, |\eta_1|\}^3), \\
(6.4.25) \quad m_3^2 &= \frac{\mu^4 v^4}{\Lambda_{2/LN}^2} (H_\nu + K_\nu) + \mathcal{O}(y_{11}, y_{12}, y_{13}; \{|\eta_{33}|, |\eta_5|, |\eta_1|\}^3),
\end{align*}

where we have introduced the quantities

\begin{align*}
(6.4.26) \quad H_\nu &= |\eta_1 + \eta_{33}^*|^2 + |\eta_5|^2 (y_{22}^2 + y_{23}^2),
\end{align*}
$$K_{\nu} = \left| (\eta_5 + \eta_{33})\eta_1^* + \eta_1(\eta_5 + \eta_{33}^*) \right| \sqrt{(y_{22}^2 + y_{23}^2)}.$$  \hspace{1cm} (6.4.27)

These quantities must satisfy $3K_{\nu} > H_{\nu} - |\eta_1|^2$ for neutrinos to form a NH, else neutrinos are organized in an IH. Note the difference with the type I seesaw; here, the singlet term corresponding to the coefficient $\eta_1$ is not suppressed. An IH would follow if the singlet term, $\eta_1$, were subdominant to $\eta_{33}$ and $\eta_5$, since then $H_{\nu}$ would dominate $K_{\nu}$. If $|\eta_{33}|, |\eta_5|$ and $|\eta_1|$ are all comparable in magnitude, then it is possible that $H_{\nu}$ and $K_{\nu}$ are likewise comparable. In this case, a NH would be produced.

**Leptonic Mixing Matrix.** The matrix $V_{\nu}$ that diagonalizes the neutrino mass matrix is defined via

$$V_{\nu} \cdot (Y_{\nu}Y_{\nu}^T) \cdot (Y_{\nu}^*Y_{\nu}^\dagger) \cdot V_{\nu}^\dagger = \mathcal{P}^T \cdot \text{diag}(m_1^2, m_2^2, m_3^2) \cdot \mathcal{P}.$$  \hspace{1cm} (6.4.28)

Here, $\mathcal{P}$ is a permutation matrix that reorders the neutrino masses according to the standard mass ordering conventions used in neutrino oscillations, following the discussion surrounding Eq. (6.4.20):

$$m_3^2 - m_2^2 > m_2^2 - m_1^2 : \mathcal{P} = \mathbb{I},$$  \hspace{1cm} (6.4.29)

$$m_3^2 - m_2^2 < m_2^2 - m_1^2 : \mathcal{P} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$  \hspace{1cm} (6.4.30)

For nontrivial $V_{\nu}$, the leptonic mixing matrix $V_{PMNS}$ is given by

$$V_{PMNS} = V_{\ell L}V_{\nu}^\dagger.$$  \hspace{1cm} (6.4.31)
similar to Eq. (6.4.9). We can anticipate some of the numerical results of Sec. 6.5 by inspecting Eqs. (6.4.14) and (6.4.22). For the type I seesaw, and assuming a NH, \( \sin \theta_{12} \) is approximately given by

\[
(6.4.32) \quad \sin \theta_{12} \sim \frac{\left| \mathcal{M}_{12}^{\nu} \right|}{\left| \mathcal{M}_{22}^{\nu} \right|} = \frac{1}{2} \frac{|\varepsilon_{\nu}| \sqrt{y_{12}^2 + y_{13}^2}}{|(y_{22} + iy_{23})\varepsilon_{\nu} - \delta_{\nu} - \xi_{\nu}|}.
\]

In the limit \( y_{12}, y_{13} \ll y_{22}, y_{23} \), this mixing angle is predicted to be small.\(^5\) A similar estimate for the type II seesaw, again assuming a NH, gives

\[
(6.4.33) \quad \sin \theta_{12} \sim \frac{\left| \mathcal{M}_{12}^{\nu} \right|}{\left| \mathcal{M}_{22}^{\nu} \right|} = \frac{\eta_{5}y_{12}}{|\eta_3y_{22} + \eta_{33}|}.
\]

From this equation, assuming \( |\eta_{33}|, |\eta_5| \) and \( |\eta_1| \) are comparable in magnitude, if \( |y_{22}| \) were approximately 1, the terms in the denominator could give a sizable cancellation. In the next section, we will show that, indeed, \( |y_{22}| \) must be approximately 1. In this case, even with \( y_{12} \ll 1 \), a sizable neutrino contribution to \( \sin \theta_{12} \) is possible.

### 6.5. Results

In this section, we numerically explore the parameter space of flavor spin and show that it provides a plausible description of all the SM flavor. We stress that the goal is not to show that there is a set of precise values for the flavor spin parameters that exactly reproduces the low-energy observables of interest to us. Setting aside that the low-energy observables are known with finite precision, attempting to find such a solution is computationally expensive and ultimately unenlightening. We demonstrate instead

\(^5\)Recall that the charged-lepton contribution to this mixing angle given by Eq. (6.4.1) with \( \varepsilon_{\nu} \rightarrow 0 \). The charged-lepton and neutrino contributions to this angle are roughly comparable, as we will see in the next section, so this conclusion is robust.
that general agreement between the predictions of flavorspin and the experimentally-
determined values of low-energy observables can be obtained by looking at specific regions
of parameter space that satisfy the constraints enumerated in Sec. 6.2.

The method used is as follows. First, random values are generated over specified ranges
of the flavorspin parameters, assuming a flat prior in these ranges, and the values for the
relevant observables are calculated for all these points. These pseudodata are binned
together in two-dimensional subspaces of the space of observables, and a likelihood $L$ is
assigned to each bin, proportional to its population, $N$. A $\Delta \chi^2$ is calculated for each bin, via

\begin{equation}
\Delta \chi^2 = 2 \ln \frac{L_0}{L} \approx 2 \ln \frac{N_0}{N},
\end{equation}

where $N_0$ and $L_0$ are the population and likelihood, respectively, of the bin with the highest
population; $\Delta \chi^2 = 0$ corresponds to the center of this bin. A smooth interpolation of
the $\Delta \chi^2$ function is calculated, and the contours along which $\Delta \chi^2 = 2.30, 5.99$ and 9.21
are drawn, corresponding approximately to the 68.3%, 95% and 99% confidence intervals
(CI)\footnote{This correspondence is only exact in the limit of vanishing bin size and a large number of pseudodata
points, but this yields a sufficiently precise approximation of the true confidence intervals for our purposes
here.} in the figures that follow, these will be represented by dark, medium and light
shadings of the color assigned to each scenario, respectively. The goal of this section is
to show that there are ranges of the flavorspin parameters such that these confidence
intervals contain the experimentally-determined values of the observables of interest with
a high degree of confidence.
Table 6.1. The values for the low-energy observables used in our analysis. We use the MS values at $\mu = 1$ TeV calculated in Ref. [3]; see text for details.

<table>
<thead>
<tr>
<th>Observable</th>
<th>MS Value, $\mu = 1$ TeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>$y_u$</td>
<td>$6.3 \times 10^{-6}$</td>
</tr>
<tr>
<td>$y_c$</td>
<td>$3.104 \times 10^{-3}$</td>
</tr>
<tr>
<td>$y_t$</td>
<td>0.8685</td>
</tr>
<tr>
<td>$y_d$</td>
<td>$1.364 \times 10^{-6}$</td>
</tr>
<tr>
<td>$y_s$</td>
<td>$2.74 \times 10^{-4}$</td>
</tr>
<tr>
<td>$y_b$</td>
<td>$1.388 \times 10^{-2}$</td>
</tr>
<tr>
<td>$y_e$</td>
<td>$2.8482 \times 10^{-6}$</td>
</tr>
<tr>
<td>$y_\mu$</td>
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</tr>
<tr>
<td>$y_\tau$</td>
<td>$1.02213 \times 10^{-2}$</td>
</tr>
<tr>
<td>$\sin \theta_{12}^q$</td>
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</tr>
<tr>
<td>$\sin \theta_{13}^q$</td>
<td>$3.770 \times 10^{-3}$</td>
</tr>
<tr>
<td>$\sin \theta_{23}^q$</td>
<td>$4.363 \times 10^{-2}$</td>
</tr>
<tr>
<td>$\sin \delta_{CP}^q$</td>
<td>0.9349</td>
</tr>
</tbody>
</table>

Charged Fermions

The starting point is the determination of the approximate ranges in which the flavorspin parameters must lie in order to reproduce the quark masses and mixing parameters. Table 6.1 shows the MS values of charged-fermion masses and quark mixing observables at the scale $\mu = 1$ TeV, which we have taken from Ref. [3]. The ranges of the parameters that we consider are as follows:

(6.5.2) $|\xi_u| \in [6 \times 10^{-3}, 8 \times 10^{-3}]$, $|\varepsilon_u| \in [1 \times 10^{-3}, 2 \times 10^{-3}]$, $|\delta_u| \in [1 \times 10^{-5}, 2 \times 10^{-5}]$,

(6.5.3) $|\xi_d| \in [0.035, 0.037]$, $|\varepsilon_d| \in [0.06, 0.07]$, $|\delta_d| \in [6 \times 10^{-4}, 7 \times 10^{-4}]$, 
\[y_{11} \in [-0.01, 0.01],\]
\[y_{22} = 1,\]

\((6.5.4)\)
\[y_{23} \in \pm [0.88, 0.92],\]
\[\Phi \equiv \sqrt{y_{12}^2 + y_{13}^2} \in [0.15, 0.16],\]
\[\varphi \equiv \arctan \left( \frac{y_{13}}{y_{12}} \right) \in [-\pi, \pi].\]

We arrive at these ranges guided by the following considerations:

(1) Ratios of masses determine the \(|\xi_X|\). For instance, \(|\xi_X|\) is approximately equal to the ratio of the second- and third-generation quark masses, per Eq. \((6.3.4)\).

(2) The largest of the \(y_{ij}\) is defined to be equal to unity using the freedom to rescale all the \(\epsilon_X\) and \(y_{ij}\). From Eqs. \((6.3.5)\) and \((6.3.12)\), we estimate that \(y_{22}, y_{23} \sim \mathcal{O}(1)\); \(y_{12}, y_{13} \sim \mathcal{O}(0.1)\); and \(y_{11} \lesssim \mathcal{O}(0.01)\).

(3) The \(|\epsilon_X|\) are estimated via their contribution to the mixing angles and to the first-generation masses. For instance, since \(m_d^2/m_b^2 \gg m_u^2/m_t^2\), we must have \(|\epsilon_d| \gg |\epsilon_u|\). Therefore, \(|\epsilon_d|\) dominates over \(|\epsilon_u|\) in Eqs. \((6.3.10)\) and \((6.3.11)\). This allows for an estimate of \(|\epsilon_d|\).

(4) At leading order, the first-generation masses are given by \(|y_{11}\epsilon_X + \delta_X|\). Therefore, \(y_{11} \lesssim \mathcal{O}(0.01)\) must hold in order to suppress the down quark mass, given the value of \(|\epsilon_d|\) in Eq. \((6.5.2)\). Furthermore, we require that \(|\delta_d|\) be at least a factor of \(10^{-2}\) smaller than \(|\epsilon_d|\); otherwise, a tuned cancellation would be required to get a small down-quark mass.
(5) Given the range of $y_{11}$ and the value of the up-quark mass, ranges for $|\varepsilon_u|$ and $|\delta_u|$ are determined.

(6) The phases on $\xi_u$, $\xi_d$, $\varepsilon_u$, $\varepsilon_d$, $\delta_u$ and $\delta_d$ are allowed to vary uniformly on $[-\pi, \pi]$.

The take-home message is that it is possible to find regions of parameter space such that the quark observables are reproduced. The ranges for the parameter ranges are later refined by comparing calculations of the observables against the values of Table 6.1 until general agreement between the two is attained.

Fig. 6.1 shows the regions of $y_2^u/y_3^u - y_2^d/y_3^d$ space covered by the ranges for the parameters in Eqs. (6.5.2) and (6.5.4) for the up-type (red) and down-type (blue) quark masses. Fig. 6.2(a) shows the regions of $\sin \theta_{12} - \sin \theta_{13}$ space covered by the same choices of parameter regions as in Eqs. (6.5.2) and (6.5.4), and Fig. 6.2(b) is the same in $\sin \theta_{23} - \sin \delta_{CP}$ space. The red regions with dashed outlines take $\xi_u$, $\xi_d$, $\varepsilon_u$, $\varepsilon_d$, $\delta_u$ and $\delta_d$ to be real, while the green regions with solid outlines allow these parameters to be complex with a phase on $[-\pi, \pi]$. Note that the red region almost completely covers the green region in Fig. 6.2(b). The six-pointed star in each panel represents the best-fit point from Table 6.1.

The phase parameters in the quark sector cannot be constrained by this analysis. Part of the reason for this is that $|\varepsilon_d| (|\varepsilon_d/\xi_d|)$ numerically dominates $|\varepsilon_u| (|\varepsilon_u/\xi_u|)$ in Eqs. (6.3.10) and (6.3.11) (Eq. (6.3.9)), so the magnitude of their difference is largely insensitive to their relative phase. Moreover, the phase of $\xi_X$ is irrelevant in determining $m_2^2/m_3^2$, and the phases on $\varepsilon_X$ and $\delta_X$ do not dramatically alter the range of possible values for $y_1^2/y_3^2$. This insensitivity to the phases is demonstrated in Fig. 6.2(b). Although there is a small preference for maximal CP violation, all possible values of $\sin \delta_{CP}$ are contained in the 95% CI for real-valued $\xi_X$, $\varepsilon_X$ and $\delta_X$. Letting these parameters be complex produces
Figure 6.1. The predicted ratio of Yukawa couplings for the up-type quarks (red), down-type quarks (blue) and charged leptons (green), calculated from the ranges in Eqs (6.5.2), (6.5.4) and (6.5.6). The phases on $\xi_u$, $\xi_d$, $\varepsilon_u$, $\varepsilon_d$, $\delta_u$ and $\delta_d$ are allowed to vary uniformly on $[-\pi, \pi]$. The 68.3% (dark), 95% (medium) and 99% (light) confidence intervals for each sector are shown. The circle, square and triangle indicate the values of the Yukawa ratios for the up-type quarks, down-type quarks and charged leptons, respectively, as given in Table 6.1.
Figure 6.2. Quark mixing parameters, calculated from the ranges in Eq. (6.5.2) and (6.5.4). The six-pointed star in each figure represents the measured values of these observables from Table 6.1. The red regions with dashed outlines are calculated assuming $\xi_X, \varepsilon_X$ and $\delta_X, (X = u, d)$ are real, while the green regions with solid outlines are calculated allowing these quantities to be complex. Note that the former almost completely covers the latter in panel (b).

no appreciable changes. The $CP$ violation that arises when these parameters are real stems from the imaginary coefficient of $Y_3$ that appears in Eq. (6.2.19). This factor of $i$, coupled with the finite spread and sign indeterminacy of the ranges in Eq. (6.5.4), is enough to populate the entire allowable range for $\sin \delta_{CP}$. Regarding the elements of $Y_5$, at this order, separate ranges for $y_{12}$ and $y_{13}$ are not specified in Eq. (6.5.4). These parameters only appear in the particular combination $(y_{12}^2 + y_{13}^2)$ in Eqs. (6.3.2), (6.3.9) and (6.3.10). Therefore, we reparametrize these as

(6.5.5) \[ y_{12} = \Phi \cos \varphi, \quad y_{13} = \Phi \sin \varphi. \]
The quark masses and mixing observables inform the range of $\Phi$, but the angle $\varphi$ is completely undetermined.

Next, we use the parameter ranges for the $y_{ij}$ found for the quarks to compute the charged lepton masses. This system of equations still has enough freedom due to the new parameters $\xi_\ell$, $\varepsilon_\ell$ and $\delta_\ell$ that determine the lepton spectrum. We obtain the following ranges for the latter:

\begin{equation}
(6.5.6) \quad |\xi_\ell| \in [0.11, 0.12], \quad |\varepsilon_\ell| \in [0.05, 0.06], \quad |\delta_\ell| \in [5 \times 10^{-4}, 6 \times 10^{-4}].
\end{equation}

The region of $y_{1}^{2}/y_{3}^{2} - y_{2}^{2}/y_{3}^{2}$ space covered by these parameter ranges and those in Eq. (6.5.4) are shown in green in Fig. 6.1. The phases on $\xi_\ell$, $\varepsilon_\ell$ and $\delta_\ell$ are varied between $[-\pi, \pi]$. The triangle represents the observed ratios of charged-lepton masses in Table 6.1.

Neutrinos

The parameter ranges obtained in Eqs. (6.5.4) and (6.5.6) for $Y_5$ are now used to determine the neutrino masses and leptonic mixing observables. Table 6.2 lists the current best-fit values for the neutrino mass-squared differences and leptonic mixing angles determined by the NuFIT collaboration \cite{4} both for a NH and for an IH of neutrino masses. While the calculation of the renormalization-group evolution of these observables has been calculated in, for instance, Ref. \cite{188 \cite{193}, we use the low-energy values in order to keep pace with current experimental observations and to avoid making model-dependent assumptions about the renormalization group flow.

We studied numerically the seesaw scenarios described in Sec. 6.4 using the same method we used for the charged fermions. As before, the values of the neutrino-specific
parameters, as well as the parameters of Eqs. (6.5.4) and (6.5.6), are scanned over specified ranges. The parameters \{\xi_X, \varepsilon_X, \delta_X, \eta_X\} are all allowed to be complex with their phases on \([-\pi, \pi]\). For each set of parameters, the low-energy observables are calculated. These observables are the three leptonic mixing angles (via \(\sin^2 \theta_{12}^l\), \(\tan^2 \theta_{13}^l\) and \(\sin^2 \theta_{23}^l\)), the lone leptonic \(CP\)-violating phase (\(\sin \delta_{CP}^l\)) and the ratio \(R_\nu\) of the neutrino mass-squared splittings,

\[
R_\nu = \begin{cases} 
\frac{m_3^2 - m_1^2}{m_2^2 - m_1^2}, & m_3^2 - m_2^2 > m_2^2 - m_1^2 \\
\frac{m_2^2 - m_1^2}{m_3^2 - m_2^2}, & m_3^2 - m_2^2 < m_2^2 - m_1^2
\end{cases}
\]

(6.5.7)

In this convention, \(R_\nu\) is positive (negative) for the NH (IH), and its magnitude is strictly greater than two.

The pseudodata then are binned in \(R_\nu\) and, using Eq. (6.5.1), \(\Delta \chi^2\) is calculated for each bin (with the most populous bin having \(\Delta \chi^2 = 0\)). A smooth interpolation of the \(\Delta \chi^2\) is calculated, and the 68.3%, 95% and 99% confidence levels (CL) are set

<table>
<thead>
<tr>
<th>Observable</th>
<th>Normal Hierarchy ((\Delta \chi^2 = 0))</th>
<th>Inverted Hierarchy ((\Delta \chi^2 = 0.83))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\Delta m_{12}^2)</td>
<td>(7.50 \times 10^{-5}) eV(^2)</td>
<td>(7.50 \times 10^{-5}) eV(^2)</td>
</tr>
<tr>
<td>(\Delta m_{13}^2)</td>
<td>(+2.524 \times 10^{-3}) eV(^2)</td>
<td>(-2.444 \times 10^{-3}) eV(^2)</td>
</tr>
<tr>
<td>(\sin^2 \theta_{12}^l)</td>
<td>0.306</td>
<td>0.306</td>
</tr>
<tr>
<td>(\sin^2 \theta_{13}^l)</td>
<td>0.02166</td>
<td>0.02179</td>
</tr>
<tr>
<td>(\sin^2 \theta_{23}^l)</td>
<td>0.441</td>
<td>0.587</td>
</tr>
<tr>
<td>(\sin \delta_{CP}^l)</td>
<td>(-0.988)</td>
<td>(-0.993)</td>
</tr>
</tbody>
</table>

Table 6.2. The values for the neutrino observables used in our analysis, from the NuFIT collaboration [4]. Shown are the NH and IH fits to oscillation data. We do not consider the renormalization-group-evolved values of these observables as we did with the quark and charged-lepton observables.
at $\Delta \chi^2 = 1.00, 3.84$ and $6.63$, respectively; in figures, these are respectively drawn as solid, dashed and dot-dashed black lines. A flat posterior is imposed on $R_\nu$, so that only pseudodata for which $30 < |R_\nu| < 35$ are kept, consistent with the measurements in Table 6.2. Separate pseudodata are generated for the NH and the IH. The pseudodata are binned in two-dimensional subspaces of the space of observables, and $\Delta \chi^2$ is calculated over each subspace, once again using Eq. (6.5.1). The 68.3%, 95% and 99% CI are drawn as the contours along which $\Delta \chi^2 = 2.30, 5.99$ and $9.21$; as before, these contours are depicted as dark, medium and light shadings of the appropriate color, respectively, in the figures that follow. Finally, a one-dimensional $\Delta \chi^2$ function is produced for $\sin \delta_{CP}$ – precisely as was done for $R_\nu$, above – both for the NH and the IH.

**Type I Neutrino Seesaw.** We consider first the type I seesaw formalism of Sec. 6.4 and scan over the neutrino parameters $\xi_\nu, \varepsilon_\nu$ and $\delta_\nu$, in addition to the parameters in Eqs. (6.5.4) and (6.5.6). These parameters are separately varied over the perturbative ranges

(6.5.8) \[ |\xi_\nu|, |\varepsilon_\nu|, |\delta_\nu| \in [0, 0.1]. \]

The results of this scan are illustrated in Figs. 6.3 and 6.4. Fig. 6.3(a) shows $\Delta \chi^2$ as a function of $R_\nu$ while in Fig. 6.3(b), $\Delta \chi^2$ is plotted as a function of $\sin \delta_{CP}$ for $30 < R_\nu < 35$ (orange) and for $-35 < R_\nu < -30$ (green). Fig. 6.4 shows confidence intervals in two-dimensional slices of the space of observables, where the orange regions are for the NH, while the green regions are for the IH. The circle and square Fig. 6.4 represent the NH and IH solutions in Table 6.2, respectively.
Figure 6.3. (a) The one-dimensional $\Delta \chi^2$ as a function of $R_\nu$ for a scan over the type I seesaw parameter ranges in Eqs. (6.5.4), (6.5.6) and (6.5.8). The dark gray band covers values of $R_\nu$ that cannot be generated. (b) The one-dimensional $\Delta \chi^2$ as a function of $\sin \delta_{CP}$ for a similar scan. The orange line corresponds to a $30 < R_\nu < 35$, while the green line corresponds to $-35 < R_\nu < -30$. In both panels, the black lines represent the 68.3% (solid), 95% (dashed) and 99% (dot-dashed) confidence levels.

From these plots, we infer that the type I seesaw in flavorspin is unlikely to simultaneously accommodate for the observed values for the mass differences and leptonic mixing angles. The NH is a somewhat better fit than the IH in the flavorspin framework for a type I seesaw scenario. In particular, the range $30 < R_\nu < 35$ is contained in the 95% CI, while the range $-35 < R_\nu < -30$ is excluded at > 99% CL. Moreover, the NH prefers small values ($\lesssim 5^\circ$) of $\theta^l_{13}$, while the IH prefers large values ($\sim 85^\circ$) thereof.

On the other hand, neither case can easily accommodate the observed value of $\sin^2 \theta^l_{12}$ at 99% CL. The NH predicts a small $\theta^l_{12}$, $\sin^2 \theta^l_{12} < 0.05$ at >99% CL, while the IH implies...
Figure 6.4. The 68.3% (dark), 95% (medium) and 99% (light) confidence intervals for \( R_\nu \) and the leptonic mixing angles produced by a scan over the type I seesaw parameter space given by Eqs. (6.5.4), (6.5.6) and (6.5.8). The NH (IH) is shown in orange (green). The dark gray bands in (a) and (c) cover values of \( R_\nu \) that cannot be generated, while light gray bands mask values of \( R_\nu \) excluded by our analysis. The circle and square represent the NH and IH solutions in Table 6.2 respectively.
Figure 6.5. (a) The one-dimensional $\Delta \chi^2$ as a function of $R_\nu$ for a scan over the type II seesaw parameter ranges in Eqs. (6.5.4), (6.5.6) and (6.5.9). The dark gray band covers values of $R_\nu$ that cannot be generated. (b) The one-dimensional $\Delta \chi^2$ as a function of $\sin \delta_{CP}$ for a similar scan. The orange line corresponds to $30 < R_\nu < 35$, while the green line corresponds to $-35 < R_\nu < -30$. See text for details. In both panels, the black lines represent the 68.3% (solid), 95% (dashed) and 99% (dot-dashed) confidence levels.

$0.4 \lesssim \sin^2 \theta_{12} \lesssim 0.6$ at 99% CL. The third angle, $\sin^2 \theta_{23}$ is similarly poorly fit; the NH prefers $\sin^2 \theta_{23} \in [0.1, 0.25]$ at 95% CL, while the IH prefers $\sin^2 \theta_{23} \gtrsim 0.95$ at 99% CL. Finally, Fig. 6.3(b) indicates that, while the NH prefers minimal $CP$ violation ($|\sin \delta_{CP}| \lesssim 0.3$) at 95% CL, the IH prefers strictly near-maximal $CP$ violation ($|\sin \delta_{CP}| \gtrsim 0.9$) at 95% CL, with every possible value allowed at 99% CL.

**Type II Neutrino Seesaw.** We scan over the parameters $\eta_{33}$, $\eta_5$ and $\eta_1$ of Eq. (6.4.12) in addition to the parameters in Eqs. (6.5.4) and (6.5.6). These parameters are separately
Figure 6.6. The 68.3% (dark), 95% (medium) and 99% (light) confidence intervals for $R_{\nu}$ and the leptonic mixing angles produced by a scan over the type II seesaw parameter space given by Eqs. (6.5.4), (6.5.6) and (6.5.9). The NH (IH) is shown in orange (green). The dark gray bands in (a) and (c) cover values of $R_{\nu}$ that cannot be generated, while light gray bands mask values of $R_{\nu}$ excluded by our analysis. The circle and square represent the NH and IH solutions in Table 6.2 respectively.
varied over the ranges

\begin{equation}
(6.5.9) \quad |\eta_{33}|, |\eta_5|, |\eta_1| \in [0,1].
\end{equation}

Note that these ranges are not perturbative.

The results are shown in Figs. 6.5 and 6.6. Fig. 6.5(a) shows $\Delta \chi^2$ as a function of $R_\nu$. The conclusion of this exploration is that it is hard to reproduce the hierarchy of mass differences in the type II seesaw. More specifically, the observed region $30 < |R_\nu| < 35$ does not occur at 99% CL away from the most likely value for this parameter, irrespective of the hierarchy.

Fig. 6.6 shows confidence intervals in two-dimensional slices of the space of observables. In these figures, the orange regions contain NH points, while the green regions contain IH points. From the figures, things are more promising regarding the mixing angles. More specifically, the NH contains all possible values of $\sin^2 \theta_{12}$ in the 95% CI. The IH prefers $\theta_{12} \sim 45^\circ$, though it can also accommodate any value at 99% CL. Both hierarchies allow for $\theta_{13}$ to either be small ($\lesssim 10^\circ$) or large ($\gtrsim 80^\circ$), but have exceedingly low probability to produce an intermediate value; the NH prefers small values and the IH prefers large values, both at $>95\%$ CL. This framework struggles only to simultaneously accommodate the large value of $\theta_{12}$ and the relatively large $\theta_{13}$, though the tension is not as severe here as it is for the type I seesaw.

Regarding $\theta_{23}$, the 95% CI for the IH contains $\sin^2 \theta_{23} \gtrsim 0.3$, and the 99% CI covers the entire allowable range. In the NH, the situation is more predictive, as the 95% CI covers the regions $0.45 \lesssim \sin^2 \theta_{12} \lesssim 0.55$ and $\sin^2 \theta_{12} \gtrsim 0.98$. While the NH solution (circle) in Fig. 6.6(a) lies inside the 95% CI, this framework generically has no preference.
Figure 6.7. (a) The one-dimensional $\Delta \chi^2$ as a function of $R_\nu$ for a scan over the general neutrino mass matrix parameter ranges in Eqs. (6.5.4), (6.5.6) and (6.5.10). The dark gray band covers values of $R_\nu$ that cannot be generated. (b) The one-dimensional $\Delta \chi^2$ as a function of $\sin \delta_{CP}^l$ for a similar scan. The orange line corresponds to a $30 < R_\nu$, while the green line corresponds to $-35 < R_\nu < -30$. See text for details. In both panels, the black lines represent the 68.3% (solid), 95% (dashed) and 99% (dot-dashed) confidence levels.

for either octant of $\theta_{23}^l$. From Fig. 6.5(b), we see that both hierarchies have a strong preference for near-maximal $CP$ violation ($|\sin \delta_{CP}^l| \gtrsim 0.9$) at 95% CL. In fact, the IH prefers $|\sin \delta_{CP}^l| \gtrsim 0.5$ at 99% CL, though every possible value is allowed at 99% CL for the NH.

**General Neutrino Mass Matrix.** For completeness, we also explored the general neutrino mass matrix introduced in Eq. (6.4.6). We briefly describe the results in this case following the methods previously described. The neutrino-specific parameter ranges over
Figure 6.8. The 68.3% (dark), 95% (medium) and 99% (light) confidence intervals for $R_\nu$ and the leptonic mixing angles produced by a scan over the general neutrino mass matrix parameter space given by Eqs. (6.5.4), (6.5.6) and (6.5.10). The NH (IH) is shown in orange (green). The dark gray bands in (a) and (c) cover values of $R_\nu$ that cannot be generated, while light gray bands mask values of $R_\nu$ excluded by our analysis. The circle and square represent the NH and IH solutions in Table 6.2, respectively.
which we scan are

\begin{equation}
|\eta_{33}|, |\eta_{5}|, |\eta_{1}|, |\eta_{35}|, |\eta_{55}|, |\eta_{355}|, |\eta_{353}| \in [0, 1],
\end{equation}

while the other relevant parameters are scanned over the ranges in Eqs. (6.5.4) and (6.5.6). The results are presented Figs. 6.7 and 6.8; the interpretation of those figures being the same as before. As with the type II seesaw, neither $30 < R_{\nu} < 35$ nor $-35 < R_{\nu} < -30$ are included in the 99% CI in Fig. 6.7(a), although the IH is significantly less likely than NH. Moreover, in this case, the NH prefers $\theta_{12}'$ at the extremes of the range: $\theta_{12}' \lesssim 20^\circ$ or $\theta_{12}' \gtrsim 70^\circ$ at 95% CL. The IH, on the other hand, is not $\theta_{12}'$-predictive; it contains all possible values of $\sin \theta_{12}'$ within the 68.3% CI.

The NH prefers small values ($\lesssim 10^\circ$) of $\theta_{13}'$ at 95% CL, while the IH prefers large values ($\gtrsim 80^\circ$) at 95% CL. While the NH (IH) may produce large (small) values of $\theta_{13}'$, these values lay outside the 99% CI, and thus do not appear in Fig. 6.8. Both hierarchies contain every possible value of $\sin^2 \theta_{23}'$ within the 95% CI. Therefore, there is nothing particularly special about the region around $\theta_{23}' = 45^\circ$. This disagrees with our theoretical prejudice that $\theta_{23}' \sim 45^\circ$ indicates that something phenomenologically interesting is happening in the lepton sector, as we saw for the type II seesaw, above. Both hierarchies in this scenario prefer near-maximal $CP$ violation: the 95% CI consists of $|\sin \delta_{CP}^l| \gtrsim 0.8$, though every possible value is allowed at 99% CL.

6.6. Flavor-Changing Neutral Currents

A full exploration of the phenomenology of the scenario we are proposing is deferred to a later study. However, it is relatively easy to show that the problem of FCNCs
is alleviated substantially in flavorspin models if the coefficients of higher-dimensional operators have a structure

\begin{equation}
\alpha(Y_3, \varepsilon Y_5, \delta \mathbb{I}),
\end{equation}

where $|\varepsilon|, |\delta| \ll 1$, mimicking the premise that was assumed before for the Yukawa couplings. Higher-dimensional operators are comprised of gauge- and Lorentz-invariant combinations of SM matter fields ($Q_L, U_R, D_R, L_L, E_R$), Higgs bosons ($H$), field strength tensors ($G^a_{\mu\nu}, W^a_{\mu\nu}, B_{\mu\nu}$) and (covariant) derivatives ($D_\mu$). After electroweak symmetry is broken, these operators are decomposed in terms of the low-energy degrees of freedom of the SM. Our analysis of nonrenormalizable operators specifically focuses on fermion bilinears of the form\(^7\)

\begin{equation}
Q_\alpha \sim c_{\alpha,ij} F_i F_j', c_{\alpha,ij} F_i F_j', c_{\alpha,ij} F_i F_j', c_{\alpha,ij} F_i F_j', X^{(t)} = U_{L,R}, D_{L,R}, E_{L,R}, \nu_L.
\end{equation}

These bilinears are, by construction, singlets of $G_{fl}$, but are not necessarily singlets of the Lorentz or SM gauge groups. Operators may contain any number of bilinears, each with its own $c_\alpha$; operator substructures unrelated to flavor are not relevant here.

We express the flavor-charged coefficients $c_\alpha$ in terms of the spurions $Y_3$ and $Y_5$. For definiteness, we have

\begin{equation}
c_\alpha = iY_3 + (1 - \xi_\alpha)Y_3^2 + \varepsilon_\alpha Y_5 + \delta_\alpha \mathbb{I} + \ldots,
\end{equation}

\(^7\)In this section, we suppress the superscript on $c$ that appeared in, for instance, Eq. 6.2.16.
where $|\varepsilon_\alpha|, |\delta_\alpha|, |\xi_\alpha| \ll 1$. Fermion bilinears may be divided into three classes based on their flavor structure.

1. $Q_1 \sim (\overline{F}_i c_{\alpha,ij} F_j^\dagger), \ F(i) = U_{L,R}, D_{L,R}, E_{L,R}$. Operators containing bilinears of this class are contributors to the most commonly searched-for FCNC processes. They yield contributions to reactions such as $b \to s\gamma$ \textsuperscript{194}, $\mu \to e\gamma$ \textsuperscript{195} and meson-antimeson oscillations \textsuperscript{196}.

2. $Q_2 \sim (F_i c_{\alpha,ij} F_j^\dagger), (\overline{F}_i c_{\beta,ij} F_j^\dagger), \ F(i) = U_{L,R}, D_{L,R}, E_{L,R}$. Bilinears in this class violate $B - L$, though the full operator need not.

3. $Q_3 \sim (\overline{\nu}_i c_{\alpha,ij} F_j), (\overline{F}_i c_{\beta,ij} \nu_j), \ F = U_{L,R}, D_{L,R}, E_{L,R}, \nu_L$. These are bilinears in which at least one fermion is a neutrino.

All the bilinears above have been expressed in the flavor basis. After EWSB, whether or not these operators lead to FCNCs is determined upon rotation into the physical basis. The rotation matrices for the charged fermions were discussed in Sec. \textsuperscript{6.2} and that of the neutrinos was discussed in Sec. \textsuperscript{6.4}. we apply these matrices in each of these cases.

In case 1, after rotation into the mass basis, the matrix $c_\alpha$ transforms to:

\begin{equation}
(6.6.4) \quad c_\alpha \to V_X c_\alpha V_{X'}^\dagger,
\end{equation}

where $V_X$ is the matrix that diagonalizes the Yukawa matrix $Y_X$, as in Eqs. \textsuperscript{6.2.27}. In the $\{\varepsilon_X, \varepsilon_\alpha\} \to 0$ limit, $V_X, V_{X'} \to V^0$, as in Eq. \textsuperscript{6.2.30}. The coefficient $c_\alpha$ is a diagonalized by this rotation, regardless of $\xi_\alpha$. Therefore, this class of bilinears yields no FCNCs at leading order in the small parameters $\varepsilon_\alpha$ and $\delta_\alpha$. Any FCNCs that do arise – and that contribute to the above flavor-changing processes – must be correspondingly suppressed.
As an illustration, consider the bilinear \( \overline{D}_L c_\alpha D_L \). When the down-type quarks are rotated into their mass basis, the flavor matrix \( c_\alpha \) of the bilinear becomes

\[
V_d c_\alpha V_d^\dagger \sim \begin{pmatrix} 0 & 0 & 0 \\ 0 & \xi_\alpha & (1 + i)(\varepsilon_d - \varepsilon_\alpha) \\ 0 & (1 - i)(\varepsilon_d - \varepsilon_\alpha) & \xi_\alpha - 2 \end{pmatrix} + \mathcal{O}(\{\varepsilon_X, \xi_X\}^2)
\]

where we have simplified this expression by assuming \( y_{22} = y_{23} = 1, y_{11} = y_{12} = y_{13} = \delta_d = \delta_\alpha = 0 \), and that the remaining flavorspin parameters are real-valued. The off-diagonal piece of this matrix is proportional to \( \varepsilon_X \), so the contributions of this bilinear to flavor-changing processes like \( b_L \to s_L + \ldots \) are suppressed by the (assumed) smallness of \( \varepsilon_X \) relative to the flavor-conserving contributions. While both quarks are left-handed in this example, we emphasize that the same conclusion applies if one or both were right-handed.

In case 2, the matrices \( c_\alpha, c_\beta \) become, after rotation into the mass basis,

\[
c_\alpha \to V_X^* c_\alpha V_{X'}^\dagger, \quad c_\beta \to V_X c_\beta V_{X'}^T.
\]

Even in the limit \( \{\varepsilon_X, \varepsilon_\alpha\} \to 0 \), \( c_\alpha \) and \( c_\beta \) are not a diagonal matrices. Bilinears of this class can then potentially induce large FCNCs. As stressed above, however, these bilinears are exotic, with the flavor coefficients connecting fermions in a \( B - L \)-violating fashion, pointing to an effective vertex that arises from an underlying \( B - L \)-violating interaction. In Sec.\textit{6.7} we will argue that these vertices can be naturally suppressed by a Froggatt-Nielsen-like mechanism\(^8\).

\(^8\)The suppression of the contributions to FCNCs from bilinears that violate \( B - L \) also applies to bilinears in class 1 of the form \( E_i c_{\alpha,ij} U_j \) or \( E_i c_{\alpha,ij} D_j \), even though these bilinears do not produce large FCNCs.
Finally, for bilinears in class 3, the matrices $c_\alpha$ and $c_\beta$ become:

\begin{align}
(6.6.7) \quad c_\alpha \rightarrow V_\nu c_\alpha V_X^\dagger, \quad c_\beta \rightarrow V_X c_\beta V_\nu^\dagger.
\end{align}

The key point here is that in the seesaw scenarios, $V_\nu$, at leading order, Eq. (6.4.28), is different from the matrices that diagonalize the charged-lepton Yukawa matrices. In the limit $\{\varepsilon_X, \varepsilon_\alpha\} \rightarrow 0$, $c_\alpha$ and $c_\beta$ can have large off-diagonal components. Therefore, higher-dimensional operators containing neutrinos will produce relatively large amplitudes for FCNC processes.

The kind of processes to be expected from this third class of bilinears include rare $\tau$, meson, Higgs and $W$ decays, the flavor-violating structure of which cannot be easily probed at experiments due to the final-state neutrinos. Some of these operators, however, give rise to potentially large nonstandard interactions (NSI) \cite{110, 197} for neutrinos. Current measurements of NSI parameters \cite{156, 198, 201} are consistent with flavorspin at the TeV scale. While gauge invariance ensures that operators containing bilinears of this class are accompanied by operators containing charged leptons, bounds on neutrino NSI from charged-lepton flavor change can be partially evaded, due to the differences between the matrices that rotate the charged leptons and the neutrinos into their respective mass bases. Over the next decade or so, a host of experiments \cite{154, 155, 200, 202, 205} will attempt to measure nonzero NSI; these will serve as a critical test of the framework we have introduced.

The existence of Majorana neutrino masses allows for lepton-number-violating processes, such neutrinoless double beta decay and $\mu^- \rightarrow e^+$ conversion in nuclei, to occur.
The connection between these phenomena has recently been discussed in Refs. [206–208]. Of particular interest is that the flavor-nondiagonal $\mu^- \rightarrow e^+$ conversion, currently constrained by the SINDRUM II experiment [209], may occur at an observable rate in upcoming experiments designed to look for $\mu^- \rightarrow e^-$ conversion, including Mu2e [210] and COMET [211, 212]. Combining these with experimental searches for neutrinoless double beta decay [213] provides an additional test of the structure that flavorspin imposes on the neutrino mass matrix, and can provide information regarding potential neutrino Majorana phases.

6.7. Discussion

In this work, we proposed a framework to attack the flavor puzzle based on the principle of decomposition of the SM Yukawas into fundamental spurions. Within this framework, we fully implemented the simplest possible case, in which the flavor structure of the SM is derived from a single horizontal $SU(2)$ flavor symmetry. With respect to flavorspin, all fermions transform as triplets of flavor $SU(2)$. In addition, we imposed some restrictions on the parameter space, in particular demanding the perturbativity of the set of parameters $\{\varepsilon_X, \delta_X, \xi_X, \eta_X\}$.

Phenomenologically desirable highlights that follow from the perturbative flavorspin scenario include:

- Naturally small masses for the first and second generations of charged fermions.
- Naturally small mixing angles in the quark sector, with the Cabibbo angle predicted to be about 100 times larger than $\theta_{13}^q$, see Eq. (6.3.14).
- Large $CP$ violation likely in the quark sector, see Fig. 6.2(b).
• A milder predicted mass hierarchy for Majorana neutrinos.
• At least one large angle predicted in the lepton sector for the case of Majorana neutrinos.
• Large $CP$ violation likely in the lepton sector, see Figs. 6.3(b), 6.5(b) and 6.7(b).
• When flavorspin is extended to nonrenormalizable operators, it naturally suppresses the most common FCNCs involving only charged fermions, while allowing for large FCNCs if neutrinos are involved, see Sec. 6.6. These could potentially been seen at long-baseline neutrino experiments.

Moreover, other features of our setup can be considered aesthetically pleasing. In particular, the quark and leptonic flavor structures both emerge from the same set of fundamental spurions. Quark and lepton flavor are unified in this sense.

Nonetheless, it should be stated that flavorspin with perturbative $\{\varepsilon_X, \delta_X, \xi_X, \eta_X\}$ appears to be somewhat restrictive. In particular, starting from a good quark fit, it does not do an entirely good job in describing flavor in the leptonic sector. The detailed results are found in Sec. 6.5 where we calculated confidence intervals for the fermion masses and mixing parameters for given ranges of the flavorspin parameters for several parametrizations of the neutrino mass matrix in terms of fundamental spurions. For the most promising Majorana possibilities, we find that although flavorspin invariably predicts large mixing angles and $CP$ violation in the lepton sector, it struggles to reproduce the neutrino mass hierarchy. Some tension is also observed between the relatively large values of $\theta^l_{12}$ and $\theta^l_{13}$. The type II scenario yields the best fit, all things considered.

Finally, we comment on the perturbativity of $\varepsilon_X$ and $\delta_X$. In the previous sections, this was taken as an assumption. However, a Froggatt-Nielsen-like principle could provide
partial justification for it. The $U(1)$ Froggatt-Nielsen symmetry would be $B - L$, under which the spurions may also be formally charged. Thus, the formal global symmetry of our model would be thus enlarged to be:

\[(6.7.1) \quad G_g = G_{fl} \times U(1)_{B-L} .\]

Specifically, suppose that in this setup a formal charge of 1 under $B - L$ is assigned to $Y_5$, while $Y_3$ is taken to be $B - L$-neutral. That is, introducing the notation $r_q$ where $r$ is the $G_{fl}$ representation and $q$ the $B - L$ charge, we would have

\[(6.7.2) \quad Y_3 \sim 3_0, \quad Y_5 \sim 5_{-1} ,\]

Now, the coefficients $\varepsilon_X, \varepsilon_\Delta$ for the corresponding operators are introduced with formal charges

\[(6.7.3) \quad \varepsilon_X, \varepsilon_\Delta \sim 0_{-1} .\]

The final form of the Yukawas, analogous to Eq. (6.2.17), necessary to render the Yukawa operator invariant under $G_g$, now under $G_{fl} \times B - L$, is given by:

\[(6.7.4) \quad Y_X \equiv f_X(Y_3, \varepsilon_X Y_5) + \delta_X I, \quad Y_\Delta \equiv f_\Delta((\varepsilon_\Delta)^2 Y_3, \varepsilon_\Delta Y_5) + \delta_\Delta I ,\]
where $|\varepsilon_X|, |\varepsilon_\Delta| \ll 1$. More generally, we take the following rule to be valid both for renormalizable and nonrenormalizable operators:

\[
\begin{align*}
\mathcal{O}^{(d)}_{\alpha, ij} & \equiv \begin{cases}
\left[ f^{(d)}_{\alpha, ij} \left( Y_3, \varepsilon^{(d)}_{\alpha} Y_5 \right) + \delta^{(d)}_{\alpha} \mathbb{I} \right] & \text{for } q = 0 \\
(\varepsilon^{(d)}_{\alpha})^q \left[ f^{(d)}_{\alpha, ij} \left( Y_3, (\varepsilon^{(d)}_{\alpha})^{-1} Y_5 \right) + \delta^{(d)}_{\alpha} \mathbb{I} \right] & \text{for } q \geq 1
\end{cases},
\end{align*}
\]

where

\[
q = B - L \text{ charge of } \mathcal{O}^{(d)}_{\alpha},
\]

and where the dimensionless $\varepsilon_{\alpha}$ parameter is assumed to be parametrically small. The consequence is that the contribution to flavor coming from the $Y_5$ spurion is suppressed with respect to $Y_3$ for $B - L$-conserving operators and vice versa for $B - L$-violating ones, à la Froggatt-Nielsen. If we assume a mild hierarchy between $Y_3$ and $Y_5$, $|Y_3| > |Y_5|$, then their contributions can be strongly hierarchical in the $B - L$-conserving case and roughly equivalent in the latter, as we found in this study. Moreover, this mechanism can also be used to suppress the flavor-singlet fermionic bilinears of case 2 mentioned in Sec. 6.6 Irrespective of its Lorentz or gauge properties, to each flavor singlet combination corresponds a $c_{\alpha}$, that would include at least two powers of $\varepsilon_{\alpha}$ if $B - L$-violating. Thus, by using the familiar $B - L$ as a Froggatt-Nielsen symmetry, this extension would make explicit the difference in flavor structure between $B - L$-conserving and $B - L$-violating operators. One may also consider gauging $U(1)_{L_\mu-L_\tau}$ as part of the flavor group; this has been studied in, for instance, Ref. 213.

Some other extensions are of potential interest. Although flavorspin provides a simple explanation for several patterns observed in the spectrum and mixings in the SM, it clearly
is not a complete theory of flavor. The parameters must be fit to the data, and it would be interesting to explore whether promoting the Yukawas to true fields and optimizing a scalar potential is beneficial in this case. On the more phenomenological side, since the flavor structure of higher-dimensional operators is determined, deviations from SM branching ratios will be correlated. A full exploration of these is beyond the scope of this work. Finally, we stress that we have only explored the simplest decomposition of the Yukawas into fundamental spurions, i.e. a sum of two spurions charged under a vectorial $SU(2)$ symmetry. This is of course not the only possibility.
CHAPTER 7

On Lepton-Number-Violating Searches for $\mu^- \rightarrow e^+$ Conversion

7.1. Introduction

Neutrino flavor oscillations imply that at least two neutrinos have nonzero masses and that there is nontrivial mixing in the lepton sector. The mechanism behind nonzero neutrino masses is currently unknown, and a definitive resolution of the neutrino mass puzzle will require input from a variety of probes of fundamental physics, including neutrino oscillation experiments, searches for lepton-number and baryon-number violation, precision measurements of charged-lepton properties and rare processes, and high-energy collider experiments.

Tests of the validity of lepton-number conservation are among the most valuable sources of information when it comes to the neutrino mass puzzle (see, for example, Ref. [215], for an overview). They provide unique information on the nature of the neutrino, i.e., whether it is a Dirac or Majorana fermion. Speculations on the origin of neutrino masses, in turn, differ dramatically depending on the nature of the neutrino. While searches for neutrinoless double beta decay ($0\nu\beta\beta$) are, by far, the most powerful available probes of lepton-number violation (see Ref. [216] for a thorough overview), the pursuit of other lepton-number-violating (LNV) observables is of the highest importance.

Searches for charged-lepton-flavor violation are also potentially powerful probes of the origin of neutrino masses (see, for example, Ref. [195, 215], for an overview). Among the
different charged-lepton-flavor-violating processes, powerful new searches for to $\mu^{-} \rightarrow e^{-}$ conversion in nuclei are currently being developed [210, 211, 217]. These are expected to improve on the current sensitivity to the $\mu^{-} \rightarrow e^{-}$ conversion rate by at least four orders of magnitude in less than a decade.

Experiments sensitive to $\mu^{-} \rightarrow e^{-}$ conversion in nuclei may also serve as laboratories to search for the LNV $\mu^{-} \rightarrow e^{+}$ conversion in nuclei (see, for example, Ref. [210, 218]). The current upper bound on this conversion rate, normalized to the capture rate, is $1.7 \times 10^{-12}$ for the transition between titanium and the ground state of calcium, obtained by the SINDRUM II collaboration [209]. Significant improvement is expected from at least a subset of the next-generation $\mu^− \rightarrow e^−$ conversion experiments.

Here, we estimate the capabilities of next-generation $\mu^- \rightarrow e^-$ conversion experiments to discover or constrain $\mu^- \rightarrow e^+$ conversion in nuclei. We also explore how these results can relate to searches for $0\nu\beta\beta$ and nonzero Majorana neutrino masses. We make use of the standard model (SM) effective operator approach – introduced in Ref. [219] and explored in, for example, Refs. [5, 6, 220, 224] – in order to gauge the impact of these future measurements on a large variety of neutrino mass models. This approach is powerful, and allows one to relate different LNV observables, including nonzero neutrino masses. Extended versions of this approach have been successfully pursued in order to relate, assuming grand unification is realized in nature, lepton-number and baryon-number violating observables [7]. For other comparisons of $\mu^- \rightarrow e^+$ conversion in nuclei to different LNV observables see, for example, Refs. [206, 210, 225]. Ref. [206], which appeared in the literature shortly before this work, asks some of the questions we address here, but our
approaches are somewhat complementary. More concretely, we analyze LNV phenomena using a different set of effective operators, as will be explained below.

This chapter is organized as follows. In Sec. 7.2 we estimate the sensitivity of different next-generation $\mu^- \rightarrow e^-$ conversion experiments to $\mu^- \rightarrow e^+$ conversion in nuclei. In Sec. 7.3 we review the effective operator approach and identify the operators of interest. We also review how the mass scale of the different effective operators can be related to the observed neutrino masses. In Sec. 7.4 we discuss a few concrete examples of how we estimate the rates for the LNV processes of interest, and in Sec. 7.5 we present and discuss our results. We present some concluding thoughts in Sec. 7.6. Appendix B.1 contains a sample ultraviolet-complete scenario that can be described using the formalism discussed here.

7.2. Sensitivities of Next-Generation Experiments

The SINDRUM II experiment at PSI was designed to investigate $\mu^- \rightarrow e^-$ conversion in nuclei. The most recent result places a limit on $\mu^- \rightarrow e^-$ conversion in gold [226],

$$R_{\mu^-e^-}^{Au} \equiv \frac{\Gamma(\mu^- + Au \rightarrow e^- + Au)}{\Gamma(\mu^- + Au \rightarrow \nu_\mu + Pt)} < 7 \times 10^{-13} \text{ (90\% CL)}.$$  \hspace{1cm} (7.2.1)

Nearly ten years earlier, the SINDRUM II collaboration also set a limit on $\mu^- \rightarrow e^+$ conversion in titanium [209],

$$R_{\mu^-e^+}^{Ti} \equiv \frac{\Gamma(\mu^- + Ti \rightarrow e^+ + Ca)}{\Gamma(\mu^- + Ti \rightarrow \nu_\mu + Sc)} < \begin{cases} 1.7 \times 10^{-12} \text{ (GS, 90\% CL)} \\ 3.6 \times 10^{-11} \text{ (GDR, 90\% CL)} \end{cases}.$$  \hspace{1cm} (7.2.2)
where the top limit (GS) assumes coherent scattering to the ground state of calcium, while the bottom limit (GDR) assumes a transition to a giant dipole resonance state. The GS limit remains the strongest on any $\mu^- \rightarrow e^+$ conversion process to date. Next-generation experiments, however, are expected to improve upon it by several orders of magnitude.

The next generation of $\mu^- \rightarrow e^-$ conversion experiments includes Mu2e [210] at Fermilab in the U.S. and DeeMe [217] and COMET [211] (and its upgrade, PRISM [227]) at J-PARC in Japan. Mu2e and COMET/PRISM are schematically similar to SINDRUM II: a proton beam impinges upon a pion production target, and the muons produced in the pion decays are directed onto an aluminum stopping target. DeeMe is similar to these, except the pion production, muon production and muon capture all take place in the same SiC target. The muons form bound states with the atomic nuclei, at which point one of the following happens: (1) the muons decay in orbit (DIO); (2) they are captured by the nucleus, and a neutrino is produced; or (3) they interact with the nucleus in a way not prescribed by the SM. DIO is one of the largest backgrounds at these experiments; the endpoint of the DIO electron spectrum coincides with the energy of the electron produced in $\mu^- \rightarrow e^-$ conversion. The spectrum of DIO electrons is calculable, however, and any unaccounted-for electrons in the region $E_e \sim m_\mu$ would constitute a signal. These experiments anticipate the following sensitivities ($R^{\text{SiC}}_{\mu^-e^-}$ and $R^{\text{Al}}_{\mu^-e^-}$ are defined analogously to Eq. (7.2.1)):

DeeMe: $R^{\text{SiC}}_{\mu^-e^-} > 5 \times 10^{-14}$ (90% CL),

Mu2e: $R^{\text{Al}}_{\mu^-e^-} > 6.6 \times 10^{-17}$ (90% CL),

COMET Phase-I: $R^{\text{Al}}_{\mu^-e^-} > 7.2 \times 10^{-15}$ (90% CL),
COMET Phase-II: \( R_{\mu^- e^-}^{\text{Al}} > 6 \times 10^{-17} \) (90% CL),

PRISM: \( R_{\mu^- e^-}^{\text{Al}} > 5 \times 10^{-19} \) (90% CL).

Here we qualitatively estimate the sensitivities of these experiments to \( \mu^- \rightarrow e^+ \) conversion. At DeeMe, COMET Phase-II, and PRISM, the electrons ejected from the stopping target are transported away from the target to the spectrometer via magnetic fields. This helps to reject background events, but also means that, naively, any produced positrons will be swept away and not detected, rendering \( \mu^- \rightarrow e^+ \) conversion searches significantly more challenging and potentially unfeasible. We are therefore not able to infer a sensitivity for these experiments. Mu2e and COMET Phase-I, however, are a different story. The aluminum stopping targets are immersed in an external magnetic field, and the energies of emitted electrons are measured by determining their trajectories after they escape the stopping target. These experiments can then directly determine if an emitted lepton is an electron or a positron. This is precisely how limits on \( R_{\mu^- e^+} \) were determined at SINDRUM II. We estimate the sensitivities of these experiments to \( \mu^- \rightarrow e^+ \) conversion as follows. In Ref. [228], the SINDRUM II collaboration set limits on \( R_{\mu^- e^-}^{\text{Ti}} \) and \( R_{\mu^- e^+}^{\text{Ti}} \) (assuming transitions to the ground state of calcium) for the same experimental run:

\[
R_{\mu^- e^-}^{\text{Ti}} < 4.3 \times 10^{-12} \text{ (90\% CL)},
\]

\[
R_{\mu^- e^+}^{\text{Ti}} < 4.3 \times 10^{-12} \text{ (90\% CL)}.\]
(That these two bounds are identical is a numerical accident.) Since these two limits are quite comparable to each other, we assume the improvements in the sensitivities to $\mu^- \to e^-$ conversion and $\mu^- \to e^+$ conversion scale commensurately and estimate that next-generation experiments will be sensitive to $\mu^- \to e^+$ rates greater than the following:

\[
\begin{align*}
\text{Mu2e:} & \quad R_{\mu^- e^+}^{\text{Al}} \gtrsim 10^{-16}, \\
\text{COMET Phase-I:} & \quad R_{\mu^- e^+}^{\text{Al}} \gtrsim 10^{-14}.
\end{align*}
\]

We emphasize that these are crude estimates. Detailed experimental analyses of the sensitivities of these experiments to $\mu^- \to e^+$ conversion do not exist in the literature and a realistic estimate can only be made in association with the existing experimental collaboration. We echo the sentiment recently expressed by the authors of Ref. [206], that such analyses should be pursued as they can potentially play a significant role in the study of LNV phenomena.

### 7.3. Effective Operator Approach

The SM Lagrangian can be augmented by operators with mass-dimension $d > 4$, that are constructed from SM matter fields ($Q, u^c, d^c, L, e^c$), Higgs bosons ($H$), field strength tensors ($G_{\mu\nu}, W_{\mu\nu}, B_{\mu\nu}$) and covariant derivatives ($D_\mu$) (and their complex conjugates) and that respect both gauge and Lorentz invariance. These operators, however, need not respect the global symmetries of baryon number and lepton number. LNV phenomena, including $0\nu\beta\beta$ and neutrino Majorana masses, arise from operators that violate lepton number by two units ($\Delta L = \pm 2$) and conserve baryon number ($\Delta B = 0$). It was recently proven in Ref. [229], and considered earlier in Refs. [7 230], that operators in the SM with
$|\Delta B - \Delta L| = 2$ must have odd mass-dimension. The operators included in our analysis are listed in Tables 7.1 (dimension-five), 7.2 (dimension-seven), and 7.3-7.5 (dimension-nine). We consider operators with $d \leq 9$ that contain neither (covariant) derivatives nor field strength tensors; the number of operators with $|\Delta L| = 2$ grows quickly when $d \geq 11$ (see Refs. [5, 6, 219]). Fields whose $SU(2)_L$ indices are contracted to form singlets are enclosed in parentheses; operators with the same field content but with different $SU(2)_L$ structure are listed separately. An operator may have multiple possible contractions of its $SU(3)_c$ and Lorentz indices. However, these different contractions lead to similar estimates – they differ by at most $O(1)$ – for the amplitudes of LNV processes of interest here and will henceforth be ignored. A simple, concrete example is discussed in Appendix B.1.

As already mentioned in the introduction, the effective operator approach employed here is complimentary to the analyses in Ref. [206], in which a different set of effective operators is used. Specifically, the operators of Ref. [206] are constructed to be invariant under the low-energy symmetry group $SU(3)_c \times U(1)_{EM}$ as opposed to the full SM gauge group. Fig. 4 of that paper, for example, depicts experimental limits and sensitivities for the Wilson coefficient of the operator

\begin{equation}
(\bar{d}\gamma^\mu P_L u) \left( \bar{d}\gamma^\mu P_L u \right) \left( \bar{e} P_L \ell \right), \quad \ell = e, \mu.
\end{equation}

This low-energy operator is descended from the following SM-gauge-invariant operators:

\begin{align}
(7.3.2) \quad \mathcal{O}_{47a} &= (L \bar{Q})(L \bar{Q})(HQ)(HQ), \\
(7.3.3) \quad \mathcal{O}_{47d} &= (\bar{L} \bar{Q})(L \bar{Q})(HQ)(H \bar{Q}),
\end{align}
Table 7.1. The dimension-five operator featured in this analysis. Naming convention follows from Refs. [5, 6]. Parentheses denote fields that have their $SU(2)_L$ indices contracted to form a singlet. While not explicitly indicated, three generations of all fermions are contained in each operator. In the third column, $\Lambda$ is the scale required to produce a neutrino mass in the range $0.05 - 0.5$ eV, with lower $\Lambda$ corresponding to higher neutrino mass. Analytic estimates of $T_{0\nu\beta\beta}$ and $R_{\mu^-e^+}$ are also listed, along with numerical estimates, assuming the operator in question is responsible for the observable neutrino masses. See text for details.

where we have used the naming convention of Ref. [5, 6]. These operators have mass-dimension eleven, and thus lie outside the scope of this work.

In the absence of neutrino masses, the SM exhibits global $U(1)$ symmetries associated with each lepton flavor. This is no longer the case in the presence of beyond-the-standard-model physics, and lepton-flavor numbers are necessarily violated if global lepton number is violated. The operators in Tables 7.1-7.5 can distribute their lepton-number violation between the lepton families. For instance, the Weinberg operator $O_1$ should be generalized to

\[
(7.3.4) \quad \frac{1}{\Lambda}(LH)(LH) \rightarrow \frac{1}{\Lambda} \left[ f_{ee}(L_eH)(L_eH) + f_{e\mu}(L_eH)(L_\mu H) + f_{e\tau}(L_eH)(L_\tau H) + \ldots \right],
\]

where $L_\alpha$, $\alpha = e, \mu, \tau$ are the electron-flavor, muon-flavor, or tau-flavor lepton doublets, $\Lambda$ is the effective energy scale of the operator, and the coefficients $f_{\alpha\beta} = f_{\beta\alpha}$, $\alpha, \beta = e, \mu, \tau$, characterize the operator’s distinct flavor components. We define $\Lambda$ such that the largest
\( f_{\alpha\beta} \) is unity. The amplitude for \( 0\nu\beta\beta \) is proportional to \( f_{ee} \), and the amplitude for \( \mu^- \rightarrow e^+ \) conversion is proportional to \( f_{e\mu} \). The series in Eq. (7.3.4) also produces rare LNV decays like \( K^+ \rightarrow \pi^-\mu^+\mu^+ \) and \( \tau^- \rightarrow \mu^+\pi^-\pi^- \), as well as lepton-number violation at collider experiments. The limits on \( f_{\alpha\beta}/\Lambda \) from these processes are not competitive with limits from \( 0\nu\beta\beta \) and \( \mu^- \rightarrow e^+ \) conversion for the relevant lepton-flavor structure, and we do not consider them here\(^1\). The \( f_{\alpha\beta} \) do not mix with one another via renormalization-group running due to SM interactions, because lepton-flavor numbers are conserved in the SM\(^2\).

We describe the relative strengths of the independent lepton-flavor components of \( d \geq 7 \) operators via coefficients \( g_{\alpha\beta\gamma...} \), \( \alpha,\beta,\gamma,... = e,\mu,\tau \). These are the analogues of \( f_{\alpha\beta} \) in Eq. (7.3.4). In this work, we assume, for simplicity, that the high-scale physics may distinguish between different lepton flavors but treats quark flavors democratically, so we suppress quark-flavor indices.

The operators listed in Tables 7.1-7.5 can also be related to Majorana neutrino masses, as discussed in Refs. [5, 6, 219]\(^3\). The idea is to postulate that UV physics explicitly violates lepton number and that, at the tree level, it manifests itself predominantly as one of the \( d \geq 7 \) operators listed in Tables 7.2-7.5\(^4\). At the loop level, SM interactions imply that the same physics will lead to nonzero neutrino masses via the Weinberg operator \( \mathcal{O}_1 \). Hence, these tree-level operators induce operators of lower mass-dimension. Their coefficients can be related by closing external legs into loops and inserting SM interactions. This procedure implies that \( f_{\alpha\beta} \) are linear combinations of the \( g_{\alpha\beta...} \).

---

\(^1\)Recent, detailed discussions and estimates can be found, for instance, in Refs. [225, 231, 235].
\(^2\)We are ignoring the possibility for neutrino Yukawa couplings, which could give rise to lepton-flavor violation at low energies.
\(^3\)The singlet operator \( \mathcal{O}_s \) is included in neither of these analyses because one requires small \( \Lambda \sim \mathcal{O}(\text{GeV}) \) in order to explain the observed neutrino masses. It is, however, discussed briefly in Ref. [7].
Table 7.2. Same as Table 7.1, for the dimension-seven operators featured in this analysis. Naming convention follows from Refs. [5] [6].

<table>
<thead>
<tr>
<th>$\mathcal{O}$</th>
<th>Operator</th>
<th>$\Lambda$ [TeV]</th>
<th>$T_{0\nu\beta\bar{\beta}}$</th>
<th>$R_{\mu^- e^+}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathcal{O}_2$</td>
<td>$(LL)(LH)e^c$</td>
<td>$4 \times 10^{6-7}$</td>
<td>$\ln (2) \left( \frac{\sqrt{2}}{G_F} \right)^2 \left( q^2 \right)^2 \left( \frac{16\pi^2}{y_{\nu\beta} v^2} \right)^2 \frac{\Lambda^2}{Q_{\nu\beta}} \sim 10^{25} - 10^{27}$ yr</td>
<td>$\frac{Q_0^6}{\Lambda^2} \sim 10^{-38} - 10^{-36}$</td>
</tr>
<tr>
<td>$\mathcal{O}_3a$</td>
<td>$(LL)(QH)d^c$</td>
<td>$2 \times 10^{4-5}$</td>
<td>$\ln (2) \left( \frac{\sqrt{2}}{G_F} \right)^2 q^2 \frac{\Lambda^2}{Q_{\nu\beta}} \left[ \left( \frac{G_F}{\sqrt{2}} \right)^2 \frac{1}{q^2} \left( \frac{y_{\nu\beta} v^2}{16\pi^2} \right)^2 + \frac{v^2}{\Lambda^2} \right]^{-1}$ $\sim 10^{24} - 10^{26}$ yr</td>
<td>$\frac{1}{q^2 \Lambda^6} \left( \frac{G_F}{\sqrt{2}} \right)^2 q^2 \left( \frac{y_{\nu\beta} v^2}{16\pi^2} \right)^2 + \frac{v^2}{\Lambda^4} \sim 10^{-37} - 10^{-36}$</td>
</tr>
<tr>
<td>$\mathcal{O}_3b$</td>
<td>$(LQ)(LH)d^c$</td>
<td>$1 \times 10^{7-8}$</td>
<td>$\ln (2) \left( \frac{\sqrt{2}}{G_F} \right)^2 q^2 \frac{\Lambda^2}{Q_{\nu\beta}} \left[ \left( \frac{G_F}{\sqrt{2}} \right)^2 \frac{1}{q^2} \left( \frac{y_{\nu\beta} v^2}{16\pi^2} \right)^2 + \frac{v^2}{\Lambda^4} \right]^{-1}$ $\sim 10^{25} - 10^{27}$ yr</td>
<td>$\frac{1}{q^2 \Lambda^6} \left( \frac{G_F}{\sqrt{2}} \right)^2 q^2 \left( \frac{y_{\nu\beta} v^2}{16\pi^2} \right)^2 + \frac{v^2}{\Lambda^4} \sim 10^{-38} - 10^{-36}$</td>
</tr>
<tr>
<td>$\mathcal{O}_4a$</td>
<td>$(L\bar{Q})(LH)\bar{u}^c$</td>
<td>$4 \times 10^{8-9}$</td>
<td>$\ln (2) \left( \frac{\sqrt{2}}{G_F} \right)^2 q^2 \frac{\Lambda^2}{Q_{\nu\beta}} \left[ \left( \frac{G_F}{\sqrt{2}} \right)^2 \frac{1}{q^2} \left( \frac{y_{\nu\beta} v^2}{16\pi^2} \right)^2 + \frac{v^2}{\Lambda^4} \right]^{-1}$ $\sim 10^{25} - 10^{27}$ yr</td>
<td>$\frac{1}{q^2 \Lambda^6} \left( \frac{G_F}{\sqrt{2}} \right)^2 q^2 \left( \frac{y_{\nu\beta} v^2}{16\pi^2} \right)^2 + \frac{v^2}{\Lambda^4} \sim 10^{-38} - 10^{-36}$</td>
</tr>
<tr>
<td>$\mathcal{O}_4b$</td>
<td>$(L)(L\bar{Q})\bar{u}^c$</td>
<td>$2 - 7$</td>
<td></td>
<td>This operator can not contribute to $0\nu\beta\bar{\beta}$.</td>
</tr>
<tr>
<td>$\mathcal{O}_8$</td>
<td>$(LH)e^c\bar{u}^c\bar{d}^c$</td>
<td>$6 \times 10^{2-3}$</td>
<td>$\ln (2) \left( \frac{\sqrt{2}}{G_F} \right)^2 q^2 \frac{\Lambda^2}{Q_{\nu\beta}} \left[ \left( \frac{G_F}{\sqrt{2}} \right)^2 \frac{1}{q^2} \left( \frac{y_{\nu\beta} v^2}{16\pi^2} \right)^2 + \frac{v^2}{\Lambda^4} \right]^{-1}$ $\sim 10^{27} - 10^{29}$ yr</td>
<td>$\frac{1}{q^2 \Lambda^6} \left( \frac{G_F}{\sqrt{2}} \right)^2 q^2 \left( \frac{y_{\nu\beta} v^2}{16\pi^2} \right)^2 + \frac{v^2}{\Lambda^4} \sim 10^{-40} - 10^{-38}$</td>
</tr>
</tbody>
</table>
Table 7.3: Same as Table 7.1 for the dimension-nine operators featured in this analysis. Naming convention follows from Refs. [5, 6], with the exception of $O_{s}$. 

<table>
<thead>
<tr>
<th>$O$</th>
<th>Operator</th>
<th>$\Lambda$ [TeV]</th>
<th>$T_{0\nu3\beta}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_{5}$</td>
<td>$(LH)(LH)(QH)d^{c}$</td>
<td>$6 \times 10^{4} - 5$</td>
<td>$\ln(2) \left( \frac{\sqrt{2}}{G_{F}} \right)^{2} q^{2} \Lambda^{2} Q^{2} \left[ \frac{G_{F}}{\sqrt{2}} \frac{1}{q^{2}} \left( \frac{y_{\nu} v^{2}}{(16\pi^{2})^{2}} \right) + \left( \frac{v}{16\pi^{2} \Lambda^{2}} + \frac{v^{3}}{\Lambda^{2}} \right)^{2} \right] -1 \sim 10^{25} - 10^{27}$ yr</td>
</tr>
<tr>
<td>$O_{6}$</td>
<td>$(LH)(LH)(\overline{QH})u^{c}$</td>
<td>$2 \times 10^{6} - 7$</td>
<td>$\ln(2) \left( \frac{\sqrt{2}}{G_{F}} \right)^{2} q^{2} \Lambda^{2} Q^{2} \left[ \frac{G_{F}}{\sqrt{2}} \frac{1}{q^{2}} \left( \frac{y_{\nu} v^{2}}{(16\pi^{2})^{2}} \right) + \left( \frac{v}{16\pi^{2} \Lambda^{2}} + \frac{v^{3}}{\Lambda^{2}} \right)^{2} \right] -1 \sim 10^{25} - 10^{27}$ yr</td>
</tr>
<tr>
<td>$O_{7}$</td>
<td>$(LH)(QH)(\overline{QH})c^{c}$</td>
<td>$4 \times 10^{1} - 2$</td>
<td>$\ln(2) \left( \frac{\sqrt{2}}{G_{F}} \right)^{2} q^{2} \Lambda^{2} Q^{2} \left[ \frac{G_{F}}{\sqrt{2}} \frac{1}{q^{2}} \left( \frac{v}{16\pi^{2} \Lambda^{2}} + \frac{v^{3}}{\Lambda^{2}} \right)^{2} \right] -1 \sim 10^{22} - 10^{24}$ yr</td>
</tr>
<tr>
<td>$O_{9}$</td>
<td>$(LL)(LL)e^{c}e^{c}$</td>
<td>$3 \times 10^{2} - 3$</td>
<td>$\ln(2) \left( \frac{\sqrt{2}}{G_{F}} \right)^{4} q^{4} \left( \frac{16\pi^{2}}{y_{\nu} v^{2}} \right)^{4} \Lambda^{2} Q^{2} \sim 10^{25} - 10^{27}$ yr</td>
</tr>
<tr>
<td>$O_{10}$</td>
<td>$(LL)(LQ)e^{c}d^{c}$</td>
<td>$6 \times 10^{2} - 3$</td>
<td>$\ln(2) \left( \frac{\sqrt{2}}{G_{F}} \right)^{2} q^{2} \Lambda^{2} Q^{2} \left[ \frac{G_{F}}{\sqrt{2}} \frac{1}{q^{2}} \left( \frac{y_{\nu} v^{2}}{(16\pi^{2})^{2}} \right) + \left( \frac{y_{\nu} v}{16\pi^{2} \Lambda^{2}} \right)^{2} \right] -1 \sim 10^{25} - 10^{27}$ yr</td>
</tr>
<tr>
<td>$O_{11a}$</td>
<td>$(LL)(QQ)d^{c}d^{c}$</td>
<td>$3 - 30$</td>
<td>$\ln(2) \left( \frac{\sqrt{2}}{G_{F}} \right)^{2} q^{2} \Lambda^{2} Q^{2} \left[ \frac{G_{F}}{\sqrt{2}} \frac{1}{q^{2}} \left( \frac{y_{\nu}^{2} v^{2}}{(16\pi^{2})^{2}} \right) + \left( \frac{y_{\nu} v}{16\pi^{2} \Lambda^{2}} \right)^{2} \right] -1 \sim 10^{22} - 10^{26}$ yr</td>
</tr>
</tbody>
</table>
Table 7.4: A continuation of Table 7.3

<table>
<thead>
<tr>
<th>Operator</th>
<th>Expression</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_{11b}$</td>
<td>$(LQ)(LQ)d^c d^c$</td>
<td>$2 \times 10^{3^{−4}} \ln \left(2 \frac{\Lambda^2}{Q^2} \frac{G_F}{\sqrt{2}} \frac{1}{q^2} \left(\frac{y_L y_L}{16\pi^2} + \frac{y_L}{16\pi^2} \right)^2 + \left(\frac{y_L y_L}{16\pi^2} \right)^2 \right)^{-1} \sim 10^{25} - 10^{27}$</td>
</tr>
<tr>
<td>$O_{12a}$</td>
<td>$(LQ)(LQ)\bar{u}^c u^c$</td>
<td>$2 \times 10^{6^{−7}} \ln \left(2 \frac{\Lambda^2}{Q^2} \frac{G_F}{\sqrt{2}} \frac{1}{q^2} \left(\frac{y_L y_L}{16\pi^2} + \frac{y_L}{16\pi^2} \right)^2 + \left(\frac{\sqrt{2}}{G_F} \right)^2 \frac{1}{\Lambda^2} \right)^{-1} \sim 10^{-38} - 10^{-36}$</td>
</tr>
<tr>
<td>$O_{12b}$</td>
<td>$(LL)(QQ)\bar{u}^c u^c$</td>
<td>$0.3 - 0.6 \frac{1}{q^2} \frac{Q^6}{\Lambda^2} \left(\frac{G_F}{\sqrt{2}} \frac{1}{q^2} \left(\frac{y_L y_L}{16\pi^2} \right)^2 + \left(\frac{y_L}{16\pi^2} \right)^2 \right) \sim 10^{-25} - 10^{-23}$</td>
</tr>
<tr>
<td>$O_{13}$</td>
<td>$(LQ)(LL)\bar{u}^c c^c$</td>
<td>$2 \times 10^{4^{−5}} \ln \left(2 \frac{\Lambda^2}{Q^2} \frac{G_F}{\sqrt{2}} \frac{1}{q^2} \left(\frac{y_L y_L}{16\pi^2} + \frac{y_L}{16\pi^2} \right)^2 + \left(\frac{\sqrt{2}}{G_F} \right)^2 \frac{1}{\Lambda^2} \right)^{-1} \sim 10^{25} - 10^{27}$</td>
</tr>
<tr>
<td>$O_{14a}$</td>
<td>$(LL)(QQ)\bar{u}^c d^c$</td>
<td>$2 \times 10^{2^{−3}} \ln \left(2 \frac{\Lambda^2}{Q^2} \frac{G_F}{\sqrt{2}} \frac{1}{q^2} \left(\frac{y_L y_L}{16\pi^2} + \frac{y_L}{16\pi^2} \right)^2 + \left(\frac{\sqrt{2}}{G_F} \right)^2 \frac{1}{\Lambda^2} \right)^{-1} \sim 10^{24} - 10^{26}$</td>
</tr>
<tr>
<td>$O_{14b}$</td>
<td>$(LQ)(LQ)\bar{u}^c d^c$</td>
<td>$6 \times 10^{4^{−5}} \ln \left(2 \frac{\Lambda^2}{Q^2} \frac{G_F}{\sqrt{2}} \frac{1}{q^2} \left(\frac{y_L y_L}{16\pi^2} + \frac{y_L}{16\pi^2} \right)^2 + \left(\frac{\sqrt{2}}{G_F} \right)^2 \frac{1}{\Lambda^2} \right)^{-1} \sim 10^{25} - 10^{27}$</td>
</tr>
<tr>
<td>$O_{15}$</td>
<td>$(LL)(LL)d^c \bar{u}^c$</td>
<td>$10^{2^{−3}} \ln \left(2 \frac{\Lambda^2}{Q^2} \frac{G_F}{\sqrt{2}} \frac{1}{q^2} \left(\frac{y_L y_L}{16\pi^2} + \frac{y_L}{16\pi^2} \right)^2 + \left(\frac{\sqrt{2}}{G_F} \right)^2 \frac{1}{\Lambda^2} \right)^{-1} \sim 10^{24} - 10^{26}$</td>
</tr>
</tbody>
</table>
Table 7.5: A continuation of Table 7.3.

| $O_{16}$ | $(LL)e^c\bar{d}e^c\bar{u}c$ | 0.2 – 2 | \[
\ln(2)\left(\frac{\sqrt{2}}{G_F}\right)^2q^2\Lambda^2 \left[\left(\frac{G_F}{\sqrt{2}}\right)^2\frac{1}{q^2}\left(\frac{y_{y_b}y_{v}v^2}{(16\pi^2)^3}\right)^2 + \left(\frac{y_{v}v}{16\pi^2\Lambda^2}\right)^2\right]^{-1} \sim 10^{16} - 10^{22} \text{ yr} \]
\]
| $O_{17}$ | $(LL)d^c \bar{d}e^c\bar{u}c$ | 0.2 – 2 | \[
\ln(2)\left(\frac{\sqrt{2}}{G_F}\right)^2q^2\Lambda^2 \left[\left(\frac{G_F}{\sqrt{2}}\right)^2\frac{1}{q^2}\left(\frac{y_{y_b}y_{v}v^2}{(16\pi^2)^3}\right)^2 + \left(\frac{y_{v}v}{16\pi^2\Lambda^2}\right)^2\right]^{-1} \sim 10^{23} - 10^{26} \text{ yr} \]
| $O_{18}$ | $(LL)d^c \bar{u}e^c\bar{u}c$ | 0.2 – 2 | \[
\ln(2)\left(\frac{\sqrt{2}}{G_F}\right)^2q^2\Lambda^2 \left[\left(\frac{G_F}{\sqrt{2}}\right)^2\frac{1}{q^2}\left(\frac{y_{y_b}y_{v}v^2}{(16\pi^2)^3}\right)^2 + \left(\frac{y_{v}v}{16\pi^2\Lambda^2}\right)^2\right]^{-1} \sim 10^{23} - 10^{26} \text{ yr} \]
| $O_{19}$ | $(LQ)d^c \bar{d}e^c\bar{u}c$ | 0.1 – 1 | \[
\ln(2)\left(\frac{\sqrt{2}}{G_F}\right)^2q^2\Lambda^2 \left[\left(\frac{G_F}{\sqrt{2}}\right)^2\frac{1}{q^2}\left(\frac{y_{y_b}y_{v}v^2}{(16\pi^2)^3}\right)^2 + \left(\frac{y_{v}v}{16\pi^2\Lambda^2}\right)^2\right]^{-1} \sim 10^{10} - 10^{19} \text{ yr} \]
| $O_{20}$ | $(LQ)d^c \bar{u}e^c\bar{u}c$ | 4 – 40 | \[
\ln(2)\left(\frac{\sqrt{2}}{G_F}\right)^2q^2\Lambda^2 \left[\left(\frac{G_F}{\sqrt{2}}\right)^2\frac{1}{q^2}\left(\frac{y_{y_b}y_{v}v^2}{(16\pi^2)^3}\right)^2 + \left(\frac{y_{v}v}{16\pi^2\Lambda^2}\right)^2\right]^{-1} \sim 10^{19} - 10^{25} \text{ yr} \]
| $O_s$ | $e^c\bar{e}u^c\bar{u}d^c\bar{d}$ | 10 – 3 | \[
\ln(2)\left(\frac{\sqrt{2}}{G_F}\right)^2q^2\Lambda^2 \left[\left(\frac{G_F}{\sqrt{2}}\right)^2\frac{1}{q^2}\left(\frac{y_{y_b}y_{v}v^2}{(16\pi^2)^3}\right)^2 + \left(\frac{y_{v}v}{16\pi^2\Lambda^2}\right)^2\right]^{-1} \sim 10^{20} - 10^{10} \text{ yr} \]
After electroweak symmetry is broken, the neutrino masses are proportional to the eigenvalues of the matrix $f_{\alpha\beta}$, and the leptonic mixing matrix $U$ is the matrix of its eigenvectors. In Refs. [5, 6], the contributions of these operators to the Weinberg operator are estimated using a procedure similar to the one we outline in Sec. 7.4. A range for $\Lambda$ is determined based on the criterion that the largest entries in the neutrino mass matrix lie within $m_\nu \in 0.05 - 0.5$ eV, with higher $\Lambda$ corresponding to lower $m_\nu$. The third column of Tables 7.1-7.5 lists these ranges of $\Lambda$.

Operators $O_{4b}$ in Table 7.2 and $O_{12b}$ in Table 7.4 require extra care. These operators are necessarily antisymmetric in the flavors of the two lepton doublets. In addition to the antisymmetry of their weak indices, the Lorentz structure of these operators requires contraction between the lepton doublets, leaving only the flavor indices to enforce the overall antisymmetry. This feature had been overlooked in previous estimates of the contributions of these operators to the neutrino mass matrix. The simplest diagrams one can write down to generate a Majorana neutrino mass for $O_{4b}$ ($O_{12b}$) are a pair of two-loop (three-loop) diagrams that sum to zero due to this antisymmetry; this is similar to what one encounters in calculating the contributions of neutrino magnetic moment operators to the neutrino mass matrix, as in Ref. [236]. Following Ref. [236], the leading contributions to the neutrino mass matrix come from inserting two Yukawa interactions into these diagrams to form either the dimension-seven equivalent of the Weinberg operator or the dimension-five Weinberg operator $O_1$ at one additional loop level. We update the estimates for the contributions of these operators to the neutrino
matrix in Ref. [5] as follows:

\begin{equation}
\mathcal{O}_{4b} : \quad m_{\alpha\beta} = g_{\alpha\beta} \left[ \frac{1}{16\pi^2} + \frac{v^2}{\Lambda^2} \right] \frac{y_t g^2 (y_{\beta}^2 - y_{\alpha}^2) v^2}{(16\pi^2)^2 \Lambda},
\end{equation}

\begin{equation}
\mathcal{O}_{12b} : \quad m_{\alpha\beta} = g_{\alpha\beta} \left[ \frac{1}{16\pi^2} + \frac{v^2}{\Lambda^2} \right] \frac{y_t g^2 (y_{\beta}^2 - y_{\alpha}^2) v^2}{(16\pi^2)^2 \Lambda},
\end{equation}

where \( y_t \) is the top-quark Yukawa coupling; \( y_{\alpha} \) is the Yukawa coupling for charged lepton \( \alpha = e, \mu, \tau \); \( g \) is the weak coupling constant; and \( v \) is the Higgs vacuum expectation value. Because \( g_{\alpha\beta} \) is antisymmetric, these matrices have vanishing diagonal elements: \( m_{ee} = m_{\mu\mu} = m_{\tau\tau} = 0 \). We recalculate the values of \( \Lambda \) for each operator such that the largest element of the mass matrix lies within \( m_\nu \in 0.05 - 0.5 \) eV; the results are listed in Tables 7.2-7.5.

It is not possible, in a model-independent way, to relate LNV processes mediated by the new physics, e.g., \( 0\nu\beta\beta \) and \( \mu^- \rightarrow e^+ \) conversion, because the different \( g_{\alpha\beta} \) are not related. Majorana neutrino masses, however, serve as a link between otherwise disconnected LNV phenomena. If the neutrino masses and the leptonic mixing matrix were known, it would be possible, assuming the physics responsible for nonzero neutrino masses was captured by one of the operators in Tables 7.1-7.5 to translate constraints on LNV processes – like those mentioned below Eq. (7.3.4) – into constraints on other LNV processes. An important consequence of the connection between Majorana neutrino masses and LNV phenomena is that the observation of any LNV decay, interaction, etc., implies that neutrinos have a Majorana component to their masses, and that the existence of a Majorana neutrino mass implies that some LNV phenomena occur [237]. Exactly which processes must occur, however, cannot be predicted a priori.
Even partial information on neutrino masses and lepton mixing allows one to relate different LNV phenomena. As an example, we discuss the connection between Majorana neutrino masses and LNV phenomena using $0\nu\beta\beta$ and $\mu^- \rightarrow e^+$ conversion assuming the Weinberg operator $O_1$ captures the bulk of LNV phenomena. If neutrino exchange dominates these processes – the case of $O_1$ – the rate of $0\nu\beta\beta$ is proportional to

\[(7.3.7) \quad |m_{ee}|^2 \equiv |U_{e1}^2 m_1 + U_{e2}^2 m_2 e^{i\alpha_1} + U_{e3}^2 m_3 e^{i\alpha_2}|^2,
\]

while the rate of $\mu^- \rightarrow e^+$ conversion is proportional to

\[(7.3.8) \quad |m_{e\mu}|^2 \equiv |U_{e1} U_{\mu1} m_1 + U_{e2} U_{\mu2} m_2 e^{i\alpha_1} + U_{e3} U_{\mu3} m_3 e^{i\alpha_2}|^2,
\]

where $m_i$ is the mass of $\nu_i$, $U_{\alpha i}$ are the elements of the leptonic mixing matrix $U$, and $\alpha_i$ are potential Majorana phases. If nothing were known about the neutrino masses and mixing parameters, nothing could be said about $m_{ee}$ in relation to $m_{e\mu}$. However, from current measurements of the leptonic mixing matrix and the neutrino mass-squared differences $[1]$, we find that $m_{ee}$ and $m_{e\mu}$ cannot simultaneously vanish, for any value of the unknown $m_1$, $\alpha_1$ and $\alpha_2$ parameters. This implies that if LNV manifests itself predominantly via $O_1$ at least one of $0\nu\beta\beta$ and $\mu^- \rightarrow e^+$ conversion must occur.

Neutrino exchange does not, however, always dominate the amplitudes for these processes, as we discuss in detail in Sec. 7.4. Even so, we have verified, for all operators in Tables 7.1-7.5, that if $m_{ee}$ ($m_{e\mu}$) is nonzero the amplitude for $0\nu\beta\beta$ ($\mu^- \rightarrow e^+$ conversion) does not vanish as long as the dominant LNV physics is captured by one of the operators
in Tables 7.1-7.5. There is no guarantee, of course, that the nonzero rate is within experimental reach. If more operators are present with commensurate strength, we cannot rule out the possibility of fortuitous cancellations.

7.4. Estimates and Comparisons

In this section, we describe the process used for estimating $0\nu\beta\beta$ half-lives ($T_{0\nu\beta\beta}$) and $\mu^- \to e^+$ conversion rates ($R_{\mu^- e^+}$), concentrating, for concreteness, on $O_{14b}$. In Section 7.4.1, we discuss $0\nu\beta\beta$, and in Section 7.4.2 we discuss $\mu^- \to e^+$ conversion in nuclei. We estimate the values of diagrams with incoming (outgoing) down quarks and outgoing (incoming) up quarks for $0\nu\beta\beta$ ($\mu^- \to e^+$ conversion), and we bypass effects from hadronic currents, nuclear matrix elements, phase-space integration, etc.. In order to make comparisons with existing and future experimental results, we take advantage of existing bounds on [20] or calculations of [238, 239] the light neutrino exchange contribution, as will become clear momentarily.

7.4.1. Neutrinoless Double Beta Decay

Here, we discuss how we estimate $T_{0\nu\beta\beta}$ for the operator $O_{14b} = (L\overline{Q})(L\overline{Q})u^c d^c$. We separate the discussion into contributions at tree level, one loop, and two loops. We reemphasize that these are rough estimates aimed at capturing the dominant contributing factors to $0\nu\beta\beta$ and comparing these different contributions. Much more thorough calculations involving hadronic currents, etc., are necessary in order to extract accurate bounds. For our purposes, however, order-of-magnitude estimates are sufficient.
Figure 7.1. Feynman diagrams contributing to $0\nu\beta\beta$ from the operator $O_{14b} = (L\bar{Q})(LQ)\bar{u}d$. The dominant contributions scaling as $\Gamma \sim \Lambda^{-10}$ (a), $\Lambda^{-6}$ (b), and $\Lambda^{-2}$ (c) are depicted.
7.4.1.1. Tree level. Fig. 7.1(a) depicts the dominant tree-level contribution from $O_{14a}$ for $0\nu\beta\beta$. The amplitude scales as $\Lambda^{-5}$ since $O_{14a}$ has mass-dimension nine. We use the variable $Q$, which has dimensions of mass and encodes all information related to phase-space, nuclear matrix elements, etc., in order to convert the diagram into a decay rate, via naive dimensional analysis. $Q$ is naively of order the $Q$-value of the decay process, a few MeV. Our estimate is

$$\Gamma^{(0)}_{0\nu\beta\beta} = |g_{ee}|^2 \frac{Q^{11}}{\Lambda^{10}},$$

where $g_{ee}$ reflects the fact that this contribution requires both of the lepton doublets to be of electron flavor.

7.4.1.2. One loop. Here we consider the diagram shown in Fig. 7.1(b). When calculating a loop contribution, we assume the momentum cutoff scale to be $\Lambda$, above which the effective field theory approach is no longer valid. Each loop also contributes a factor of $(16\pi^2)^{-1}$ to the amplitude. We estimate the contribution of this loop to the amplitude to be

$$\int \frac{d^4p}{(2\pi)^4} \sim \frac{\Lambda^2}{16\pi^2}.$$

The amplitude, therefore, scales as $\Lambda^{-3}$. The Higgs boson can be replaced by its vacuum expectation value $v$ which multiplies its coupling to the up-type quark in the loop. We choose to take all effective operators to be quark-flavor universal, so the largest contribution to this diagram comes from the top quark, proportional to $y_t$, the top quark Yukawa coupling. The $W-$boson propagator and couplings contribute a factor of $G_F/\sqrt{2}$. The dominant contribution from the neutrino propagator scales like $1/q^2$, which we estimate is
of order \((100 \text{ MeV})^{-2}\), the typical distance scale between nucleons. Therefore, we estimate

\[
\Gamma_{0\nu\beta\beta}^{(1)} = |g_{ee}|^2 \left( \frac{G_F}{\sqrt{2}} \right)^2 \left( \frac{1}{q^2} \right) \left( \frac{v y_t}{16\pi^2} \right)^2 Q^{11} \frac{1}{\Lambda^6}.
\]

Since the neutrino propagator is not exactly point-like, the phase-space-matrix-element-etc.-\(Q^2\) factor here is not identical to the one in Eq. (7.4.1). The difference – not more than an order of magnitude – is too small to impact our results and will be ignored.

**7.4.1.3. Two loop.** The dominant contribution at two-loop order comes from the diagram shown in Fig. 7.1(c). Here, one loop contributes the same factor discussed above, and the second contributes the same factor but with the bottom quark Yukawa coupling \(y_b\) instead of the top quark Yukawa coupling \(y_t\). Additionally, there are two \(W^-\) boson propagators instead of one. The neutrino propagator contributes a factor proportional to \(1/q^2\) on top of the mass-insertion associated to the two-loop diagram. The estimate, therefore, is

\[
\Gamma_{0\nu\beta\beta}^{(2)} = |g_{ee}|^2 \left( \frac{G_F}{\sqrt{2}} \right)^4 \left( \frac{1}{q^2} \right)^2 \left( \frac{y_t y_b v^2}{(16\pi^2)^2} \right)^2 Q^{11} \left( \frac{G_F}{\sqrt{2}} \right)^4 \left( \frac{1}{q^2} \right)^2 \left| m_{ee} \right|^2 Q^{11}.
\]

This diagram is exactly the neutrino exchange process discussed in Section 7.3, hence we have rewritten the width as proportional to \(\left| m_{ee} \right|^2\). For \(O_{14}\), the neutrino mass matrix in the flavor basis is estimated to be

\[
m_{\alpha\beta} = \frac{g_{\alpha\beta} y_t y_b v^2}{\Lambda \left( 16\pi^2 \right)^2},
\]

\[(7.4.5)\]
\(\alpha, \beta = e, \mu, \tau\). As in the case of Eq. \((7.4.3)\), the phase-space-matrix-element-etc.-\(Q^2\) factor here is not identical to the one in Eq. \((7.4.1)\) but the difference can, given our goals, be safely ignored.

We use the results from the KamLAND-Zen experiment, along with the upper bound they compute for \(|m_{ee}|\), in order to extract the value of \(Q^{11}\) by requiring that Eq. \((7.4.4)\) exactly reproduces the KamLAND-Zen result, i.e., we obtain the lower bound on the half-life for the quoted upper bound on \(|m_{ee}|\). Concretely, the bound \(T_{0\nu\beta\beta} > 1.07 \times 10^{26} \) (90\% CL) from KamLAND-Zen, which can be translated into \(m_{ee} < 100 \) meV – here we make a concrete choice about the relevant nuclear matrix element – results into \(Q = 11 \) MeV.

For \(\mathcal{O}_{14_b}\), the tree-level, one-loop, and two-loop processes add incoherently, so \(\Gamma_{0\nu\beta\beta} \equiv \Gamma^{(0)}_{0\nu\beta\beta} + \Gamma^{(1)}_{0\nu\beta\beta} + \Gamma^{(2)}_{0\nu\beta\beta}\). Fig. 7.2 depicts the half-life \(T_{0\nu\beta\beta} = \log(2)/\Gamma_{0\nu\beta\beta}\) as a function of \(\Lambda\). Also shown are the current bound on \(T_{0\nu\beta\beta} > 1.07 \times 10^{26} \) yr (90\% CL) from the KamLAND-Zen experiment \[20\] along with the range of \(\Lambda\) where \(\mathcal{O}_{14_b}\) leads to neutrino masses between 0.05 and 0.5 eV, as listed in Tables 7.3-7.5. Generically, a subset of the tree-level, one-loop and two-loop diagrams may interfere with one another for a given operator. If so, then the transitions between different \(\Lambda\)-dependencies in Fig. 7.2 will be smoothed out. If we assume \(|g_{ee}|^2 = 1\) and that \(\mathcal{O}_{14_b}\) is responsible for neutrino masses, we estimate \(T_{0\nu\beta\beta} \sim 10^{25} - 10^{27}\) years. On the other hand, assuming \(|g_{ee}|^2 = 1\), the current bounds on \(T_{0\nu\beta\beta}\) translates into \(\Lambda \gtrsim 10^5\) TeV. The current upper bound on \(T_{0\nu\beta\beta}\) implies that the dominant contribution to \(0\nu\beta\beta\) coming from UV physics that manifests itself at the tree-level as \(\mathcal{O}_{14_b}\) comes from massive neutrino exchange.
Figure 7.2. The $0\nu\beta\beta$ half-life $T_{0\nu\beta\beta}$ as a function of the scale of new physics $\Lambda$ for operator $O_{14b}$. The pink line displays the current bound (assuming $|g_{ee}|^2 = 1$) by the KamLAND-Zen experiment [20], $T_{0\nu\beta\beta} > 1.07 \times 10^{26}$ yr (90% CL), and the grey region shows the range of $\Lambda$ necessary to generate neutrino masses between 0.05 and 0.5 eV. Three distinct regions are visible on the graph, where $T \propto \Lambda^{10}$, $\Lambda^6$, and $\Lambda^2$. These regions correspond to when the diagrams in Fig. 7.1(a), (b), and (c) are dominant in this process, respectively.

7.4.2. $\mu^- \rightarrow e^+$ conversion

In order to estimate the rate of $\mu^- \rightarrow e^+$ conversion, we first address the muon capture rate. As this is a weak-interaction process, it is proportional to the probability density function of the incoming muon $|\psi_{100}(0)|^2$ (which we assume to be in the 1s ground state
of the atom), so we estimate

\begin{equation}
\Gamma(\mu \text{ capture}) \sim \left( \frac{G_F}{\sqrt{2}} \right)^2 Q^2 \left( \frac{Z_{\text{eff}}^3}{\pi (a_0 m_e/m_{\mu})^3} \right),
\end{equation}

where \( a_0 \) is the Bohr radius and \( Q \) is a number with dimensions of mass that contains information regarding phase-space, nuclear matrix elements, etc., similar to the equivalent variable in the \( 0\nu\beta\beta \)-decay discussion. Note that, here, the \( Q \)-value of the reaction is of order the muon mass. The last factor in parenthesis is \( |\psi_{100}(0)|^2 \). The rate for \( \mu^- \rightarrow e^+ \) conversion depends on \( |\psi_{100}(0)|^2 \) as well, which cancels out in estimating \( R_{\mu^-e^+} \).

Fig. 7.3 shows the dominant diagrams contributing at tree-level (a), one loop (b), and two loops (c) to \( \mu^- \rightarrow e^+ \) conversion. These are similar to Figs. 7.1(a), (b), and (c), respectively. The contributions to \( R_{\mu^-e^+} \) from Figs. 7.3(a), (b), and (c) can be estimated following the same steps that led to Eqs. (7.4.1), (7.4.3), and (7.4.4), respectively. We find

\begin{align}
R^{(0)}_{\mu^-e^+} &= |g_{e\mu}|^2 \left( \frac{\sqrt{2}}{G_F} \right)^2 \frac{Q^6}{\Lambda^{10}}, \\
R^{(1)}_{\mu^-e^+} &= |g_{e\mu}|^2 \left( \frac{1}{q^2} \right) \left( \frac{y_t v}{16 \pi^2} \right)^2 \frac{Q^6}{\Lambda^6}, \\
R^{(2)}_{\mu^-e^+} &= |g_{e\mu}|^2 \left( \frac{G_F}{\sqrt{2}} \right)^2 \left( \frac{1}{q^2} \right)^2 \left( \frac{y_t y_b v^2}{(16 \pi^2)^2} \right)^2 \frac{Q^6}{\Lambda^2}.
\end{align}

Similar to Eq. (7.4.4), Eq. (7.4.9) can be written as a coefficient times \( |m_{e\mu}|^2 \), see Eq. (7.4.5). As in Sec. 7.4.1 the \( Q^2 \) factors are not strictly the same for the tree-level, one-loop, and two-loop contributions, but we assume that differences are sufficiently small and can be safely ignored.
Figure 7.3. Feynman diagrams contributing to $\mu^{-} \rightarrow e^{+}$ conversion from the operator $\mathcal{O}_{14b} = (L\bar{Q})(LQ)\bar{W}d\bar{e}$. The dominant contributions scaling as $\Gamma \sim \Lambda^{-10}$ (a), $\Lambda^{-6}$ (b), and $\Lambda^{-2}$ (c) are shown.
Refs. [238, 239] estimated $R_{\mu^- e^+}$ for light neutrino exchange,

\begin{equation}
R_{\mu^- e^+} = (2.6 \times 10^{-22}) |\mathcal{M}_{e\mu^+}|^2 \frac{|m_{e\mu}|^2}{m_e^2},
\end{equation}

where $m_e$ is the electron mass and $|\mathcal{M}_{e\mu^+}|$ is the nuclear matrix element, estimated to lie, for titanium, between 0.03 and 0.5. Similar to what we did in the previous subsection, we solve for $Q$ in the estimates above so that Eq. (7.4.9) matches the more precise estimate, Eq. (7.4.10), for $|\mathcal{M}_{e\mu^+}| = 0.1$, which we assume is the value of the nuclear matrix element for aluminum to sodium transition.

As with $0\nu\beta\beta$, these diagrams add incoherently, so $R_{\mu^- e^+} = R_{\mu^- e^+}^{(0)} + R_{\mu^- e^+}^{(1)} + R_{\mu^- e^+}^{(2)}$. Fig. 7.4 depicts the normalized conversion rate $R_{\mu^- e^+}$ as a function of $\Lambda$. Also shown is the range of $\Lambda$ where $\mathcal{O}_{14b}$ leads to neutrino masses between 0.05 and 0.5 eV, as listed in Tables 7.3-7.5. As before, interference between the tree-level, one-loop and two-loop diagrams would smooth out the transitions between different $\Lambda$-dependencies in Fig. 7.4 for a generic operator. If we assume that $\mathcal{O}_{14b}$ is responsible for neutrino masses, $\Lambda \sim 6 \times 10^{4-5}$ TeV and we estimate that $R_{\mu^- e^+} \simeq 10^{-38} - 10^{-36}$, further assuming $|g_{e\mu}|^2 = 1$. The current bound on $R_{\mu^- e^+} < 1.7 \times 10^{-12}$ from the SINDRUM II collaboration, again assuming $|g_{e\mu}|^2 = 1$, implies $\Lambda \gtrsim 10$ GeV. As discussed in Sec. 7.2, we expect the Mu2e experiment will be sensitive to $R_{\mu^- e^+} \gtrsim 10^{-16}$ and is hence expected to observe $\mu^- \rightarrow e^+$ conversion if $\Lambda \lesssim 40$ GeV.

### 7.5. Results

We follow the steps outlined for $\mathcal{O}_{14b}$ in Sec. 7.4 and estimate the rates for $0\nu\beta\beta$ and $\mu^- \rightarrow e^+$ conversion for all effective operators listed in Tables 7.1-7.5. Analytic results
Figure 7.4. The $\mu^- \to e^+$ conversion rate $R_{\mu^- e^+}$ as a function of the scale of new physics $\Lambda$ for operator $O_{14b}$. The black line displays the current bound by the SINDRUM II Collaboration, while the blue line indicates our estimate of the reach of the Mu2e experiment, both assuming $|g_{e\mu}|^2 = 1$. The grey region highlights the range of $\Lambda$ necessary to generate neutrino masses between 0.05 and 0.5 eV. Three distinct regions are visible on the graph, where $T \propto \Lambda^{10}$, $\Lambda^6$, and $\Lambda^2$. These regions correspond to when the diagrams in Fig. 7.1(a), (b), and (c) are dominant in this process, respectively.

are listed in Tables 7.1-7.5. The results for $0\nu\beta\beta$ agree with the estimates presented in Ref. [5], while the $\mu^- \to e^+$ conversion rates are the main results of this paper.
Table 7.6. Constants used for estimating $T_{0\nu\beta\beta}$ and $R_{\mu^- e^+}$. The $Q$-value for $0\nu\beta\beta$ refers to the isotope $^{136}$Xe and the $Q$-value for $\mu^- \rightarrow e^+$ refers to the isotope $^{27}$Al.

<table>
<thead>
<tr>
<th>Constant</th>
<th>$G_F$ [GeV$^{-2}$]</th>
<th>$g$</th>
<th>$\langle r \rangle$</th>
<th>$v$ [GeV]</th>
<th>$Q$ [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>$1.17 \times 10^{-5}$</td>
<td>0.653</td>
<td>(100 MeV)$^{-1}$</td>
<td>174</td>
<td>11.0 ($0\nu\beta\beta$), 15.6 ($\mu^- \rightarrow e^+$)</td>
</tr>
</tbody>
</table>

In order to convert analytic expressions into numerical estimates for observables or the sensitivity to the new physics scale $\Lambda$, we use the values listed in Tables 7.6 and 7.7 for various SM parameters. $y_f$ denotes the Yukawa coupling of fermion $f$, $g$ denotes the weak gauge coupling, and $v$ denotes the vacuum expectation value of the Higgs field. The variables $Q$ – different for $R_{\mu^- e^+}$ and $T_{0\nu\beta\beta}$ – were defined in Sec. 7.4 and are used to map our rough estimates to more precise computations of $R_{\mu^- e^+}$ and $T_{0\nu\beta\beta}$. We further assume that the operator coefficients $g_{\alpha\beta...}$ are all $\mathcal{O}(1)$. As discussed in Section 7.3, this is not necessarily the case and should be kept under advisement. Several operators, e.g., $O_{13}$, contain four or more leptons, and the resulting $0\nu\beta\beta$ and $\mu^- \rightarrow e^+$ amplitudes depend on a weighted sum of coefficients $g_{\alpha\beta\gamma\delta}$, typically of the form $\sum_{\gamma} g_{\alpha\beta\gamma\gamma} y_{\ell\gamma}$, where $y_{\ell\gamma}$ is the Yukawa coupling of the lepton of flavor $\gamma$. In these instances, we assume that $g_{\alpha\beta\gamma\delta} \sim g_{\alpha\beta\mu\mu} \sim g_{\alpha\beta\tau\tau}$ and only list the largest contribution, usually due to the latter thanks to the relatively large tau Yukawa coupling. Numerical estimates for all observables under investigation are also listed in Tables 7.1-7.5, assuming the operator in question is responsible for the observable neutrino masses, i.e., the value of $\Lambda$ agrees with the associated tabulated values of $\Lambda$. 

Table 7.7. A continuation of Table 7.6.

<table>
<thead>
<tr>
<th>Constant</th>
<th>$y_t$</th>
<th>$y_b$</th>
<th>$y_e$</th>
<th>$y_\mu$</th>
<th>$y_\tau$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Value</td>
<td>0.9</td>
<td>$2 \times 10^{-2}$</td>
<td>$3 \times 10^{-6}$</td>
<td>$6 \times 10^{-4}$</td>
<td>$10^{-2}$</td>
</tr>
</tbody>
</table>
Figure 7.5. Bounds on the effective scale associated with the dimension-five operator $O_1$ from the KamLAND-Zen experiment for $0\nu\beta\beta$ (blue) and SINDRUM-II experiment for $\mu^- \to e^+$ (black). Also shown are the estimated sensitivity for the Mu2e experiment (pink) and the range of $\Lambda$ for which $m_{\alpha\beta} \sim 0.05 - 0.5$ eV (grey). We assume $g_{\alpha\beta...} = 1$ for all coefficients here. See text for details.

Figs. 7.5, 7.6, and 7.7 depict the currently allowed values of $\Lambda$ assuming current and future experimental bounds for operators of mass-dimension five, seven, and nine, respectively. For each operator, we depict the estimated bound for $\Lambda$ using the bound on $R_{\mu^-e^+}$ from SINDRUM II (black), the estimated sensitivity of Mu2e (pink) and the estimated bound on $\Lambda$ using the results on $T_{0\nu\beta\beta}$ from the KamLAND-ZEN experiment (blue). All estimates are valid for $g_{\alpha\beta...} = \mathcal{O}(1)$). A hierarchical structure among the flavor coefficients could impair the ability to place a bound on $\Lambda$ from $0\nu\beta\beta$ or $\mu^- \to e^+$ conversion, for instance. Also shown for each operator is the range of $\Lambda$ such that $m_{\alpha\beta} \simeq 0.05 - 0.5$ eV.

As before, we direct the reader’s attention to $O_{4_b}$ and $O_{12_e}$. These operators must have vanishing $g_{ee}$ due to the flavor-antisymmetry of the lepton doublets, meaning neither of these operators can produce $0\nu\beta\beta$, as indicated in Tables 7.2 and 7.3. There is no such restriction on $g_{e\mu}$. This means that, in principle, $\mu^- \to e^+$ conversion could occur at an observable rate in next-generation experiments in the complete absence of $0\nu\beta\beta$ if either of these operators were the only source of lepton-number violation. We note, however, that the neutrino mass matrices in Eqs. (7.3.5) and (7.3.6) have vanishing diagonal elements,
resulting in a mass matrix with relatively few independent degrees of freedom. This produces strong correlations among the neutrino masses and leptonic mixing parameters, such that current neutrino oscillation data preclude either of these operator from being the dominant contribution to neutrino masses and mixings (see, for instance, Refs. [240–242]).

7.6. Discussion and Conclusions

The observation of LNV phenomena would imply that the neutrinos are Majorana fermions and would help point the community to a subset of ideas for the new physics behind nonzero neutrino masses. The absence of LNV phenomena would not necessarily
Figure 7.7. The same as Figure 7.6 but for the dimension-nine operators considered in our analysis. See text for details.
allow one to conclude that neutrinos are Dirac fermions, but a prolonged absence, assuming many different probes, would lead one to ultimately suspect this is the case and would point the search for the origin of nonzero neutrino masses down a different path. Hence, deep and broad searches for the validity of lepton-number conservation are among the highest priorities of experimental particle physics today.

Here, we concentrated on understanding the reach of searches for $\mu^- \rightarrow e^+$ conversion in nuclei, partially motivated by the fact that, in the foreseeable future, several new experiments are aiming at improving the sensitivity to $\mu^- \rightarrow e^-$ conversion by four or more orders of magnitude. We opted for an effective operator approach that allows one to compare a large number of new physics scenarios.

At face value, future searches for $\mu^- \rightarrow e^+$ conversion are sensitive to new, LNV physics at a wide range of effective energy scales, from 100 MeV to 10 TeV. This sensitivity pales in comparison with searches for $0\nu\beta\beta$, as revealed in Figs. 7.5, 7.6, and 7.7. Comparisons between different LNV observables, however, need to be interpreted with care. Flavor effects can, as is well known, render the rate for $0\nu\beta\beta$ infinitesimally small and need not impact different LNV observables in the same way.

LNV new physics ultimately leads to nonzero neutrino masses. Figs. 7.5, 7.6, and 7.7 also reveal that if the dominant contribution to the neutrino masses is captured individually by any of the effective operators discussed here, the expected rates for $\mu^- \rightarrow e^+$ conversion are well beyond the reach of next generation experiments, with one trivial

\[4\text{Except for } O_9. \text{ For } \Lambda \gtrsim 1 \text{ GeV, the effective operator approaches is still valid for } \mu^- \rightarrow e^+ \text{ conversion in nuclei, as long as the new physics is not weakly coupled. It is, however, difficult to imagine that, for } \Lambda \lesssim 100 \text{ GeV, the existence of these new degrees of freedom is not severely constrained by probes of new phenomena that do not involve lepton-number violation. The exploration of such constraints cannot, however, be pursued within the formalism adopted here.}\]
All of these observations imply that, should $\mu^- \rightarrow e^+$ conversion be discovered in the next round of experiments, we will be able to conclude that (i) neutrinos are Majorana fermions, (ii) flavor effects, or something equivalent, significantly suppress the rate for $0\nu\beta\beta$, and (iii) the physics behind nonzero neutrino masses, assuming all new degrees of freedom are heavy, does not manifest itself at tree level via one of the effective operators investigated here but, instead, is captured by a non-trivial combination of operators whose contribution to the Majorana neutrino masses are significantly smaller than the contributions of any one operator.

**Note added:** After this work was completed, Ref. [208] appeared on the preprint archive. In it, the authors present a detailed calculation of the rate of $\mu^- \rightarrow e^+$ conversion for a model with a doubly-charged scalar, as well as a discussion of how to map specific models of new physics onto effective operator coefficients.

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5If $O_s$ were responsible for nonzero neutrino masses, its effective scale would be around 1 GeV and either $0\nu\beta\beta$-decay or $\mu^- \rightarrow e^+$ conversion should have been observed a long time ago, along with many more non-LNV observables.
CHAPTER 8

Constructing Chiral Fermion Sectors in Nonabelian Gauge Models

8.1. Introduction

The standard model of particle physics (SM) is a chiral $SU(3) \times SU(2) \times U(1)$ gauge theory. Considering all fermion fields in the theory as, for example, left-handed Weyl spinors, this means that (1) all fermions are charged under the gauge symmetry, and (2) there are no fermions with equal-and-opposite quantum numbers. These imply that fermion mass terms are forbidden by gauge invariance and all nonzero fermion masses are consequences of gauge symmetry breaking. An attractive feature of the SM is all masses are proportional to same, unique source of mass, the scale of electroweak symmetry breaking.

Chiral gauge theories are, in general, anomalous. In the SM, quantum numbers are such that the contributions of the chiral fermions to the different anomalies cancel exactly. This minor miracle implies that – per generation – all SM fermions are required in the sense that if any of them were absent, then the theory would be mathematically inconsistent. Considerations of anomaly cancellations contributed to the hypothesized existence of the bottom and top quarks, and of the tau-type neutrino, years before direct discovery. The peculiar quantum numbers of the fermion fields, required by anomaly cancellations, also
imply that the SM Lagrangian is invariant under accidental global symmetries, including baryon and lepton numbers.

The SM is known to be incomplete. The dark matter puzzle and nonzero neutrino masses imply that degrees of freedom outside of the SM exist. It is interesting to take the SM Lagrangian as guidance and investigate whether the new degrees of freedom are also chiral fermions, charged under a gauge symmetry. Identifying possible chiral gauge theories is a nontrivial exercise, mostly because of the anomaly-cancellation requirement [243, 244].

Here, we discuss a novel yet powerful mechanism for generating chiral, anomaly-free gauge theories. We refer to these models as *imperfect mirrors* of the SM. In a nutshell, we start with simple gauge theories that are anomaly-free and admit complex representations – these include $SO(10)$, $SO(14)$, and $E_6$ – and identify gauge symmetries with subgroups of the theory and the fermion fields with representations of the simple gauge group. The mechanism is discussed in detail and is easy to implement. We explore, using mostly $SO(10)$ and the 16 representation, several chiral, anomaly-free gauge theories, including quasi-perfect copies of the SM, and discuss qualitatively general properties of such theories and how they might shed light on the the neutrino mass and dark matter puzzles.

### 8.2. Chiral $U(1)$ theories from Simple Orthogonal Groups

In Ref. [245], a general method was described to obtain anomaly-free abelian theories with chiral particle content. Let us briefly review those results. The starting point is a gauge field theory based on a simple, anomaly-free Lie group $G$. Such groups were identified by Georgi and Glashow in Ref. [246]. The complete list is:
(1) $SU(2)$.

(2) The infinite sequence $Sp(2N)$.

(3) The infinite sequences $SO(2N + 1)$ and $SO(2N + 2)$ with the exception of $SO(6)$.

(4) The 5 exceptional groups: $G_2$, $F_4$, $E_6$, $E_7$ and $E_8$.

Consider an anomaly-free simple group $\mathcal{G}$ and a semisimple group $\mathcal{G} \subset \mathcal{G}$ which is not necessarily anomaly-free. Starting from a representation $R$ of $\mathcal{G}$, one can construct anomaly-free theories based on the gauge group $\mathcal{G}'$ by decomposing $R$ into a direct sum of representations $R'_i$ of $\mathcal{G}'$, and introducing the corresponding fermionic content. Such a procedure, however, may lead to nonchiral $\mathcal{G}'$ theories, i.e., to trivial cancellations of anomalies. Focusing on the abelian case, $\mathcal{G}' \equiv U(1)$, in order to end up with a chiral $\mathcal{G}'$ gauge theory, it is necessary for the initial $\mathcal{G}$ representation $R$ to be a complex representation $[245]$.

Of the anomaly-free groups listed above, only those of the form $SO(4N + 2)$ and the exceptional group $E_6$ have complex representations. The group with lowest dimensionality of these is $SO(10)$, a well-known unification group $[247, 248]$. For any $SO(4N + 2)$ algebra, the smallest complex representation is the fundamental spinor of dimension $2^{2N}$. Hence, the simplest representation that satisfies all requirements is the $16$ of $SO(10)$. Most of this work thus focuses on $\mathcal{G} \equiv SO(10)$ and $R \equiv 16$, although we will mention other possibilities in Section 8.5.

Without loss of generality, we can identify $\mathcal{G}'$ with a $U(1)$ subgroup generated by an element $H \in \mathcal{H}$ of the Cartan subalgebra of $\mathcal{G}$. The charges of the fermionic matter content with respect to $\mathcal{G}'$ are then given by the eigenvalues of $H$. We denote the $\mathcal{G}'$ charges by $q_i$ with $i = 1, \ldots, d$, where $d$ is the dimension of the $\mathcal{G}$ representation $R$. Note
that for compact $G$, $H$ can be assumed Hermitian which implies that the $q_i$ can be taken to be real.

A generic element of the Cartan subalgebra in the 16 representation of $SO(10)$ has the form:

$$H(a, b, c, d, e) = \frac{1}{N} \text{diag}\{a + b + c + d + e, a - b + c + d - e, a + b - c + d - e, a - b - c + d + e, a + b - c - d - e, a - b + c - d + e, -a + b - c + d - e, -a - b + c + d + e, -a + b + c - d - e, -a - b + c - d - e, -a + b + c - d - e, -a - b - c + d + e, -a + b + c + d - e, -a - b - c - d + e, -a + b - c + d - e, -a - b - c - d - e, -a - b - c - d - e, -a + b - c - d + e\},$$

where $a, b, c, d$ and $e$ are arbitrary real numbers and $N$ is a normalization factor. These eigenvalues form the list of $G'$ charges $\{q_i\}$. For generic values of $a, b, c, d, e$, for any $q \in \{q_i\}$, $-q \not\in \{q_i\}$. One can quickly check that for any $a, b, c, d, e$, the $\{q_i\}$ are solutions to the anomaly $G' \equiv U(1)$ equations,

$$\sum_{i=1}^{16} q_i = 0, \quad \sum_{i=1}^{16} q_i^3 = 0. \quad (8.2.2)$$

An anomaly-free $G'$ model is specified by a choice of $\{a, b, c, d, e\}$. Some properties of Eq. (8.2.1) are of note. Chirality is destroyed if at least one of $a, b, c, d$ or $e$ vanishes. In that case, for every $q$ in Eq. (8.2.1), $-q$ is also present. Hence, in order to obtain a chiral theory, it is necessary to take all of $a, b, c, d$ and $e$ different from zero.
Consider next the effect of flipping the sign of one of \{a, b, c, d, e\}. We find

\[ H(-a, b, c, d, e) = H(a, -b, c, d, e) = H(a, b, -c, d, e) = H(a, b, c, -d, e) = H(a, b, c, d, -e) = -H(a, b, c, d, e). \]  

(8.2.3)

Flipping the sign of one among \{a, b, c, d, e\} is equivalent to a model where all the charges have been reversed in sign. Since the overall sign of the charges is a convention, this implies that there is no loss of generality in considering all of \(a, b, c, d, e\) strictly positive. This has an immediate corollary: The largest \(G'\) charge is \(a + b + c + d + e\) and it appears only once, the absolute values of all other charges being necessarily smaller. Hence, in every anomaly-free model derived following this method, there can be only one state with highest gauge abelian charge.

This is particularly important since, in the following section, we will extend the procedure to the case in which \(G'\) has nonabelian components in addition to the \(U(1)\) symmetry. The particle content in \(R\) will organize into multiplets of the nonabelian symmetry, and all states in a multiplet must have the same abelian charge. Hence, the state with highest \(U(1)\) charge must transform as a singlet under any nonabelian piece of \(G'\). As an example, consider the SM. The state with highest hypercharge (the \(U(1)\) inside \(G'\) in that case) is the left-handed antielectron \(e^c\). This analysis implies that the \(e^c\) must be a singlet of both color \(SU(3)\) and weak \(SU(2)\), as it is indeed the case.

It is useful to introduce a geometric picture of this procedure. The Cartan subalgebra of a group forms a vector space, which in the case of \(SO(10)\) is five-dimensional. Taking into account that the absolute scale of charges is a matter of convention, choosing specific values for \(a, b, c, d\) and \(e\) amounts to selecting a one-dimensional subspace, i.e., a ray,
Figure 8.1. Cross sections of the \( \{a, b, c, d, e\} \) vector space. Figure (A) represents the plane \( a + b + c = 3d, \ d = e \) with \( a, b, c > 0 \). The centroid of the triangle corresponds to the \( SU(5) \) model, the medians correspond to the \( SU(2) \times SU(2) \) models \( (d = e, \ a = b) \). Nonchiral models live in the edges of the triangle where at least one of \( a, b \) or \( c \) vanishes. Figures (B) and (C) represent the tetrahedron \( a + b + c + d = 4e \) for positive \( a, b, c, d \). The lines joining (B) the vertex with the opposite face of the tetrahedron and (C) the midpoints of two opposing edges have been drawn. They represent models with larger symmetry.

in \( \{a, b, c, d, e\} \) space. Nonchiral models are located within hyperplanes where at least one coordinate vanishes, while chiral theories live inside a hyperquadrant. Sections of \( \{a, b, c, d, e\} \) space are shown in Fig. 8.1.

Next, we restrict discussion to theories with integer charges. From this requirement, either none, two, or four out of \( a, b, c, d \) and \( e \) can be half-integers, while the rest are integers. Example theories include:

- \( a = b = c = d = e \). This case comprises one model up to charge rescalings, that is a ray in \( \{a, b, c, d, e\} \) space. For \( a = 1 \), we obtain the following charges and multiplicities:

<table>
<thead>
<tr>
<th>Charge</th>
<th>5</th>
<th>-3</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity</td>
<td>1</td>
<td>5</td>
<td>10</td>
</tr>
</tbody>
</table>

We call this model the \( (5) \).
• \( a = b = c = d, \ e. \) Here, different models can be specified by the ratio \( r = e/a \) which labels the specific ray in the space of the Cartan subalgebra along which we intend to gauge. For instance, the following model is achieved with \( a = b = c = d = 1/2, \ e = 1 \), corresponding to \( r = 2 \):

<table>
<thead>
<tr>
<th>Charge</th>
<th>3</th>
<th>-2</th>
<th>1</th>
<th>0</th>
<th>-1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity</td>
<td>1</td>
<td>4</td>
<td>6</td>
<td>4</td>
<td>1</td>
</tr>
</tbody>
</table>

We call any model of this type, a (4, 1). Note that as long as we are building purely \( U(1) \) models, neutral states and pairs of opposite charges give a vanishing contribution to the anomaly equations, Eq. (8.2.2), and can be removed from the list of states. From this point of view, the model above has ten chiral fermions.

• \( a = b = c, \ d = e. \) Again, we define \( r = e/a \). For \( a = b = c = 1, \ d = e = 1/2 \) \((r = 1/2)\), we find:

<table>
<thead>
<tr>
<th>Charge</th>
<th>4</th>
<th>-3</th>
<th>-2</th>
<th>2</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multiplicity</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>1</td>
<td>3</td>
</tr>
</tbody>
</table>

We call any model of this type, a (3, 2). The model above contains eleven chiral fermions.

More generally, we label models where the set \( \{a, b, c, d, e\} \) can be split into subsets of \( j_1, \ldots, j_k \) equal numbers, \((j_1, \ldots, j_k)\) models. Clearly, for the \( 16 \) of \( SO(10), \sum j_i = 5 \), that is, the \( j_i \) constitute a partition of 5.

The alert reader will have noticed that the charges in these examples organize suggestively. In particular, in the (3, 2) case the charges seem to organize into multiplets resembling the SM particle content. A bit of experimentation shows that in all these
models, although the charges themselves depend on \( r \), the number of particles with identical charges does not. In the \((5)\) case, for example, the charges mimic the multiplets in the \(SU(5)\) Georgi-Glashow unification model \[249\]. We prove next that this resemblance is not accidental.

### 8.3. Nonabelian Symmetries

The \(\{a, b, c, d, e\}\) formalism can also be used to identify gauge theories based on non-abelian groups. The key fact is the following result: *Any \((j_1, \ldots, j_k)\) model accepts the simultaneous introduction of nonabelian, anomaly-free \(SU(j_i)\) gauge groups for any \(j_i \geq 2\).*

We begin by illustrating the result for the case of \(SU(2)\). Without losing generality, we show that there is an \(SU(2)\) subalgebra that commutes with \(H(a, a, \ldots)\). The proof proceeds by construction. The \(2^N\)-dimensional spinor representation of \(SO(2N + 2)\) acts on a vector space that is conveniently represented as the tensor product of \(N\) 2-dimensional vector spaces \[250\]. We choose a basis in this space with its elements given by:

\[
(8.3.1) \quad |k_1\rangle|k_2\rangle\ldots|k_N\rangle
\]

where \(k_i = \pm 1\).

Generators of \(SO(2N + 2)\) can be written as tensor product operators composed of Pauli matrices acting independently on the 2-dimensional vector subspaces. We define a basis of generators as follows:

\[
(8.3.2) \quad H^s = \sigma^s_3, \quad \text{for } s = 1, \ldots, N,
\]

\[
(8.3.3) \quad H^5 = \sigma^1_3 \otimes \sigma^2_3 \otimes \cdots \otimes \sigma^N_3,
\]
\[ A^s_i = \left( \bigotimes_{r=1}^{s-1} \sigma^r_3 \right) \otimes \sigma^s_i, \quad \text{for } s = 1, \ldots, N, \] (8.3.4)

\[ B^s_i = \sigma^s_i \otimes \left( \bigotimes_{r=s+1}^{N} \sigma^r_3 \right), \quad \text{for } s = 1, \ldots, N, \] (8.3.5)

\[ M^{st}_{ij} = \sigma^s_i \otimes \left( \bigotimes_{r=s+1}^{t-1} \sigma^r_3 \right) \otimes \sigma^t_j, \quad \text{for } s, t = 1, \ldots, N, \ s \neq t, \] (8.3.6)

where \( \sigma^r_i \) acts on the \( r \)th vector subspace; subspaces not explicitly identified are acted on by the identity. The goal is to prove that there is an \( SU(2) \) subalgebra that commutes with the generator

\[ H = \sum_{a=1}^{5} \beta_a H^a, \] (8.3.7)

if \( \beta_1 = \beta_2 \).

Without loss of generality, we define the following:

\[ T_1 = \frac{1}{4} \left( M^{12}_{11} + M^{12}_{22} \right), \quad T_2 = \frac{1}{4} \left( M^{12}_{12} - M^{12}_{21} \right), \quad T_3 = \frac{1}{4} \left( H^2 - H^1 \right). \] (8.3.8)

The commutators among these are

\[ [T_1, H] = \frac{i}{2} (\beta_1 - \beta_2) \left( M^{12}_{12} - M^{12}_{21} \right) = 2i (\beta_1 - \beta_2) T_2, \] (8.3.9)

\[ [T_2, H] = \frac{i}{2} (\beta_1 - \beta_2) \left( M^{12}_{11} + M^{12}_{22} \right) = 2i (\beta_1 - \beta_2) T_1, \] (8.3.10)

\[ [T_3, H] = 0, \] (8.3.11)

\[ [T_1, T_2] = \frac{i}{4} \left( H^2 - H^1 \right) = iT_3. \] (8.3.12)
The generators $T_{1,2,3}$ form an $SU(2)$ subalgebra belonging to $SO(10)$ that commutes with $H$ if $\beta_1 = \beta_2$ (regardless of $\beta_3, \beta_4, \ldots$), which is what we wanted to prove.

In order to extend the proof to an $SU(K)$ subgroup, we need to construct the corresponding subalgebra for $\alpha^1 = \alpha^2 = \cdots = \alpha^K$. Such a subalgebra can be defined by the following choice of generators:

\begin{align*}
F^n &= \frac{1}{\sqrt{2^N n(n+1)}} \left[ \sum_{i=1}^{n} H^i - nH^{n+1} \right], \quad \text{for } n = 1, \ldots, K - 1, \\
E^{lm} &= \begin{cases} \\
\frac{1}{\sqrt{2^N n+1}} (M_{11}^{lm} + M_{22}^{lm}), & \text{for } l, m = 1, \ldots, \min(K, N); \ l < m, \\
\frac{1}{\sqrt{2^N n+1}} (A_l^1 - B_l^1), & \text{for } l = 1, \ldots, K - 1; \ m = K, \\
\end{cases} \\
E^{lm} &= \begin{cases} \\
\frac{1}{\sqrt{2^N n+1}} (M_{12}^{lm} - M_{21}^{lm}), & \text{for } l, m = 1, \ldots, \min(K, N); \ l < m, \\
\frac{1}{\sqrt{2^N n+1}} (A_l^2 - B_l^2), & \text{for } l = 1, \ldots, K - 1; \ m = K. \\
\end{cases}
\end{align*}

The second lines of Eqs. (8.3.14) and (8.3.15) are only required to complete the subalgebra when $K$ is maximal, i.e., when $K = N + 1$. It is straightforward to check that this choice of generators indeed satisfies the $SU(K)$ commutation relations.

As we have stressed before, the numbers \{a, b, c, d, e\} span a vector space in which each model corresponds to a ray. The set of models corresponds therefore to 4D projective space. A graphical representation of some features of this space is depicted in Fig. 8.1.

In Fig. 8.1(A), a planar cross section of 4D projective space in the coordinates \{a, b, c\} is shown. The conditions selecting this hyperplane are

\begin{equation}
(8.3.16) \quad d = e, \quad a + b + c = 3d.
\end{equation}
The restriction to positive $a, b, c, d, e$ extracts an equilateral triangle out of this plane whose centroid, the point $a = b = c = d = e$, has maximal $SU(5)$ symmetry. The medians of the triangle also have enhanced symmetry, in this case $SU(2) \times SU(2) \times U(1)$. Note that the conditions in Eq. (8.3.16) are invariant under simultaneous rescalings of all coordinates as befits a projective space.

A solid cross section is shown in Fig. 8.1(B) and Fig. 8.1(C) corresponding the requirement $a + b + c + d = 4e$. The barycenter of the tetrahedron is again the maximally symmetric point $a = b = c = d = e$, and the segments depicted, dropping from a vertex to the centroid of the opposite face or joining the midpoints of two opposite edges, have again enhanced symmetry, $SU(3)$ and $SU(2) \times SU(2)$ respectively.

In summary, we have shown that chiral gauge theories based on the $16$ representation of $SO(10)$ are in a one-to-one correspondence with a set of five strictly positive numbers. The substitution of these in Eq. (8.2.1) yields charges with respect to a chiral, anomaly-free $U(1)$ symmetry. If two or more among $\{a, b, c, d, e\}$ are equal, the model can also accommodate enhanced, nonabelian symmetries, as described above.

8.4. Applications

The formalism developed above can be used to quickly explore the infinite space of chiral gauge theories. Here, we discuss several models, highlighting some of their main features and how they may be useful for addressing phenomenology questions. In this section, we concentrate on scenarios seeded by the $16$ representation of $SO(10)$. We will briefly comment on higher-dimensional representations of $SO(10)$, the $64$ representation of $SO(14)$, and the $27$ representation of $E_6$ in Sec. 8.5.
Simple chiral $U(1)$ theories have been explored in, for example, Refs. [243, 245], and it is possible to organize and classify them using different criteria. We can use the highest charge as an organizing principle. If we impose that all $U(1)$ charges are integers, the model characterized by $(a = b = c = d = 1/2, e = 1) \equiv \{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1\}$ is such that the charge of the highest-charged fermion is as small as possible (and equal to 3). There is only one model with highest charge 3. The three models with highest charge 4 are $\{\frac{1}{2}, \frac{1}{2}, 1, 1, 1\}$, $\{\frac{1}{2}, \frac{1}{2}, 1, \frac{3}{2}\}$, and $\{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 2\}$. There are more models with highest charge 5, 6, etc. The number of models is roughly proportional to the combinatorial partitions of the highest charge.

One can also characterize $U(1)$ models by the number of chiral fermions. Starting from the 16 representation of $SO(10)$, chiral $U(1)$ models will contain at most 16 chiral fermions. On the other hand, the smallest number of chiral fermions is 5, as can be demonstrated quite generally: theories with 1, 2, 3, and 4 chiral fermions cannot satisfy the anomaly-cancellation conditions Eqs. (8.2.2) [243, 245]. The following solution of Eqs. (8.2.2) with highest charge 10 requires only five fields: $q_1 = 2, q_2 = 4, q_3 = -7, q_4 = -9, q_5 = 10$. This is the $\{\frac{1}{2}, \frac{3}{2}, 2, \frac{5}{2}, \frac{7}{2}\}$ model.

The scalar sector of the theory, responsible for $U(1)$ symmetry breaking, also helps define the phenomenological consequences of the model. If none of the fermions acquire Majorana masses, models with an odd number of chiral fermions will contain one massless Weyl fermion. This is the case of the SM with its minimal Higgs sector (i.e., only one Higgs doublet $H$). For each generation there are fifteen fermions, and there is one

---

1Keep in mind that fermions with charge zero and pairs of fermions with opposite charge are not chiral and contribute trivially to the anomaly-cancellation constraints.

2Forbidding Majorana masses is equivalent to requiring the Yukawa sector to preserve a subset of accidental global symmetries.
massless left-handed neutrino after spontaneous gauge symmetry breaking. The existence
of a Higgs triplet $T$, such that the $LTL$ Yukawa interaction is allowed, violates lepton
number, and $\langle T \rangle \neq 0$ would lead to neutrino Majorana masses. The scenario explored
in Ref. [245] also contains an odd number of hidden-sector fermions (eleven), and one of
them is massless after $U(1)_e$ symmetry breaking. The Yukawa sector of the theory is such
that accidental global symmetries prevent this left-handed antineutrino from acquiring a
Majorana mass [245].

For a generic chiral $U(1)$ model, one can compute the smallest number of scalar fields
required to make sure that (1) at most one fermion is massless after spontaneous symmetry
breaking, and (2) all massive fields are Dirac fermions. In the SM, and in the model
explored in Ref. [245], this number is one. In the scenario with the smallest number
of fermions ($\{\frac{1}{2}, \frac{3}{2}, 2, \frac{5}{2}, \frac{7}{2}\}$, above), two scalar fields are required. We investigated the
fraction of models where Dirac masses for all fermions (except at most one) can come
from the vacuum expectation value of only one scalar field. As a function of the highest
charge, the fraction of scenarios with only one Higgs decreases, as depicted in Fig. 8.2.
Oscillations arise because these scenarios are more likely for an even highest charge.

The same procedure can be used to generate chiral $U(1)^N$ theories. In the $SO(10)$-
seeded scenarios under consideration here, $N \leq 5$. Models with $U(1)^2$ symmetry, for
example, correspond to a pair of vectors $\{a_1, b_1, c_1, d_1, e_1\}$, $\{a_2, b_2, c_2, d_2, e_2\}$ that are linearly independent, while $U(1)^4$ models correspond to four linearly independent vectors
in the $\{a, b, c, d, e\}$ space. In general, $U(1)^N$ models will include particles nontrivially
charged under all $U(1)$ symmetries. Models with $N > 5$ can also be constructed, but they
Figure 8.2. Fraction $f$ of $U(1)$ models where all fermions, except at most one, obtain nonzero Dirac masses from the expectation value of one scalar field, as a function of the highest charge $N$.

require the use of other seed groups, including $E_6$, which can accommodate $U(1)^6$ chiral models and $SO(14)$, which can accommodate $U(1)^7$ chiral models.

Turning to the nonabelian scenarios, anomaly-free $SU(N)$ theories have been investigated in, for instance, Ref. [251]. In our formalism, the (5) model, introduced in Sec. 8.2, corresponds to $\{a,a,a,a,a\}$. As shown in Sec. 8.3 we can choose an $SU(5)$ subgroup of $SO(10)$ that commutes with the $U(1)$ subgroup characterized by $\{a,a,a,a,a\}$ such that the emerging particle content can be organized into a chiral, gauge-invariant $SU(5) \times U(1)$
theory. For $a = 1$, $\{1, 1, 1, 1, 1\}$ translates into

\begin{equation}
\text{(8.4.1)}
10_1, \quad 5_{-3}, \quad 1_5,
\end{equation}

where the number in boldface refers to the $SU(5)$ representation and the subscript to the $U(1)$ charge. As emphasized before, there is an $SU(5)$ singlet, and the singlet has the highest $U(1)$ charge. In the $(5)$ scenario, the particle content and charge assignments are unique, modulo an overall (unphysical) rescaling of all $U(1)$ charges. The particle content also agrees with that of the $SO(10)$ grand-unified theory (GUT) where the GUT symmetry-breaking follows the path $SO(10) \rightarrow SU(5) \times U(1)$. The $U(1)$ in this case is sometimes referred to as $U(1)_X$, and is a unique linear combination of $U(1)_{B-L}$ and $U(1)_Y$, where $B - L$ refers to baryon number minus lepton number.

While we used the $U(1)$ subgroup of $SO(10)$ to identify the chiral $SU(5)$ particle content, one is allowed to turn off the $U(1)$ symmetry. The leftover $SU(5)$ theory is still guaranteed to be anomaly-free. Investigating Eq. (8.4.1), we can conclude that a chiral $SU(5)$ model with one $10$ and one $\bar{5}$ is anomaly free, as is well known. This is the only chiral $SU(5)$ model one can derive from the $16$ of $SO(10)$.

The $(4, 1)$ models, introduced in Sec. 8.2 can be interpreted as chiral $SU(4) \times U(1)$ models. In particular, the $U(1)$ is characterized by $\{a, a, a, a, e\}$, and translates into the following $SU(4) \times U(1)$ particle content, for $a = 1, r = e/a$:

\begin{equation}
\text{(8.4.2)}
6_r, \quad 4_{2-r}, \quad \bar{4}_{-2-r}, \quad 1_{4+r}, \quad 1_{-4+r}.
\end{equation}

The number in boldface refers to the $SU(4)$ representation and the subscript to the $U(1)$ charge. There are, in general, two singlets, and the highest $U(1)$ charge is $4 + r$. Similar
to the $SU(5) \times U(1)$ case, the $SU(4)$ particle content is unique. In this case, one can also choose to ignore the $U(1)$ part of the theory, and only explore the $SU(4)$ model with the particle content spelled out in Eq. (8.4.4), ignoring the singlet fields. This model, unlike the $SU(5)$ model in Eq. (8.4.1), is not chiral since there is both a 4 and a $\bar{4}$, which can combine into a Dirac fermion, and a 6, which is a real representation and allows for a vectorlike mass term. In summary, while the $SU(4) \times U(1)$ is a chiral model for any value of $r \neq 0$, the $SU(4)$ model is not.

Given that the rank of $SO(10)$ is greater than that of $SU(4) \times U(1)$, it is possible to gauge a different $U(1)$ and consider chiral $SU(4) \times U(1)^2$ models. The two $U(1)$s are characterized by, for example, $\{1, 1, 1, 1, r\}$ and $\{1, 1, 1, 1, s\}$, $r \neq s$. Note that an analogous choice is to pick the second $U(1)$ to be nonchiral, e.g., $\{0, 0, 0, 0, s'\}$. The reason is that $\{1, 1, 1, 1, r\}$, $\{1, 1, 1, 1, s\}$, and $\{0, 0, 0, 0, s'\}$ are not linearly independent: $\{1, 1, 1, 1, s\} + \{0, 0, 0, 0, s'\} = \{1, 1, 1, 1, r\}$, where $r = s + s'$.

One scalar field with a nonzero vacuum expectation value is sufficient to render all fermions in Eq. (8.4.4) massive. Explicitly, if we add to the theory a scalar 4-plet of $SU(4)$ with $U(1)$ charge $-2$, $4^H_{-2}$, the following Yukawa Lagrangian preserves gauge invariance,

\[
\mathcal{L}_{\text{Yukawa}} = \lambda_1 4^H_{-2} 6, 4_{-2} - r + \lambda_2 4^H_{-2} 1_{4+r}, \bar{4}_{-2-r} + \lambda_3 (4^H_{-2})^\dagger 6, \bar{4}_{-2-r} + \lambda_4 (4^H_{-2})^\dagger 1_{-4+r}, 4_{-2-r} + h.c.,
\]

where the $(4^H_{-2})^\dagger$ transforms like a $\bar{4}$ with charge $+2$. The case $r = 4$ is special. Here, one of the $SU(4)$ singlets has zero $U(1)$ charge and is allowed to have a Majorana mass, unrelated to the $SU(4) \times U(1)$ symmetry breaking scale. In the $r = 4$ case, one may also
consider a model with a reduced particle content, in which the gauge-singlet fermion is ignored.

For illustrative purposes, we discuss in more detail the \( SU(4) \times U(1) \) model without the gauge-singlet fermion. The Yukawa Lagrangian is given by Eq. (8.4.3) with \( \lambda_4 \equiv 0 \), and the number of chiral fermions is odd. Following the symmetry-breaking pattern \( SU(4) \times U(1) \to SU(3) \times U(1)' \), 14 of the 15 fields get Dirac masses, except for part of the \( 4_{-1} \), which remains massless. The degrees of freedom reorganize into triplets, anti-triplets and singlets of \( SU(3) \), as follows:

\[
\begin{align*}
6_2 &\to 3_{1/3} \oplus 3_{2/3}, \\
4_{-1} &\to 3_{-1/3} \oplus 1_0, \\
\bar{4}_{-3} &\to 3_{-2/3} \oplus 1_{-1}, \\
1_4 &\to 1_1,
\end{align*}
\]

while \( 4^H_1 \to 3^H_{-1/3} \oplus 1^H_0 \), including the degrees of freedom eaten by the heavy vector bosons. Here, the subscripts indicate the corresponding \( U(1)' \) charges. The broken generators (of which there are seven) manifest themselves as massive gauge bosons \( W_3 \), which are \( 3_{-1/3} \), and \( Z_3 \), which is an \( SU(3) \times U(1)' \) singlet. From the \( SU(3) \times U(1)' \) point of view, it is easy to see that there are two massive Dirac “quarks” (with \( U(1)' \) charge 1/3 and 2/3), one massive Dirac “electron” (with \( U(1)' \) charge 1) and a massless Weyl fermion that we will refer to as the left-handed antineutrino. The \( SU(4) \times U(1) \) model has an accidental \( U(1)_\ell \) (\( \ell \) for ‘hidden lepton number’) global symmetry (which, not surprising, agrees with the \( \{0, 0, 0, s'\} \) nonchiral \( U(1) \) discussed above), under which the \( 4_{-1} \) and the \( \bar{4}_{-3} \) have the same charge, which is opposite to that of the \( 6_2 \) and \( 1_{-1} \). Note that the vacuum expectation value of \( 4^H_1 \) does not break the hidden-lepton-number symmetry.
As far as phenomenology is concerned, in the absence of interactions that connect the hidden sector $SU(4) \times U(1)$ model to the SM, the lightest $U(1)'$-charged hidden-sector particle is stable, along with the massless antineutrino. Assuming the hidden $SU(3)$ gauge theory confines in the infrared, the lightest $U(1)'$ particle could be the “electron” or an $SU(3)$-neutral baryon-like state. Note that, unlike the SM, there is no separate baryon-number and lepton-number symmetry in this hidden sector. The $W_3$-mediated interactions, for example, connect “electron” and “quark” states. The presence of massive, stable particles allows one to explore whether there is a viable dark matter candidate in this hidden sector.\footnote{The long-range $U(1)'$ force poses an interesting challenge that may require further model building. There is also the possibility that the dark matter is made up of hidden sector “atoms”.} We refrain from addressing this in any detail here.

Yukawa interactions between the SM neutrinos and the hidden sector antineutrinos are forbidden by the SM and the $SU(4) \times U(1)$ gauge symmetries. The dimension-five operator

\begin{equation}
\mathcal{L}_5 = \frac{(LH)(4_{-1}(4^H_{-1})^l)}{\Lambda} + h.c.,
\end{equation}

however, after spontaneous symmetry breaking, leads to nonzero neutrino Dirac masses of order $v v_4/\Lambda$, where $v$ and $v_4$ are the vacuum expectation values of the SM Higgs boson and $4^H_{-1}$, respectively, and $\Lambda$ is the effective messenger scale. Eq. (8.4.5) explicitly breaks the $U(1)_\ell$ global symmetry and the SM global $U(1)_{B-L}$ symmetry down to a diagonal global lepton number $U(1)_{B-L_\text{tot}}$, under which both the SM leptons and all hidden sector fermions transform.

The (3, 2) models, introduced in Sec. 8.2, can be interpreted as chiral $SU(3) \times SU(2) \times U(1)$ models. In particular, the $U(1)$ characterized by $\{a, a, a, d, d\}$ translates into the
following $SU(3) \times SU(2) \times U(1)$ particle content:

\[(8.4.6) \quad (3, 2)_a, \quad (\bar{3}, 1)_{-a+2d}, \quad (\bar{3}, 1)_{-a-2d}, \quad (1, 2)_{-3a}, \quad (1, 1)_{3a+2d}, \quad (1, 1)_{3a-2d}, \]

where $(A, B)_q$ represent a state that transforms as an $A$-plet of $SU(3)$, a $B$-plet under $SU(2)$, and has $U(1)$ charge $q$. Like in the (5) and (4,1) models described above, the (3,2) model is unique as far as the $SU(3) \times SU(2)$ quantum numbers are concerned. Like the (5) model, but unlike the (4,1) model, the $SU(3) \times SU(2)$ obtained by discarding the $U(1)$ piece of $SU(3) \times SU(2) \times U(1)$ is also a chiral gauge theory.

The SM is the (3,2) model characterized by $\{1, 1, 1, \frac{3}{2}, \frac{3}{2}\}$. The (3,2) model can be augmented by another chiral $U(1)$ symmetry characterized by $(a, a, d', d')$, where $d' \neq d$. Alternatively, one can choose the nonchiral $U(1)$ symmetry characterized by $(a, a, d, d')$ – in the SM case, this is is $U(1)_{B-L}$ – or $(0, 0, 0, d, d)$ – in the SM this is a right-handed global $U(1)_R$, where the quark singlets have opposite charge, and the right-handed electron and neutrino also have opposite charge.\footnote{The $U(1)_R$ symmetry is broken by the Yukawa interactions. It is easy to see that the Higgs boson has charge $2d$ and hence does not break $U(1)_{B-L}$.} Combined with hypercharge, the $U(1)_{B-L}$ and $U(1)_R$ charges are not independent.

Phenomenologically, the (3,2) models provide several interesting opportunities. Since the SM is a (3,2) model, one is allowed to identify some or all of the $SU(3) \times SU(2) \times U(1)$ with SM simple gauge groups. For example, one can consider adding to the SM a distorted fourth family, where all hypercharge assignments correspond to a different value of $a, d$, i.e., $(a, d) \neq (1, 3/2)$. These distorted quarks and leptons would all get masses from the SM Higgs boson, but their electric charges would be different from the SM counterparts.

Another possibility is to augment the SM to a gauged, chiral $SU(3) \times SU(2) \times U(1) \times$
$U(1)_{\text{new}}$ theory, where the $U(1)_{\text{new}}$ charges of the SM particles are characterized by some choice of $(a, d) \neq (1, 3/2)$. This is a generalized version of gauging the $U(1)_{B-L}$ symmetry.

The $(2,2,1)$ models can be interpreted as $SU(2)^2 \times U(1)$ chiral gauge theories. In particular, the $U(1)$ characterized by $\{a, a, c, e\}$ translates into the following $SU(2)^2 \times U(1)$ particle content:

\[
\begin{align*}
(1,2)_{-2a-e} & , \quad (1,2)_{2a-e} & , \quad (2,1)_{-2c-e} & , \quad (2,1)_{2c-e} & , \quad (2,2)_{e} , \\
(1,1)_{-2a-2c+e} & , \quad (1,1)_{-2a+2c+e} & , \quad (1,1)_{2a-2c+e} & , \quad (1,1)_{2a+2c+e} .
\end{align*}
\]

These models can be maximally extended to $SU(2)^2 \times U(1)^3$ chiral gauge theories by choosing three linearly independent sets of $(a, c, e)$, one for each $U(1)$.

The $(3,1,1)$ and $(2,1,1,1)$ models can be interpreted as $SU(3) \times U(1)$ and $SU(2) \times U(1)$ chiral gauge theories, respectively. They can be maximally extended, within the $SO(10)$ framework, to $SU(3) \times U(1)^2$ and $SU(2) \times U(1)^3$. The $(3,1,1)$ models are of the form $\{a, a, a, d, e\}$. For generic values of $(a, d, e)$ the particle content is unique: two $3$s, two $\bar{3}$s, all with potentially different $U(1)$ charges, and two singlets, one of which has the highest charge, $3a + d + e$. While the $SU(3) \times U(1)$ is chiral as long as none of $a, d, e$ vanish, the $SU(3)$ theory, which one can define by turning off all $U(1)$ charges, is vectorlike. It is possible to choose $(a, d, e)$ such that a $3, \bar{3}$ pair has opposite charge or such that one of the singlets has zero charge. In these scenarios, the particle content is smaller. The $(2,1,1,1)$ models are of the form $\{a, a, c, d, e\}$. For generic values of $(a, c, d, e)$ the particle content is unique: four $2$s, and eight singlets, all with potentially different $U(1)$ charges. One of which has the highest charge, $2a + c + d + e$. For specific choices of $(a, c, d, e)$ charge-zero
or vectorlike pairs of 2s or singlets might emerge, and the chiral particle content might be smaller.

8.5. Extensions

In the previous sections, we concentrated our discussions on chiral gauge theories seeded by $SO(10)$ and the 16 representation. In this section, we briefly discuss higher-dimensional complex representations of $SO(10)$ and other anomaly-free simple gauge theories, including $SO(14)$ and $E_6$. As we will illustrate with a few concrete example, higher-dimensional representations are required if one is interested in models with more than sixteen fermionic degrees of freedom. Furthermore, larger gauge groups allow one to consider chiral gauge theories with rank larger than five.

Another reason for pursuing larger groups and higher-dimensional representations is that the 16 of $SO(10)$ might be too restrictive a starting point. In Section 8.4, only a few representations of $SU(N)$ were found when generating the different chiral gauge theories. In particular, in all of Sec. 8.4, only the fundamental representations of $SU(N)$ appear. This is not an accident, but a direct consequence of the fact that we started with the fundamental spinor representation of $SO(10)$.

8.5.1. Higher-Dimensional Representations of $SO(10)$

For higher-dimensional complex representations of $SO(10)$, we need an expression for generic elements of the $SO(10)$ Cartan subalgebra, similar to Eq. (8.2.1). For any complex representation $R$ of $SO(10)$, these will still be functions of five parameters and can

\footnote{These are the totally antisymmetric representations, corresponding to the single-column Young tableaux. They include the 10, 10, 5, and 5 of $SU(5)$, the 6, 4, 4 of $SU(4)$, the 3 and 3 of $SU(3)$, and the 2 of $SU(2)$.}
also be thought of as vectors on a five-dimensional vector space, \( \{a, b, c, d, e\}_R \). The reason for this, of course, is that \( SO(10) \) has rank five. Note that, for any complex representation of \( SO(10) \), we can still choose all \( a, b, c, d, e \geq 0 \), i.e., Eq. (8.2.3) is representation independent.

Starting from the \( 126 \) representation of \( SO(10) \), we find that the particle content of the \( SU(5) \times U(1) \) model corresponding to \( \{1, 1, 1, 1, 1\}_{126} \), the \( (5) \) model, is,

\[
(8.5.1) \quad 1_5, \quad 5_1, \quad 10_3, \quad 15_{-3}, \quad 45_{-1}, \quad 50_1.
\]

Here, representations of \( SU(5) \) other than the \( 5 \) and \( 10 \) appear, unlike the \( (5) \) associated to the \( 16 \) of \( SO(10) \), Eq. (8.4.1). Like the \( (5) \) model associated to the \( 16 \) of \( SO(10) \), the simple \( SU(5) \) theory, which one can obtain by simply ignoring the existence of the \( U(1) \) group, is also chiral.

On the other hand, starting from the \( 144 \) representation of \( SO(10) \), \( \{1, 1, 1, 1, 1\}_{144} \) corresponds to

\[
(8.5.2) \quad 5_7, \quad 45_3, \quad 5_3, \quad 40_{-1}, \quad 15_{-1}, \quad 10_{-1}, \quad 24_{-5}.
\]

This scenario has some qualitative differences from the \( 16 \)- and \( 126 \)-seeded models, Eq. (8.4.1) and Eq. (8.5.1), respectively. Eq. (8.5.2) has no \( SU(5) \) singlets and, hence, the highest \( U(1) \) charge is not unique. In this case, the highest \( U(1) \) charge is 7 and is five-fold degenerate (where the five fermions combine into a \( 5 \) of \( SU(5) \)).

Some technical comments are in order. By only investigating the degeneracy of \( U(1) \) charges, it is not possible to distinguish a representation from its complex conjugate. It is also not possible to determine, from the \( U(1) \) charges alone, whether a set of degenerate
charges corresponds to one or several representations of the nonabelian group. This is the case in Eq. (8.5.2), where the $\mathbf{45}$ and the $\mathbf{5}$ have the same $U(1)$ charge, and so do the $\mathbf{40}$, the $\mathbf{15}$ and the $\mathbf{10}$. In order to extract all this information, one needs to investigate in detail how the different representations of $SO(10)$ organize themselves in terms of representations of the $SU(N)$ nonabelian subgroup of interest. In more detail, we make our assignments by examining how the weight spaces of these representations decompose when $SO(10)$ is broken. For computing the weights of different representations associated to different gauge groups, we made ample use of Ref. [252].

The $(4,1)\, SU(4) \times U(1)$ model corresponding to $\{1,1,1,1,r\}_{126}$ has the following particle content. In what follows, the $\mathbf{4}$s and $\mathbf{\bar{4}}$s, and the $\mathbf{20}$s and $\mathbf{\bar{20}}$ form vectorlike pairs and hence do not contribute to the anomaly cancelation conditions, and could be safely ignored.

\[
\mathbf{4}_{-6}, \quad \mathbf{20}_{-2}, \quad \mathbf{4}_{-2}, \quad \mathbf{20}_{2}, \quad \mathbf{\bar{4}}_{2}, \quad \mathbf{4}_{6}, \quad \mathbf{\bar{10}}_{-4-2r}, \quad \mathbf{10}_{1-2r},
\]

\[
(8.5.3) \quad \mathbf{15}_{-2r}, \quad \mathbf{20'}_{2r}, \quad \mathbf{1}_{2r}, \quad \mathbf{1}_{-8+2r}, \quad \mathbf{6}_{-4+2r}, \quad \mathbf{6}_{4+2r}, \quad \mathbf{1}_{8+2r}.
\]

Similar to the $(5)$ model, here we also obtain larger representations of $SU(4)$. Nonetheless, as in the $\mathbf{16}$ case, Eq. [8.4.4], the $SU(4)$-only model is not chiral, keeping in mind that the $\mathbf{6}$, $\mathbf{15}$ and $\mathbf{20'}$ representations are real. We also examined the $SU(4) \times U(1)$ associated to $\{1,1,1,1,r\}_{144}$. There, the $SU(4)$-only particle content is also not chiral.

8.5.2. $SO(14)$

$SO(14)$ has rank 7, and its smallest complex representation is the fundamental spinor $\mathbf{64}$. All results and intuition developed for and from the $\mathbf{16}$ of $SO(10)$ apply. Here, the
elements of the Cartan subalgebra live in a seven-dimensional vector space that can be labelled by \{a, b, c, d, e, f, g\}. Chiral models correspond to all \(a, b, c, d, e, f, g \neq 0\) and degeneracies among \(a, b, c, d, e, f, g\) allow one to consider nonabelian chiral gauge theories.

Starting from the 64 of \(SO(14)\), one can explore a larger space of models. The following models are too large to fit into \(SO(10)\) but can be accommodated by \(SO(14)\): (7), (6, 1), (5, 2), (4, 3), (4, 2, 1), (3, 2, 2), etc. For example, the (7) model corresponding to \{1, 1, 1, 1, 1, 1\} allows one to define a chiral \(SU(7) \times U(1)\) model with particle content

\[
1_7, \quad \overline{7}_{-5}, \quad 21_3, \quad \overline{35}_{-1}.
\]

As is the case of the 16 of \(SO(10)\), the highest charge is a singlet and only fundamental representations of \(SU(7)\) appear. On the other hand, the (6,1) model corresponding to \{1, 1, 1, 1, 1, 1, r\} can be mapped into an \(SU(6) \times U(1)\) model with particle content

\[
16_{+r}, \quad 1_{r-6}, \quad 6_{4-r}, \quad \overline{6}_{-4-r}, \quad 15_{2+r}, \quad \overline{15}_{r-2}, \quad 20_{-r}.
\]

The \(SU(6)\) part of the model is not chiral (the 20 representation of \(SU(6)\) is real).

Finally, we discuss a couple of larger imperfect mirrors of the SM that mimic the \(SU(M) \times SU(N)\) SM structure, \(M \neq N \geq 2\) structure of the SM. These include the \{1, 1, 1, 1, r, r, r\} \(SU(4) \times SU(3) \times U(1)\) chiral gauge theory, which has particle content

\[
(1, 1)_{4+3r}, \quad (4, 3)_{2+r}, \quad (1, \overline{3})_{4-r}, \quad (6, 1)_{3r}, \quad (4, 1)_{2-3r},
\]

(8.5.6)

\[
(6, \overline{3})_{-r}, \quad (4, 3)_{r-2}, \quad (4, 1)_{-2-3r}, \quad (1, 1)_{3r-4}, \quad (1, \overline{3})_{-4-r}.
\]

The \(SU(4) \times SU(3)\) model is also chiral.
On the other hand, the \{1,1,1,1,1,r,r\} SU(5) × SU(2) × U(1) chiral gauge theory has particle content

\[(1,1)_{5+2r}, \ (5,2)_3, \ (1,1)_{5-2r}, \ (10,1)_{1+2r}, \]
\[(10,1)_{1-2r}, \ (\overline{10},2)_{-1}, \ (\overline{5},1)_{-2r-3}, \ (\overline{5},1)_{2r-3}, \ (1,2)_{-5}. \]

8.5.3. \(E_6\)

The exceptional group \(E_6\) has rank 6, and its smallest complex representation is the \(27\)

As in the \(SO(10)\) and \(SO(14)\) cases, we can represent the elements of the \(E_6\) Cartan subalgebra as six-dimensional vectors, labelled \(\{a,b,c,d,e,z\}\). Explicitly, the elements of the Cartan subalgebra for one of the \(27\) representations can be written as

\[
H(a,b,c,d,e,z) \propto \text{diag}\{a+b+c+d+e+z, a+b+c-d-e+z, a+b-c+d-e+z, a-b+c+d-e+z, a-b-c+d-e+z, a-b+c-d+e+z, a+b-c+d-e+z, a+b-c-d+e+z, a-b+c-d-e+z, a-b-c+d-e+z, a-b-c-d+e+z, 2a-2z, 2b-2z, 2c-2z, 2d-2z, 2e-2z, -2e-2z, \}
\]

There are two inequivalent complex, 27-dimensional representations of \(E_6\)
The first sixteen charges look remarkably similar to the entries in Eq. (8.2.1). This is, of course, not an accident; $E_6$ contains $SO(10) \times U(1)$ as a maximal subgroup, and the 27 decomposes into $16_1 \oplus 10_{-2} \oplus 1_4$, where the subscript indicates the $U(1)$ charge. Consequently, the first sixteen charges in Eq. (8.5.8) are the $U(1)$ charges of the 16 of $SO(10)$ up to an additive factor of $z$. If $z \neq 0$, then the charges of the 16, by themselves, do not satisfy the anomaly equations, Eq. (8.2.2). However, when one factors in the eleven remaining charges, the linear and cubic anomalies vanish. In this scenario, the chiral fermions of the 16 are necessarily accompanied by vectorlike fermions which belong to the 10 and 1 representations.

The discussion of the interpretation of these charge assignments follows our discussion in Sec. 8.4. The coefficients $a, b, c, d, e$ inform us about how states are grouped into representations of nonabelian subgroups, depending on which subsets of coefficients are equal, as before. The number $z$ describes a uniform shift of the $U(1)$ charges within each multiplet of $SO(10)$, while maintaining that the 27 charges in Eq. (8.5.8), taken together, are nonanomalous. As before, we are free to impose that $a, b, c, d, e$ are all positive without loss of generality. However, $z$ must be allowed to have either sign; we highlight this by showing the charge assignments in the two cases \(\{a, b, c, d, e, z\} = \{1, 1, 1, 1, +1\}\) and \(\{1, 1, 1, 1, -1\}\), which both possess $SU(5) \times U(1)$ symmetry:

\[
\{1, 1, 1, 1, +1\} : \quad 1_6, \quad \bar{5}_{-2}, \quad 10_2, \quad 5_{-4}, \quad \bar{5}_0, \quad 1_4.
\]

\[
\{1, 1, 1, 1, -1\} : \quad 1_4, \quad \bar{5}_{-4}, \quad 10_0, \quad 5_0, \quad \bar{5}_4, \quad 1_{-4}.
\]
Both scenarios are different from one another and different from Eq. (8.4.1).

8.6. Discussion

Chirality is an intriguing feature of nature. Quantum anomalies render generic chiral gauge theories inconsistent, and yet, in the SM, these are mysteriously absent thanks to a set of delicate cancellations. It seems pertinent to ask the questions: How do these cancellations come to happen? Do anomaly cancellations reveal that there is more structure at small distance scales?

The standard explanation is to posit that the SM is embedded into a complex representation of a higher-dimensional, anomaly-free unification gauge theory, such as $SO(10)$. If $SO(10)$ unification is realized in Nature, then anomaly cancellations are naturally explained and the existence of chiral fermions is simple to understand. On top of explaining why anomalies cancel, an $SO(10)$ GUT also predicts the unification of the gauge couplings, the existence of new, ultra-heavy particles, proton decay, etc. In this work we concentrated on a humbler, more agnostic task. If chirality were a fundamental principle, and not assuming unification, we have asked what are other chiral, anomaly-free gauge theories. Inspired by the SM embedding in the $SO(10)$ – but making no assumptions regarding gauge coupling unification or the existence of a GUT gauge theory – we have devised a general method to construct such theories from scratch.

Due to the anomaly-cancellation conditions, these imperfect mirrors of the SM are necessarily nonminimal. In Ref. [245], a concrete $U(1)$ chiral gauge theory was explored. There, it was demonstrated how the rich, chiral structure provides the necessary ingredients for simultaneously addressing the dark matter and neutrino mass puzzles. In this
chapter, we provide an algorithm that makes it possible to characterize and study an infinite number of qualitatively different chiral models, many of which could have interesting phenomenological applications.

In order to prove the statements and claims in this chapter, relatively heavy use of group theory was made. Nonetheless, it should be emphasized that an important result advocated here is that much information about chiral models can be obtained without any group theory analysis whatsoever. In particular, a result of this work is that the particle content of anomaly-free, chiral models, including charges and nonabelian representations, can be easily obtained by following the procedure described in Secs. 8.2 and 8.3. A summary of the procedure, for imperfect mirrors based on the 16 of $SO(10)$, is as follows: (1) Pick the gauge group of the model of the form $G = SU(n_1) \times \ldots SU(n_k) \times U(1)^m$ subject to the requirements that the rank of $G \leq 5$, $n_1 + \ldots + n_k \leq 5$, and $m \geq 1$; (2) pick $m$ sets of five numbers $\{a, b, c, d, e\}$ such that they can be divided into sets of $n_1, \ldots, n_k$ equal numbers, and such that the $m$ different sets are linearly independent; and (3) introduce fermions with $U(1)$ charges given by Eq. (8.2.1). The fermions will automatically organize into anomaly-free multiplets of $G$. For example, the choice $\{1, 1, \frac{1}{2}, \frac{1}{2}, 2\}$, $\{\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{3}{2}, 1\}$ will yield a set of chiral fermions nontrivially charged under $SU(2)^2 \times U(1)^2$.

This algorithm, which does not require group theory savviness, works for models based on complex representations of groups of the form $SO(4N + 2)$. Models based on the group $E_6$ – the only other compact, anomaly-free Lie group with complex representations – can be treated similarly, as briefly outlined in Sec. 8.5, although the identification of nonabelian symmetries is not as straightforward.
Some well-known extensions of the standard model, even ones that can be obtained by descending from $SO(10)$ unification, cannot be directly obtained from the procedure proposed here. The most prominent example is the Pati-Salam model \cite{253} based on the gauge group $\mathcal{G} = SU(4) \times SU(2)_L \times SU(2)_R$. The problem is readily apparent: the ranks of the Pati-Salam group and $SO(10)$ are the same, but the numbers $n_i$ in this case satisfy $n_1 + n_2 + n_3 = 8$. However, a simple generalization of our procedure to account for this case, under investigation, seems to exist.

While it was not the purpose of this work to focus on specific models, we did briefly discuss, as examples of the power of this procedure, chiral models with large gauge groups that can arise out of the $16$ of $SO(10)$. We believe that many of these are interesting in their own right. They include: (1) a unique $SU(5) \times U(1)$ model, essentially the Georgi-Glashow $SU(5)$ unification; (2) a new class of $SU(4) \times U(1)^2$ scenarios that have not, as far we as can tell, been explored before and that, in particular, do not correspond to Pati-Salam unification; and (3) $SU(3) \times SU(2) \times U(1)$ models that mimic the nonabelian representations of the SM but where the charges with respect to the abelian counterpart of hypercharge are different from those of the SM fermions. Finally, we also discussed, very briefly, models one can construct starting with larger, complex representations of $SO(10)$, or with larger simple gauge groups: $SO(14)$ and $E_6$. 
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APPENDIX A

Appendix to Chapter 4

A.1. Three-Neutrino Fits to Three-Neutrino Data

In this appendix, we present the results of simulating and analyzing DUNE data consistent with the three-neutrino hypothesis. This is done, in part, to validate our simulation and analysis tools, and in order to facilitate comparisons between the three-neutrino and the four-neutrino scenarios. We also comment on the ability of the DUNE experiment to constrain the solar parameters $\Delta m_{12}^2$ and $\theta_{12}$.

Fig. A.1 depicts the expected sensitivity contours at 68.3% (blue), 95% (orange), and 99% (red) CL as measured by DUNE with six years of data collection (3 years with the neutrino beam, three years with the antineutrino one), a 34 kiloton detector, and a 1.2 MW beam, assuming the data are consistent with a three-neutrino scenario. The figure also depicts one-dimensional $\Delta \chi^2$ plots for each parameter, with the 68.3% (blue), 95% (orange), and 99% (red) CL highlighted. Quoted measurement bounds are for 68.3% CL.

The input values of the mixing angles are $\sin^2 \theta_{12} = 0.308$, $\sin^2 \theta_{13} = 0.0235$, and $\sin^2 \theta_{23} = 0.437$. Results from solar neutrino experiments and KamLAND are included here as Gaussian priors for the values of $|U_{e2}|^2 = 0.301 \pm 0.015$ and $\Delta m_{12}^2 = (7.54 \pm 0.24) \times 10^{-5}$ eV$^2$. This scenario assumes a normal mass hierarchy, i.e., $\Delta m_{13}^2 = +2.43 \times 10^{-3}$ eV$^2$, and that the $CP$-odd phase is $\delta_{CP} = \pi/3$. Distributions are sampled using a Markov Chain Monte Carlo (MCMC) method [131]. We find that the measurement precisions of the
mixing angles and mass-squared differences are safely comparable to the projected results in Ref. [8].

Throughout, with one exception, our analyzes include only data to be collected by the DUNE experiment. We do not include, for example, data from reactor experiments, [55, 56, 100] nor do we include existing or simulated data from the long-baseline experiments currently in operation [101, 254–256]. The main reason for this is that we anticipate DUNE data will provide the most significant information when it comes to measurements of $\sin^2 \theta_{13}$, $\sin^2 \theta_{23}$, $\Delta m^2_{13}$ (including the sign), and $\delta_{CP}$. We do, however, include results from solar data and from the KamLAND experiment when it comes to constraining the solar parameters $\Delta m^2_{12}$ and $\theta_{12}$. The reason for this is that DUNE’s ability to, in isolation, determine the solar parameters is rather limited. To illustrate this fact, we perform a DUNE-only fit to the DUNE data. The results for a subset of the three-neutrino oscillation parameters ($\Delta m^2_{12}$, $\tan^2 \theta_{12}$, $\delta_{CP}$) are depicted in Fig. A.2.

While DUNE is not very sensitive to $\tan^2 \theta_{12}$ or $\Delta m^2_{12}$ (note the logarithmic scales), it can exclude nonzero values for each parameter, and is still able to observe $CP$-invariance violation and measure $\delta_{CP}$ even if external information on the solar parameters is not included in the data analysis. The uncertainty on $\delta_{CP}$, as expected, is significantly larger (cf. Fig. A.1).

Finally, we repeat the analysis discussed in Sec. 4.3.3, where appearance and disappearance channels are analyzed independently, this time assuming the data are consistent with the three-neutrino scenario. Fig. A.3 depicts the results. As in Sec. 4.3.3 we see that the appearance channel is sensitive to the product $\sin^2 \theta_{13} \sin^2 \theta_{23}$ while the disappearance
Figure A.1. Expected sensitivity contours at 68.3% (blue), 95% (orange), and 99% (red) CL as measured by DUNE with six years of data collection (3y $\nu + 3y \bar{\nu}$), a 34 kiloton detector, and a 1.2 MW beam given a three-neutrino scenario. On the far-right, one-dimensional $\Delta \chi^2$ plots for each parameter display the 68.3% (blue), 95% (orange), and 99% (red) CL bounds. Quoted measurement bounds are for 68.3% CL. Mixing angles here are $\sin^2 \theta_{12} = 0.308$, $\sin^2 \theta_{13} = 0.023$, and $\sin^2 \theta_{23} = 0.437$. Results from solar neutrino experiments are included here as Gaussian priors for the values of $|U_{e2}|^2 = 0.301 \pm 0.015$ and $\Delta m^2_{12} = (7.54 \pm 0.24) \times 10^{-5} \text{eV}^2$. This scenario assumes the normal hierarchy, i.e. $\Delta m^2_{13} = +2.43 \times 10^{-3} \text{eV}^2$, and that $\delta_{CP} = \pi/3$. 

### 3 years $\nu + \bar{\nu}$

- $\Delta m^2_{12} = (7.540 \pm 0.240) \times 10^{-5} \text{eV}^2$
- $\Delta m^2_{13} = 2.430 \times 10^{-3} \text{eV}^2$
- $\sin^2 \theta_{12} = 0.308$
- $\sin^2 \theta_{13} = 0.023$
- $\sin^2 \theta_{23} = 0.437$
- $\delta_{CP} = 1.047$
- $|U_{e2}|^2 = 0.301 \pm 0.015$
channel is mostly sensitive to $|U_{e3}|^2(1 - |U_{\mu 3}|^2)$. Unlike the scenario discussed in Sec. 4.3.3 (see Fig. 4.7), here the fits to the different data sets are in agreement.

### A.2. Four-Neutrino Fits to Four-Neutrino Data

Here we display the full results we obtain when analyzing the different four-neutrino scenarios (see Table 4.1) assuming the four-neutrino hypothesis. Figs. A.4, A.5, and A.6 depict the expected sensitivity contours at 68.3% (blue), 95% (orange), and 99% (red)
Figure A.3. Expected sensitivity contours at 68.3%, 95%, and 99% for neutrino and antineutrino appearance channels (blue, orange, red) vs. neutrino and antineutrino disappearance channels (green, teal, blue) in the \( \sin^2 \theta_{13} \) - \( \sin^2 \theta_{23} \) plane assuming a three neutrino hypothesis with parameters from Ref. [1], indicated with a star in the figure.

CL at DUNE with six years of data collection (3y \( \nu \) + 3y \( \bar{\nu} \)), a 34 kiloton detector, and a 1.2 MW beam, given the existence of a fourth neutrino with parameters from Case 1, Case 2, and Case 3 in Table 4.1, respectively. Results from solar neutrino experiments are included here as Gaussian priors for the values of \( |U_{e2}|^2 = 0.301 \pm 0.015 \) and \( \Delta m^2_{12} = 7.54 \pm 0.24 \times 10^{-5} \text{ eV}^2 \) [1]. Distributions are sampled using a Markov Chain Monte Carlo (MCMC) method [131]. These results are discussed in Sec. 4.3.2.
3 years $\nu + \bar{\nu}$

$\Delta m^2_{12} = (7.540 \pm 0.240) \times 10^{-5} \text{ eV}^2$

$\Delta m^2_{34} = 2.430 \times 10^{-3} \text{ eV}^2$

$\Delta m^2_{14} = 0.930 \text{ eV}^2$

$\sin^2 \phi_{12} = 0.315$

$\sin^2 \phi_{13} = 0.024$

$\sin^2 \phi_{23} = 0.456$

$\sin^2 \phi_{34} = 0.002$

$\sin^2 \phi_{45} = 0.003$

$\eta_1 = \pi/3$

$\eta_2 = -\pi/4$

$|U_{e2}|^2 = 0.301 \pm 0.015$

$|U_{\mu2}|^2 = 0.280 \pm 0.003$

$\theta_{12} = 34.2 \pm 0.6^\circ$

$\theta_{13} = 25.3 \pm 0.8^\circ$

$\theta_{23} = 59.5 \pm 0.3^\circ$

$\theta_{14} = 11.69 \pm 0.29^\circ$

$\Delta m^2_{23} = 2.430 \times 10^{-3} \text{ eV}^2$

$\Delta m^2_{34} = 7.540 \pm 0.240 \times 10^{-5} \text{ eV}^2$

Figure A.4. Expected sensitivity contours at 68.3% (blue), 95% (orange), and 99% (red) CL at DUNE with six years of data collection ($3\nu + 3\bar{\nu}$), a 34 kiloton detector, and a 1.2 MW beam given the existence of a fourth neutrino with parameters from Case 1 in Table 4.1. On the far right, one-dimensional $\Delta \chi^2$ plots for each parameter display 68.3% (blue), 95% (orange), and 99% (red) CL bounds. Quoted measurement bounds are for 68.3% CL. Results from solar neutrino experiments are included here as Gaussian priors for the values of $|U_{e2}|^2 = 0.301 \pm 0.015$ and $\Delta m^2_{12} = 7.54 \pm 0.24 \times 10^{-5} \text{ eV}^2$ [1].
3 years $\nu + \bar{\nu}$

$\Delta m_{12}^2 = (7.540 \pm 0.240) \times 10^{-5}$ eV$^2$

$\Delta m_{13}^2 = 2.430 \times 10^{-3}$ eV$^2$

$\Delta m_{14}^2 = 10^{-2}$ eV$^2$

$\sin^2 \theta_{12} = 0.315$

$\sin^2 \theta_{13} = 0.024$

$\sin^2 \theta_{23} = 0.456$

$\sin^2 \theta_{14} = 0.022$

$\sin^2 \phi_{34} = 0.030$

$\eta_3 = \pi/3$

$\eta_4 = -\pi/4$

$|U_{e2}|^2 = 0.301 \pm 0.015$

Figure A.5. Expected sensitivity contours at 68.3% (blue), 95% (orange), and 99% (red) CL at DUNE with six years of data collection (3y $\nu + 3y \bar{\nu}$), a 34 kiloton detector, and a 1.2 MW beam given the existence of a fourth neutrino with parameters from Case 2 in Table 4.1. On the far right, one-dimensional $\Delta \chi^2$ plots for each parameter display 68.3% (blue), 95% (orange), and 99% (red) CL bounds. Quoted measurement bounds are for 68.3% CL. Results from solar neutrino experiments are included here as Gaussian priors for the values of $|U_{e2}|^2 = 0.301 \pm 0.015$ and $\Delta m_{12}^2 = 7.54 \pm 0.24 \times 10^{-5}$ eV$^2$ [II].
3 years $\nu + \bar{\nu}$

$\Delta m^2_{12} = (7.54 \pm 0.24) \times 10^{-5}$ eV$^2$

$\Delta m^2_{13} = 2.43 \times 10^{-3}$ eV$^2$

$\Delta m^2_{14} = 10^{-5}$ eV$^2$

$\sin^2 \theta_{12} = 0.321$

$\sin^2 \theta_{13} = 0.024$

$\sin^2 \theta_{23} = 0.659$

$\sin^2 \theta_{14} = 0.040$

$\sin^2 \theta_{24} = 0.326$

$\eta_1 = \pi/3$

$\eta_2 = -\pi/4$

$|U_{e2}|^2 = 0.301 \pm 0.015$

Figure A.6. Expected sensitivity contours at 68.3% (blue), 95% (orange), and 99% (red) CL at DUNE with six years of data collection (3y $\nu + 3y \bar{\nu}$), a 34 kiloton detector, and a 1.2 MW beam given the existence of a fourth neutrino with parameters from Case 3 in Table 1.1. On the far right, one-dimensional $\Delta \chi^2$ plots for each parameter display 68.3% (blue), 95% (orange), and 99% (red) CL bounds. Quoted measurement bounds are for 68.3% CL. Results from solar neutrino experiments are included here as Gaussian priors for the values of $|U_{e2}|^2 = 0.301 \pm 0.015$ and $\Delta m^2_{12} = 7.54 \pm 0.24 \times 10^{-5}$ eV$^2$ [1].
B.1. An Explicit New Physics Scenario

Here we outline an ultraviolet-complete scenario of new physics in order to illustrate how the effective operators of Tables 7.1–7.5 might arise, as well as to illustrate the procedure for estimating the contributions of such operators to the LNV phenomena of interest.

Concretely, we add two scalar fields, \( \rho \) and \( \Phi \), to the SM particle content. Their charges under the SM gauge group are

\[
\rho \sim (3, 1)_{-1/3}, \quad \Phi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \sim (3, 2)_{1/6},
\]

where the notation indicates in parentheses the \( SU(3)_c \) and \( SU(2)_L \) representations, followed by the hypercharges.

In addition to the standard kinetic and mass terms for \( \rho \) and \( \Phi \), the symmetries of the SM allow for the following interactions:

\[
\Delta \mathcal{L} = -\mu \rho (\Phi^\dagger H) - \lambda_1^\alpha \rho^\dagger (L^c_\alpha Q) - \lambda_2^\beta (\Phi L_\beta) d^c - \kappa^\alpha \rho e^c c^c + h.c. ,
\]
where, as before, parentheses denote fields whose $SU(2)_L$ indices have been contracted, and $\alpha, \beta$ are lepton-flavor indices; all other indices have been suppressed. We continue to assume that the new physics is independent of quark flavor.

Integrating out $\rho$ and $\Phi$ using Eq. (B.1.2) induces a tree-level contribution to the operator $O_{3b}$. Explicitly,

\[(B.1.3)\]

\[O_{3b} = \frac{g_{\alpha\beta}}{\Lambda^3} (L^\alpha Q) (L^\beta H) d^c,\]

where

\[(B.1.4)\]

\[\frac{g_{\alpha\beta}}{\Lambda^3} = \frac{\lambda_1^\alpha \lambda_2^\beta \mu}{M^4}.\]

Here $M$ are the masses of $\rho$ and $\Phi$, which we assume are identical for simplicity. Choosing the largest $g_{\alpha\beta} = 1$, as discussed in the text, Eq. (B.1.4) is the definition of the effective scale $\Lambda$ associated to the effective operator $O_{3b}$ while $g_{\alpha\beta} \propto \lambda_1^\alpha \lambda_2^\beta$. If $\mu \sim M$ – which one may argue is a reasonable criterion, from the point of view of naturalness – then $\Lambda \sim M$ if $\lambda_1, \lambda_2 \sim 1$. As is well known, if, for example, the new physics is very weakly coupled ($\lambda_1, \lambda_2 \ll 1$) the masses of the new degrees of freedom are much lighter than the effective scale of the operator that describes the low-energy consequences of the new physics.

At low energies, integrating out $\rho$ and $\Phi$ also leads to $O_8$, its coefficient proportional to $\kappa^\alpha \lambda_2^\beta$. However, assuming $\lambda_1^\alpha \sim \kappa^\alpha$, the contributions of $O_{3b}$ to LNV phenomena overwhelm those from $O_8$ – see Table 7.2. For this reason, we restrict our remaining discussions to $\kappa^\alpha = 0$, for simplicity and clarity.
Fig. B.1(a) depicts the tree-level contribution to $0\nu\beta\beta$ within this model, and Fig. B.1(b) depicts the one-loop contribution. While the contribution from Fig. B.1(a) is already captured by Eq. (B.1.4), after integrating out the heavy scalars (note that we refer to $\varphi_2$ in the diagram, as we are interested in the broken phase), we must execute a loop integral in order to determine the contribution of Fig. B.1(b). This contribution is finite and, assuming a vanishing down-quark mass, is given by

$$
(B.1.5) \quad \lambda_1^e \lambda_2^e \int \frac{d^4p}{(2\pi)^4} \frac{\mu \times \phi\phi}{(p^2 - M^2)^2 \cdot p^2 \cdot p^2} = \frac{(-i)\lambda_1^e \lambda_2^e \mu}{(4\pi)^2 M^2} \sim \frac{1}{A^3} \left(\frac{-iA^2}{16\pi^2}\right),
$$
where in the last step we assume $\mu \sim M \sim \Lambda$ and $\lambda_1^e, \lambda_2^e \sim 1$. The familiar factor $\Lambda^2/16\pi^2$ is directly related to the prescription described in Eq. (7.4.2). There are more detailed discussions of the validity of this prescription, including concrete examples, in Refs. [5, 6].

An in-depth analysis of this model is well beyond the scope of this work; instead, we outline some simple phenomenological considerations. The potential of the new scalars must be such that neither acquires a vacuum expectation value, or else $SU(3)_c$ gauge invariance would be spontaneously broken. Moreover, they must be sufficiently heavy in order to elude searches for new heavy colored states at the Large Hadron Collider (LHC) and in order to bypass severe constraints from flavor observables. From Table 7.2, $\Lambda \gtrsim O(10^7)$ TeV is required if the physics responsible for $O_3$ is directly related to the observed neutrino masses. This means that, assuming $M \sim \Lambda$, the new degrees of freedom are heavy enough that collider or flavor constraints are easily satisfied.

It is easy to check that Eq. (B.1.2) conserves baryon-number (both $\rho$ and $\Phi$ can be assigned baryon-number $+1/3$) so there are no constraints from proton decay or other baryon-number-violating phenomena. On the other hand, Eq. (B.1.2) violates lepton-number – indeed, it was designed to do just that – but does so only if all three new-physics couplings $\lambda_1$, $\lambda_2$, and $\mu$ are nonzero. This implies that LNV observables are, necessarily, proportional to the product $\lambda_1 \lambda_2 \mu$ and that nonzero Majorana neutrino masses occur only at the one-loop level.

\footnote{$\rho$ or $\Phi$ exchange potentially mediate, at the tree-level, $\mu^- \to e^-$ conversion in nuclei.}