Instructor: Kevin Beach

* please read the syllabus (in class handout + online pdf)
* regularly visit the <u>class website</u> (http://www.phy.olemiss.edu/~kbeach/courses) for lectures and assignments

<u>Condensed Matter</u>

* somewhat broader than "solid state"
  → includes regular and amorphous solids
  liquid crystals
  glasses
  superfluids
  ⋮
  any many-particle system more complicated than a conventional gas

* domain of physics that deals with <u>agglomerations</u> of matter whose properties are determined on length (Å) and energy scales (eV) typical of most chemical and biological processes

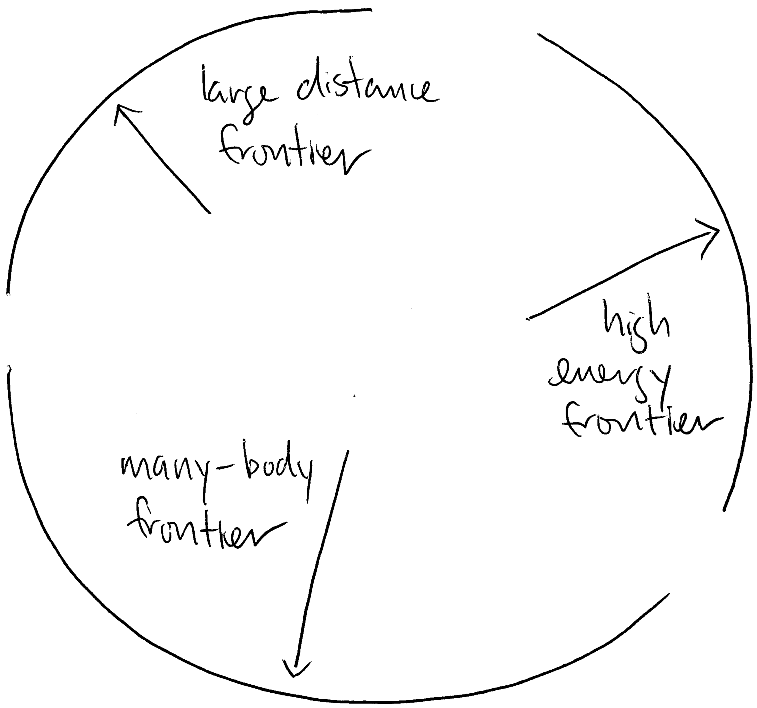
Physics Frontiers

e.g. Cosmology

- determine the structure of space-time and the nature of gravity

e.g. Particle physics

- search for fundamental laws and correct zoology of particles



e.g. Condensed matter

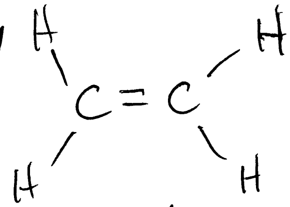
- all physical laws are <u>known</u>
- try to understand the behaviour of many interacting particles (in a material environment)
- concerned with ordered phases of matter and transitions between phases
- low-energy effective theories are the main conceptual tool: think in terms of ordered ground state + low-lying excitations
- search for new <u>emergent</u> phenomena (non-obvious from the microscopic model)

- good and marginal Fermi Liquids
- superconductors
- Mott insulators + quantum magnets
- heavy fermions / Kondo effect
- integer + fractional quantum Hall systems

Energy scales

Energy

- 10^{19} GeV Planck scale
- ~150 GeV expected Higgs mass
- ~100 GeV electroweak scale
- GeV — 0.938 GeV proton rest mass
- 100 MeV QCD strong interactions
- 22 MeV binding energy of deuterium nucleus
- 14 MeV energy of neutron produced in deuterium/tritium fusion: $^2H + ^3H \rightarrow ^4He + n$
- MeV — ~1 MeV energy of a single bacterium to replicate
- 0.12 MeV energy to completely ionize a uranium atom
- keV — 8 keV x-rays with a wavelength on the order of atomic spacing (~1.5 Å)
- 13.6 eV (Rydberg) energy to ionize hydrogen
- 8.8 eV triple covalent bond in acetylene H−C≡C−H
- 6.6 eV double covalent bond in ethylene



- 2-5 eV typical single covalent bond between carbon atoms

string theory

particle physics

nuclear physics

atomic physics

condensed matter

chemistry

400 GeV

LHC energy range

1 GeV

chemistry

condensed matter

eV — 1.1 eV silicon band gap

0.17–0.3 eV ionic bond

0.2 eV hydrogen bond

1–200 meV magnetic exchange energy

44 meV van der Waals bond

26 meV average energy associated with rotation of a diatomic molecule in a gas at room tem

meV — ~ 1 meV Cooper pair energy in a conventional superconductor

Practical units

$$1\,\text{Å} = 0.1\ \text{nm} = 10^{-10}\ \text{m}$$

$$1\ \text{eV} = 1.602 \times 10^{-19}\ \text{J}$$

$$k_B T_{room} = k_B (300\ \text{K}) = 0.02585\ \text{eV}$$

$$\frac{e^2}{4\pi\varepsilon_0} = 14.4\ \text{eV}\cdot\text{Å}$$

visible spectrum

THz

789	666	606	526	508	484	400
violet	blue	green	yellow	orange	red	
380	450	495	570	590	620	750

nm

3.26 eV photon

1.65 eV photon

Conversion factors

$1\ eV = k_B \cdot (11{,}605\ K)$

$k_B = 8.617 \times 10^{-5}\ eV \cdot K^{-1}$

$\hbar = 6.582 \times 10^{-16}\ eV \cdot s$

$hc = 1{,}240\ eV \cdot nm = 12{,}400\ eV \cdot \text{Å}$

* Consider the example of metallic copper
  → all the action is in the (outer-shell) valence electrons

$$Cu : [Ar]\, 3d^{10}\, 4s^1$$

→ energies around a few eV; low with respect to atomic physics

[Energy]	thermal $k_B[\text{Temp}]$	optical $h[\text{Freq}]$, $hc/[\text{Length}]$	coulomb $\frac{e^2}{4\pi\varepsilon_0 [\text{Length}]}$
0.11 eV	1357 K melting temp of copper crystal		
~2 eV		525 THz, 5711 Å yellow/orange color of copper	
~5 eV			3 Å length of the Cu–Cu bond

Review of quantum mechanics

* mostly interested in the non-relativistic description of electrons moving in a background ionic potential

* single quantum particle described by a wavefunction $\psi(\vec{r},t)$
  - → function of its real-space position and time
  - → complex-value probability amplitude
  - → $|\psi(\vec{r},t)|^2$ corresponds to the measured classical probability

* evolution of the w.f. proceeds according to the time-dependent Schrödinger equation (TDSE)

$$i\hbar \frac{\partial}{\partial t}\psi = H\psi = \Big(\underbrace{-\frac{\hbar^2\nabla^2}{2m}}_{\text{kinetic energy operator}} + \underbrace{U(\vec{r})}_{\text{external "one-body" potential}} \Big)\psi(\vec{r},t)$$

* well-defined particle must satisfy a normalization condition

$$\int_{\text{physical volume}} d^3r \; |\psi(\vec{r},t)|^2 = 1 \quad \text{for all } t$$

* the corresponding requirement in each infinitesimal volume d^3r is a local conservation law

$$\frac{dn}{dt} = \mathrm{div}\, J$$

where $n = |\psi|^2$ is a probability density and J is a probability current.

→ explicitly,

$$\frac{\partial|\psi|^2}{\partial t} = \frac{\partial\psi^*}{\partial t}\cdot\psi + \psi^*\frac{\partial\psi}{\partial t}$$

$$= (i\hbar H\psi)^* + \psi^*(i\hbar H\psi)$$

$$= -i\hbar\left(-\frac{\hbar^2\nabla^2\psi^*}{2m} + U\psi^*\right)\psi + i\hbar\psi^*\left(-\frac{\hbar^2\nabla^2\psi}{2m} + U\psi\right)$$

$$= \frac{\hbar}{2mi}\left[\psi^*\nabla^2\psi - (\nabla^2\psi^*)\psi\right] + \cancel{i\hbar U|\psi|^2} - \cancel{i\hbar U|\psi|^2}$$

$$= \vec{\nabla}\cdot\vec{J} \quad \text{where } \vec{J} = \frac{\hbar}{2mi}\left[\psi^*\vec{\nabla}\psi - (\vec{\nabla}\psi^*)\psi\right]$$

* Some observations:

→ the actual flow of the particle has no <u>explicit</u> dependence on the potential $U(\vec{r})$

→ real-valued wavefunctions (usually corresponding to stationary bound states) have no net current

* free propagation corresponds to a plane wave $\psi(\vec{r},t) \sim e^{i(\vec{k}\cdot\vec{r}-\omega t)}$

$$\vec{J}[\psi] \approx \frac{\hbar}{2mi}\left[e^{-i\vec{k}\cdot\vec{r}}\, i\vec{k}\, e^{i\vec{k}\cdot\vec{r}} - (-i\vec{k}\cdot\vec{r})\, e^{-i\vec{k}\cdot\vec{r}}\, e^{i\vec{k}\cdot\vec{r}}\right] = \frac{\hbar\vec{k}}{m}$$

→ has units of velocity
since $\vec{p} = \hbar\vec{k}$ is the momentum
$\left(\vec{p}\, e^{i\vec{k}\cdot\vec{r}} = \frac{\hbar}{i}\vec{\nabla} e^{i\vec{k}\cdot\vec{r}} = \hbar\vec{k}\, e^{i\vec{k}\cdot\vec{r}}\right)$

→ becomes a pure rate if we include the $(\text{volume})^{-1/3}$ normalization factor for the plane wave

* for a general w.f. $\psi(\vec{r},t) = \underbrace{\psi_0(\vec{r},t)}_{\text{real-valued amplitude}} \underbrace{e^{i\theta(\vec{r},t)}}_{\text{phase factor}}$

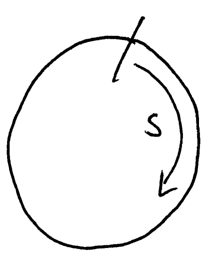
$$\to \psi^* \nabla \psi - (\nabla \psi^*)\psi = \psi_0^2 e^{-i\theta}\left[\cancel{(\vec{\nabla}\psi_0)} e^{i\theta} + i\psi_0(\vec{\nabla}\theta)e^{i\theta}\right]$$
$$- \psi_0^2\left[\cancel{(\vec{\nabla}\psi_0)} e^{-i\theta} - i\psi_0(\vec{\nabla}\theta)e^{-i\theta}\right]e^{i\theta}$$
$$= 2i\psi_0^2 \vec{\nabla}\theta$$

→ probability current $J[\psi] = \frac{\hbar\psi_0^2}{m}\vec{\nabla}\theta$ flows in the direction of the phase gradient

→ physical charge current $J_Q = +e\frac{\hbar\psi_0^2}{m}\vec{\nabla}\theta$

→ this means that we can <u>induce</u> an electrical current by imposing a phase twist across the sample

e.g. ring of length L (boundary-free system with a nontrivial topology) carrying a persistent current



$\psi_n(s) = \psi_0 e^{i2\pi n s/L}$ is required by continuity alone: $\psi(0) = \psi(L)$

The overall amplitude is set by the normalization

$$\int_0^L ds\, |\psi|^2 = \psi_0^2 L = 1$$

hence, we get a set of current-carrying states

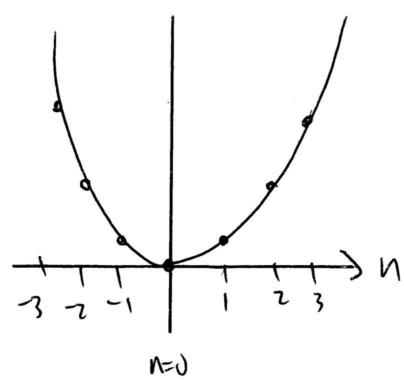
$$\psi_n(s) = \frac{1}{\sqrt{L}} e^{i2\pi n s/L} \quad \text{for integer } n$$

and a corresponding charge current

$$J_{Q,n} = + \frac{e\hbar}{mL} \cdot \frac{2\pi n}{L} = \frac{he}{mL^2} \times \text{integer}$$

discrete set of allowed current values with this common spacing; continuous variations in the current are only possible for a macroscopic ($L \to \infty$) wire

For a Hamiltonian with kinetic energy alone $\left(H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial s^2}\right)$ the quantized energy levels are $E_n = \frac{hn^2}{2mL^2}$

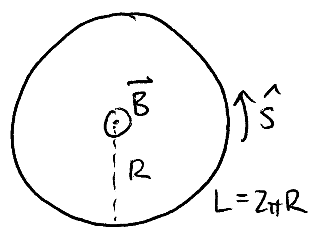


* currents are driven by the electromagnetic field
  - → usually specify a static, semiclassical vector potential $\vec{A}$ (the field itself has no dynamics, and we haven't quantized it into its photon modes)
  - → work with minimal coupling in the "velocity gauge"

$$H = -\frac{\hbar^2 \nabla^2}{2m} + U = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla}\right)^2 + U = \frac{1}{2m}p^2 + U$$

becomes $\frac{1}{2m}(\vec{p} - e\vec{A})^2 = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} - e\vec{A}\right)^2$

e.g. back to the ring ...



$$\vec{A} = \frac{\Phi}{2\pi R}\hat{s} = \frac{\Phi}{L}$$

$$\text{Flux } \Phi = \int_{\text{Ring}} \vec{B}\cdot d(\text{Area}) = \int_{\text{circumference}} \vec{A}\cdot d(\text{line})$$

$$H\psi_n = \frac{1}{2m}\left(\frac{hn}{L} - eA\right)^2 \psi_n$$

leads to energy levels $E_n = \frac{1}{2m}\left(\frac{hn}{L} - eA\right)^2 = \frac{h^2}{2mL^2}\left(n - \frac{\Phi}{\Phi_0}\right)^2$

where $\Phi_0 = \frac{h}{e}$ is a unit of flux

The current is now $J[\psi] = \frac{\hbar}{2mi}(\psi^* \nabla\psi - \psi\nabla\psi^*) + \frac{e}{m}\vec{A}|\psi|^2$

or $J_\phi = \frac{he}{mL^2} \times n + \frac{e^2}{m}A|\psi|^2 = \frac{he}{mL^2}\left(n + \frac{\Phi}{\Phi_0}\right)$

* For free particles, $U(\vec{r}) = U_0 = \text{const}$, there is a continuum of states and an arbitrary wave packet is given by the Fourier transform

$$\psi(r,t) = \int \frac{d^3k}{(2\pi)^3} \tilde{\psi}_k \, e^{i(\vec{k}\cdot\vec{r} - E_k t/\hbar)}$$

Here, the TDSE imposes a dispersion relation

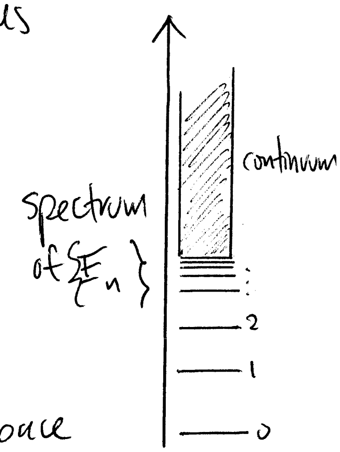
$$\hbar\omega \rightarrow E_k = \frac{\hbar^2 k^2}{2m} + U_0$$

* For a particle in an arbitrary potential,

$$\psi(\vec{r},t) = \sum_n \tilde{\psi}_n \, \phi_n(r) \, e^{-iE_n t/\hbar}$$

↑ sum over continuum and any discrete bound states

→ Here, $\{\phi_n(\vec{r})\}$ is a complete set of eigenstates satisfying the eigen-equation $H\phi_n = E_n \phi_n$



→ coefficients $\tilde{\psi}_n$ fixed at time zero

$$\tilde{\psi}_n = \int d^3r \, \phi_n^*(\vec{r}) \, \psi(\vec{r}, t=0)$$

$$= \int d^3r \, \langle r|\phi_n\rangle^* \langle r|\psi\rangle$$ ← view w.f. as real-space representation of some state vector

$$= \int d^3r \langle \phi_n | r\rangle\langle r|\psi\rangle$$

$$= \langle \phi_n | \left(\int d^3r \, |r\rangle\langle r| \right) |\psi\rangle$$

$$= \langle \phi_n | \psi \rangle$$

↑ representation of unity (completeness relation on $\vec{r}$)

→ full time evolution given by

$$\psi(\vec{r},t) = \underbrace{e^{-iHt/\hbar}}_{\text{evolution operator}} \psi(r, t=0)$$

which is the formal solution to $i\hbar \frac{\partial \psi}{\partial t} = H\psi$

Abstract state vectors

* we'll sometimes want to use "bra" and "ket" notion to denote state vectors living in a Hilbert space appropriate to the problem
* view wavefunction as an overlap

$$\psi(r,t) = \langle r | \psi(t) \rangle = \langle r | e^{-i\hat{H}t/\hbar} | \psi(t=0) \rangle$$

we've added a "hat" to indicate that the Hamiltonian is an abstract operator acting on $|\psi(t)\rangle$ (and no longer a differential operator)

* Hence $|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(t=0)\rangle$

$$= e^{-i\hat{H}t/\hbar} \left(\sum_n |\phi_n\rangle\langle\phi_n| \right) |\psi(t=0)\rangle$$

insert complete, orthonormal set of eigenstates: $\langle\phi_n|\phi_{n'}\rangle = \delta_{nn'}$

$$= e^{-i\hat{H}t/\hbar} \sum_n \tilde{\psi}_n |\phi_n\rangle$$

$$= \sum_n \tilde{\psi}_n e^{-iE_n t/\hbar} |\phi_n\rangle$$

* For a basis $\{|\alpha\rangle\}$ that is not orthonormal, it is still the case that each eigenstate has an expansion

$$|\phi_n\rangle = \sum_\alpha \tilde{\phi}_\alpha^{(n)} |\alpha\rangle$$

→ the eigenequation $\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$ has a matrix form

$$\sum_\beta \langle\alpha|\hat{H}|\beta\rangle \tilde{\phi}_\beta^{(n)} = E_n \sum_\beta \langle\alpha|\beta\rangle \tilde{\phi}_\beta^{(n)}$$

which we understand as a generalized eigenvalue problem

$$H\phi^{(n)} = E^{(n)} S \phi^{(n)}$$

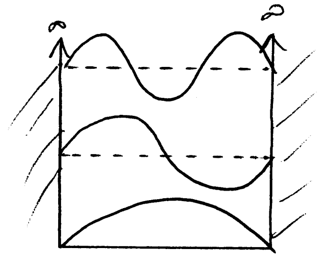
hamiltonian matrix elements

matrix of overlaps with off-diagonal entries

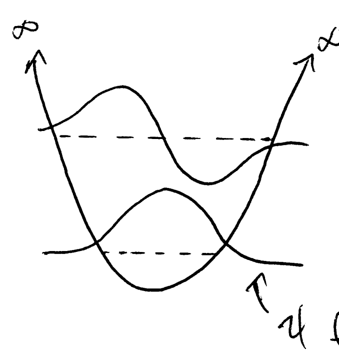
Electron bound to an ion

* infinitely high potentials give localized states with a discrete spectrum

e.g. particle in a box



ψ vanishes everywhere outside the box



ψ falls off exponential fast beyond the classical turning points

* the Coulomb potential $U(r) = -\frac{Ze^2}{r}$ is infinitely deep at $r=0$, but it never exceeds $U=0$.

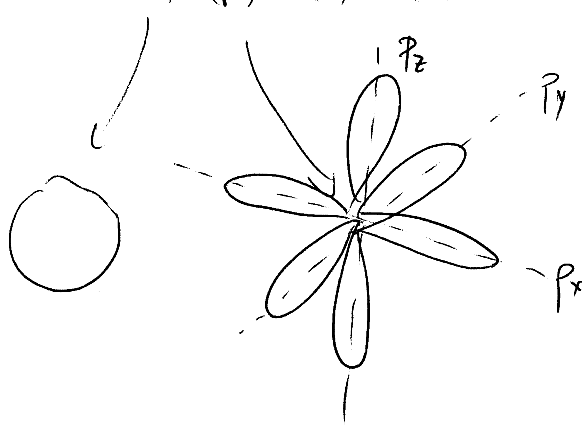
* effective Hamitonian in radial coordinates

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)R + \frac{2\mu}{\hbar^2}\left[E + \frac{Ze^2}{r} - \frac{l(l+1)\hbar^2}{2\mu r^2}\right]R = 0$$

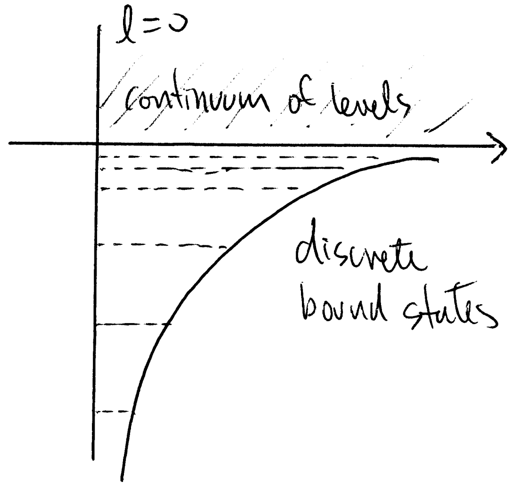
→ separation of variables $\psi(\vec{r}) = \psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$

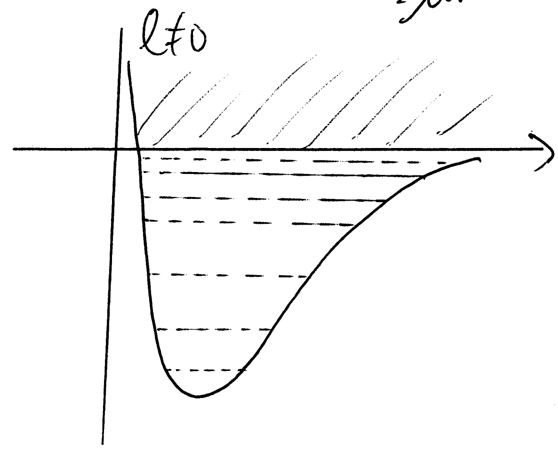
→ μ is the reduced mass of electron and nucleus

→ $l = 0, 1, 2, 3, \ldots$ is an angular momentum quantum number
(s) (p) (d) (f)



→ electron sees a radial potential $-\frac{Ze^2}{r} + \frac{l(l+1)\hbar^2}{2\mu r^2}$





Many-particle states

* generalize w.f. to N variables $\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$ with a Hamiltonian

$$H = \sum_{i=1}^{N} \left(-\frac{\hbar^2 \nabla_i}{2m_i} + U(\vec{r}_i) \right) + \sum_{i<j} V(\vec{r}_i, \vec{r}_j) + \text{three and higher body terms}$$

* requires imposition of particle "statistics", by which we mean their parity under interchange

$$\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{i-1}, \vec{r}_{i+1}, \vec{r}_i, \vec{r}_{i+2}, \ldots, \vec{r}_N, t) = \psi(\vec{r}_1, \ldots, \vec{r}_N)$$

if particles i and $i+1$ are bosons

$$= -\psi$$

if they are fermions

* for systems of all one species, we can write the w.f. as a <u>Slater determinant</u> (or <u>permanent</u>)

$$\psi(\vec{r}_1, \ldots, \vec{r}_N) = \frac{1}{\sqrt{N!}} \sum_P (\mp)^P \phi_a(\vec{r}_{P_1}) \phi_b(\vec{r}_{P_2}) \cdots \phi_w(\vec{r}_{P_N})$$

Sum over all N! permutations on N elements

Sign of the permutation appears for <u>fermions</u>

$$= \begin{vmatrix} \phi_a(\vec{r}_1) & \phi_b(\vec{r}_1) & \cdots & \phi_w(\vec{r}_1) \\ \phi_a(\vec{r}_2) & \phi_b(\vec{r}_2) & \cdots & \phi_w(\vec{r}_2) \\ \vdots & & & \\ \phi_a(\vec{r}_N) & \phi_b(\vec{r}_N) & \cdots & \phi_w(\vec{r}_N) \end{vmatrix}_{\mp}$$

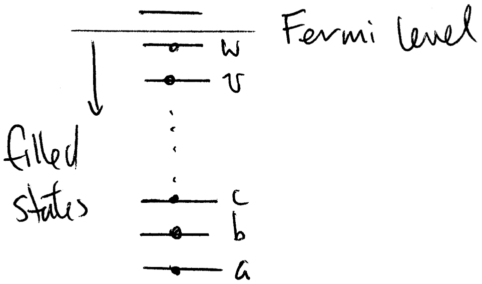
* fermionic w.f. vanishes if any of the labels $a, b, c, \ldots, w$ are duplicated

  → implies that no two particles can be in the same quantum state (Pauli exclusion) e.g. $\psi(r_1, r_2) = \frac{1}{\sqrt{2}}[\phi_a(r_1)\phi_b(r_2) - \phi_b(r_1)\phi_a(r_2)]$ $= 0$ if $a = b$

* In terms of single-particle levels $H\phi_a = E_a \phi_a$, the Hamiltonian of a non-interacting many-body system is

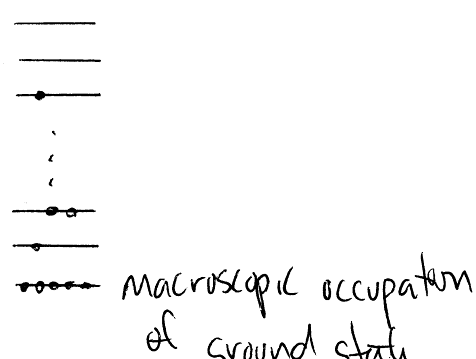
$$H\psi = (E_a + E_b + \cdots + E_w)\psi$$

fermions



→ energy of uppermost filled fermionic state sets a new energy scale

bosons



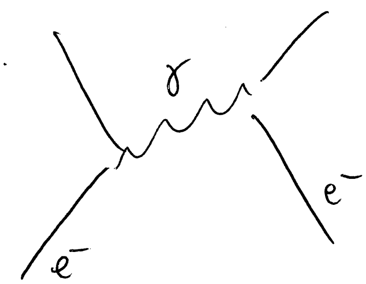
→ possible to achieve condensation of all bosons into a single level

* particles in the condensed matter context ...

fermions: electrons, protons, ^{3}He

bosons: composite objects involving an even number of bound fermions (^{4}He)

* some bosons are not conserved; these are excitations that mediate interactions and can be created and destroyed



e.g. emission and absorption of a photon

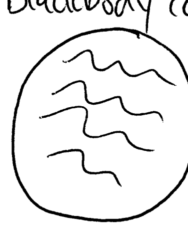
→ these don't condense at $T=0$

container

^{4}He
fixed number

macroscopic occupation of ground state as $T \to 0$

blackbody cavity



photons → 0 as $T \to 0$