Quantum mechanics of a collection of mutually interacting, nonrelativistic particles

- Wave function \( \Psi (\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N, t) \)

- Probability amplitude

- Coordinates positions of the N particles

- Global time clock

- Governed by the Schrödinger equation

\[
\left\{ -\frac{\hbar^2}{2m} \sum_{j=1}^{N} \nabla_j^2 + \sum_{j<j'} \mathcal{V}(\vec{r}_j - \vec{r}_{j'}) + \sum_{j} \mathcal{U}(\vec{r}_j) \right\} \Psi
\]

- Hamiltonian = operator expression of the total system energy

- Two-body interaction term

- "Theory of Everything"
$\rightarrow$ phase of $\Psi$ is ambiguous with respect to the classical probability $|2\Psi|^2$

$\Psi (\text{particle at A, particle at B})$

$= e^{i\theta} \Psi (\text{particle at B, particle at A})$

\[ \Rightarrow \]

phase arising from exchange

Indistinguishability implies that

\[ e^{2i\theta} = 1 \quad \text{or} \quad e^{i\theta} = \begin{cases} +1 & \text{bosons} \\ -1 & \text{fermions} \end{cases} \]
Second quantization is the key technical innovation

\[ \rightarrow \text{connection between } |\Psi(t)\rangle \text{ and } \Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N, t) \]

ket in the abstract state space \hspace{2cm} many body wavefunction

is overlap with a ket \( |\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N\rangle \) in the position representation

\[ \rightarrow \text{Suppose the existence of single-body creation operator } \hat{a}(\vec{r})^+ \text{ such that} \]

\[ |\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N\rangle = \hat{a}(\vec{r}_1)^+ \hat{a}(\vec{r}_2)^+ \ldots \hat{a}(\vec{r}_N)^+ |\text{Vac}\rangle \]

vacuum state

then

\[ \Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N, t) = \langle \text{vac} | \hat{a}(\vec{r}_1)^\dagger \ldots \hat{a}(\vec{r}_N)^\dagger | \Psi(t) \rangle \]

dual bra
Exchange statistics impose the operator algebra

\[ \Phi(\vec{r}_1, \vec{r}_2) = \langle \text{vac} | \hat{\Phi}(\vec{r}_2) \hat{\Phi}(\vec{r}_1) | \Phi \rangle \]

\[ \Phi(\vec{r}_2, \vec{r}_1) = \pm \Phi(\vec{r}_1, \vec{r}_2) \quad \vec{r}_1 \neq \vec{r}_2 \]

\[ = \pm \langle \text{vac} | \hat{\Phi}(\vec{r}_1) \hat{\Phi}(\vec{r}_2) | \Phi \rangle \]

\[ \Rightarrow \hat{\Phi}(\vec{r}_1) \hat{\Phi}(\vec{r}_2) = \pm \hat{\Phi}(\vec{r}_2) \hat{\Phi}(\vec{r}_1) \]

 Bosons commute

 Fermions anticommute

\[ \Phi(\vec{r}_2, \vec{r}_1) = - \Phi(\vec{r}_1, \vec{r}_2) \]


Pauli exclusion

\[ \Phi(\vec{r}_2, \vec{r}_1) = - \Phi(\vec{r}_1, \vec{r}_2) \]

\[ \vec{r}_2 \Rightarrow \vec{r}_1 \quad \Phi(\vec{r}_1, \vec{r}_2) = - \Phi(\vec{r}_2, \vec{r}_1) \equiv 0 \quad \text{no weight} \]
In the fermion case

\[ \hat{a}(\vec{r})^2 = \hat{a}(\vec{r}) \hat{a}(\vec{r}) = 0 \]

Schematically:

**Vacuum State**

- bosons
- fermions

**1-particle State**

- \( \hat{a}(\vec{r}_1)^+ \)
- \( \hat{a}(\vec{r}_1)^+ (\text{Vac}) \)
- \( \hat{a}(\vec{r}_2)^+ \)

**3-particle State**

- \( \hat{a}(\vec{r}_3)^+ \)
- \( \hat{a}(\vec{r}_2)^+ \)
- \( \hat{a}(\vec{r}_1)^+ \)
bosons  \[ \left( \hat{\psi}(\vec{r}_1)^\dagger \right)^2 \hat{\psi}(\vec{r}_2)^\dagger \left| \text{vac} \right> \] 

free to swap

\[ = \left( \hat{\psi}(\vec{r}_1)^\dagger \right)^2 \hat{\psi}(\vec{r}_2)^\dagger \left| \text{vac} \right> \]  (canonical ordering)

fermions

\[ \hat{\psi}(\vec{r}_1)^\dagger \hat{\psi}(\vec{r}_2)^\dagger \hat{\psi}(\vec{r}_2)^\dagger \left| \text{vac} \right> \]

\[ = - \hat{\psi}(\vec{r}_1)^\dagger \hat{\psi}(\vec{r}_2)^\dagger \hat{\psi}(\vec{r}_3)^\dagger \left| \text{vac} \right> \]

\[ \Rightarrow \hat{\psi}(\vec{r}_1)^\dagger \left( \hat{\psi}(\vec{r}_2)^\dagger \right)^2 \left| \text{vac} \right> \equiv 0 \]

& Commutation / anticommutation relations

\[ \left[ \hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}')^\dagger \right] = \hat{\psi}(\vec{r}) \hat{\psi}(\vec{r}')^\dagger + \hat{\psi}(\vec{r}')^\dagger \hat{\psi}(\vec{r}) \]

\[ = \delta(\vec{r} - \vec{r}') \]

\[ \left[ \hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}') \right] = \left[ \hat{\psi}(\vec{r})^\dagger, \hat{\psi}(\vec{r}')^\dagger \right] = 0 \]
Hamiltonian expressed in terms of field operators

\[ \hat{H} = \int d^3 r \, \hat{\psi}^\dagger(r) T(r) \hat{\psi}(r) + \frac{1}{2} \int d^3 r \, d^3 r' \, \hat{\psi}^\dagger(r) \hat{V}(r,r') \hat{\psi}(r') \hat{\psi}(r) \]

1-body kinetic energy

\[ \hat{\psi}^\dagger(r) \hat{\psi}(r) = \frac{\hbar^2 \nabla^2}{2m} \]

2-body interaction potential

\[ \hat{V}(r,r') = \text{note the ordering (encompasses fermi and bose cases)} \]

\[ = \hat{H}_0 + \hat{V} \]

→ customary to express the field operators in terms of creation/annihilation ops for the 1-body modes that satisfy the eigenvalue \[ T \hat{\phi}_k = E_k \hat{\phi}_k \]

\[ \hat{\psi}^\dagger(r) \equiv \sum_k \phi_k^* (r) \, C_k \]

\[ \hat{\psi} (r) \equiv \sum_k \phi_k (r) \, C_k^\dagger \]

\( c \) usually written \( c \) for fermions and \( a \) for bosons

(occasionally momentum or crystal wave)
\[ \rightarrow \text{the } \phi_k(\vec{r}) \text{ states form an orthonormal set, so} \]
\[ \int d^3r \; \phi_k^*(\vec{r}) \phi_{k'}(\vec{r}) = \delta_{kk'} \]

and \[ \sum_k \phi_k(\vec{r})^* \phi_k(\vec{r}') = \delta(\vec{r}-\vec{r}') \]

\( \rightarrow \text{generic, } \text{local } 1\)-body operator (bilinear in the fields) looks like

\[ \hat{\mathbf{J}} = \int d^3r \; \hat{\phi}^*(\vec{r}) \hat{J}(\vec{r}) \hat{\phi}(\vec{r}) \]

\[ = \int d^3r \; \sum_k \phi_k(\vec{r})^* C_k^+ \hat{J}(\vec{r}) \sum_{k'} \phi_{k'}(\vec{r}) C_{k'} \]

\[ = \sum_{kk'} \left\langle \sum_{k} \int d^3r \; \phi_k^*(\vec{r}) \hat{J}(\vec{r}) \phi_k(\vec{r}) \right\rangle C_k^+ C_{k'} \]

\[ = \sum_{kk'} \langle k | \hat{J} | k' \rangle C_k^+ C_{k'} \]
e.g. number-density operator

\[ \hat{n}(\vec{r}) = \hat{c}(\vec{r})^\dagger \hat{c}(\vec{r}) \]

\[ = \sum_{kk'} \phi_k(\vec{r})^\dagger \phi_{k'}(\vec{r}) \, c_k^\dagger c_{k'} \]

and the total particle number

\[ \hat{N} = \int d^3r \, \hat{n}(\vec{r}) = \sum_{kk'} \int d^3r \, \phi_k^*(\vec{r}) \phi_{k'}(\vec{r}) \, c_k^\dagger c_{k'} \]

\[ = \sum_k c_k^\dagger c_k = \sum_k \hat{n}_k^\dagger \hat{n}_k \]

\[ \hat{n}_k = c_k^\dagger c_k \] is the occupation number operator on each mode \( k \)
Example: Degenerate electron gas

→ interacting gas of negative charges in a uniformly distributed background of compensating positive charge

![Diagram of a volume with electrons]

\[ \text{Volume } V = L^3 \]

\[ \rho \text{ charge density } + eN/V \]

\[ N \text{ electrons} \]

Single-particle wave functions

\[ \phi_{k\alpha}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k} \cdot \vec{r}} \chi_{\alpha} \]

\[ \chi_{\uparrow} \text{ (spin up)} \]

\[ \chi_{\downarrow} \text{ (spin down)} \]

necessary for \( S=1/2 \) particles.
\[ \mathbf{p} = \frac{2\pi}{L} (L, L, L) \] because of periodic boundary conditions.

The Hamiltonian is sum of three terms:

\[ H = H_{el} + H_{b} + H_{el-b} \]

\[ H_{el} = \sum_{i=1}^{n} \frac{p_{i}^{2}}{2m} + \frac{1}{2} \sum_{i \neq j} e^{-\mu |\mathbf{r}_{i} - \mathbf{r}_{j}|} \] (we'll take \( \mu \to 0 \) at the end).

\[ H_{b} = \frac{1}{2} \int d^{3}r \Delta \mathbf{v} \cdot \mathbf{p}(\mathbf{r}) \mathbf{p}(\mathbf{v}') e^{-\mu |\mathbf{r} - \mathbf{v}'|} \]

\[ H_{el-b} = -D \sum_{i=1}^{n} \int d^{3}r \mathbf{p}(\mathbf{r}) e^{-\mu |\mathbf{r} - \mathbf{r}_{i}|} \]

\[ \mathbf{v} \] changes the density of background for regularization.
Background is inert (no dynamical quantum degrees of freedom)

\[ p = eN \sqrt{\frac{m}{V}} \]

\[ H = \frac{1}{2} e^2 \left( \frac{N}{V} \right)^2 \int d^3r d^3r' \, e^{-\mu (r - r')} \]

\[ = \frac{1}{2} e^2 \left( \frac{N}{V} \right)^2 \cdot V \cdot \int d^3r \, \frac{e^{-\mu r}}{V} \quad \text{(transl. invariance)} \]

\[ = \frac{1}{2} e^2 \frac{N^2}{V} \cdot \frac{4\pi}{m^2} \quad \text{(divergent as } m \to 0) \]

\[ H_{el-b} = -e^2 \sum_{i=1}^{N} \frac{N}{V} \int d^3r \, e^{-\mu (r - \vec{r}_i)} \]

\[ = -e^2 \sum_{i=1}^{N} \frac{N}{V} \int d^3r \, \frac{e^{-\mu r}}{V} \]

\[ = -e^2 \frac{N^2}{V} \frac{4\pi}{m^2} \]

Hamiltonian reduces to

\[ H = -\frac{1}{2} e^2 \frac{N^2}{V} \frac{4\pi}{m^2} + H_{el} \]
All the interesting physical effects are contained in the kinetic energy part...

\[
\langle \hat{E}_k \xi_1 | T | \hat{E}_k \xi_2 \rangle = \frac{1}{V} \int \hat{d}^3 r \ e^{-i \hat{E}_k \cdot \hat{r}} \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \\
\times e^{i \hat{E}_k \cdot \hat{r}} \xi_2 \end{array}
\]

\[
= \frac{\hbar^2 k_z^2}{2mV} \delta_{\xi_1, \xi_2} \int \hat{d}^3 r \ e^{-i (k_z - k_z') \cdot \hat{r}} \end{array}
\]

\[
= \frac{\hbar^2 k_z^2}{2m} \delta_{\xi_1, \xi_2} \delta_{k_z, k_z'}
\]

\[
\hat{T} = \sum_{k_\alpha} \frac{\hbar^2 k_\alpha^2}{2m} \frac{c^+_k c_k}{k_\alpha}
\]
potential energy part

$\langle \vec{k}_1 \alpha_1 \vec{k}_2 \alpha_2 | V | \vec{k}_3 \alpha_3 \vec{k}_4 \alpha_4 \rangle$