Part I: Non-Relativistic Quantum Many-Body Theory

2. Identical Particles: $\hat{=}$ same properties like mass, spin, charge

2.1 Distinguishable Particles:

Classical description: Lagrangian of n identical particles

$$L(\vec x_1,\dots,\vec x_n;\dot{\vec x}_1,\dots,\dot{\vec x}_n) = \sum_{\nu=1}^{n} \frac{M}{2}\dot{\vec x}_\nu^{\,2} - \underbrace{V(\vec x_1,\dots,\vec x_n)}$$

$$= \underbrace{\sum_{\nu=1}^{n} V_1(\vec x_\nu)}_{\hat{=}\ \text{external}} + \underbrace{\frac{1}{2}\sum_{\nu=1}^{n}\sum_{\mu=1}^{n} \overbrace{V_2(\vec x_\nu-\vec x_\mu)}^{=V_2(\vec x_\mu-\vec x_\nu)}}_{\hat{=}\ \text{internal}}$$

Newton's "actio = − reactio" law

Euler-Lagrange equations: $\frac{\partial L}{\partial \vec x_\nu} - \frac{d}{dt}\frac{\partial L}{\partial \dot{\vec x}_\nu} = 0 \; ; \; \nu = 1,\dots,n$

Newton equations:

$$M\ddot{\vec x}_\nu = -\frac{\partial V_1(\vec x_\nu)}{\partial \vec x_\nu} - \sum_{\mu=1}^{n}\frac{\partial V_2(\vec x_\nu-\vec x_\mu)}{\partial \vec x_\nu}$$

Transition to Hamilton mechanics: canonically conjugated momenta

$$\vec p_\nu = \frac{\partial L}{\partial \dot{\vec x}_\nu} = M\dot{\vec x}_\nu$$

Legendre transformation from Lagrangian to Hamiltonian:

$$H = \sum_{\nu=1}^{n} \vec p_\nu \dot{\vec x}_\nu - L = H(\vec p_1,\dots,\vec p_n;\vec x_1,\dots,\vec x_n)$$

$$= \sum_{\nu=1}^{n}\frac{\vec p_\nu^{\,2}}{2M} + \sum_{\nu=1}^{n} V_1(\vec x_\nu) + \frac{1}{2}\sum_{\nu=1}^{n}\sum_{\mu=1}^{n} V_2(\vec x_\nu-\vec x_\mu)$$

Hamilton equations:

$$\dot{\vec x}_\nu = \frac{\partial H}{\partial \vec p_\nu} = \frac{\vec p_\nu}{M}$$

$$\dot{\vec p}_\nu = -\frac{\partial H}{\partial \vec x_\nu} = -\frac{\partial V_1(\vec x_\nu)}{\partial \vec x_\nu} - \sum_{\mu=1}^{n}\frac{\partial V_2(\vec x_\nu-\vec x_\mu)}{\partial \vec x_\nu}$$

$\hat{=}$ Newton's equation

Transition to quantum mechanics: observables $\longrightarrow$ operators

$\vec x_\nu \longrightarrow \hat{\vec x}_\nu$, $\vec p_\nu \longrightarrow \hat{\vec p}_\nu$, $H(\vec p_1,\dots,\vec p_n;\vec x_1,\dots,\vec x_n) \longrightarrow \hat H = H(\hat{\vec p}_1,\dots,\hat{\vec p}_n;\hat{\vec x}_1,\dots,\hat{\vec x}_n)$

Canonical commutation relations $\hat{=}$ Heisenberg uncertainty relation

$$[\hat x_{j\nu},\hat x_{k\mu}]_- = [\hat p_{j\nu},\hat p_{k\mu}]_- = 0, \quad [\hat p_{j\nu},\hat x_{k\mu}]_- = \frac{\hbar}{i}\,\delta_{jk}\,\delta_{\nu\mu}$$

$[\hat A,\hat B]_- = \hat A\hat B - \hat B\hat A$ commutator

Time evolution of a state $|\psi(t)\rangle$: Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat H\,|\psi(t)\rangle$$

Spatial representation: special basis

$$\hat{\vec x}_\nu|\vec x_1,\dots,\vec x_n\rangle = \vec x_\nu|\vec x_1,\dots,\vec x_n\rangle \qquad \text{eigenvalue equation}$$

$$\langle\vec x_1,\dots,\vec x_n|\vec x'_1,\dots,\vec x'_n\rangle = \delta(\vec x_1-\vec x'_1)\cdots\delta(\vec x_n-\vec x'_n) \qquad \text{orthonormality}$$

$$\int d^3x_1\cdots\int d^3x_n\,|\vec x_1,\dots,\vec x_n\rangle\langle\vec x_1,\dots,\vec x_n| = 1 \qquad \text{completeness}$$

Jordan rule: $\langle\vec x_1,\dots,\vec x_n|\,\hat{\vec p}_\nu = \frac{\hbar}{i}\frac{\partial}{\partial\vec x_\nu}\langle\vec x_1,\dots,\vec x_n|$

wave function: expansion coefficients

$$|\psi(t)\rangle = \int d^3x_1\cdots\int d^3x_n\,\underbrace{\langle\vec x_1,\dots,\vec x_n|\psi(t)\rangle}_{=\psi(\vec x_1,\dots,\vec x_n;t)}\,|\vec x_1,\dots,\vec x_n\rangle$$

Projection: $i\hbar\frac{\partial}{\partial t}\underbrace{\langle\vec x_1,\dots,\vec x_n|\psi(t)\rangle}_{\psi(\vec x_1,\dots,\vec x_n;t)} = \underbrace{\langle\vec x_1,\dots,\vec x_n|\,\hat H}\,|\psi(t)\rangle$

$$= H\left(\frac{\hbar}{i}\frac{\partial}{\partial\vec x_1},\dots,\frac{\hbar}{i}\frac{\partial}{\partial\vec x_n};\vec x_1,\dots,\vec x_n\right)\langle\vec x_1,\dots,\vec x_n|$$

$$i\hbar\frac{\partial}{\partial t}\psi(\vec x_1,\dots,\vec x_n;t) = \hat H\,\psi(\vec x_1,\dots,\vec x_n;t)$$

$$= \sum_{\nu=1}^{n}\left\{-\frac{\hbar^2}{2M}\Delta_\nu + V_1(\vec x_\nu)\right\} + \frac{1}{2}\sum_{\nu=1}^{n}\sum_{\mu=1}^{n} V_2(\vec x_\nu-\vec x_\mu)$$

no explicit time dependence of V_1, V_2: separation ansatz

$$\psi(\vec x_1,\dots,\vec x_n,t) = \psi(\vec x_1,\dots,\vec x_n)\,e^{-\frac{i}{\hbar}Et}$$

$$\hat H\,\psi(\vec x_1,\dots,\vec x_n) = \underbrace{E}_{\text{energy eigenvalue}}\;\underbrace{\psi(\vec x_1,\dots,\vec x_n)}_{\text{energy eigenfunction}}$$

2.2 Bosons and Fermions:

identical particles $\hat{=}$ indistinguishable
$\hat{=}$ expectation values of operators do not change when the enumeration of two particles is swapped

$$\int d^3x_1 \cdots \int d^3x_n \, \Psi^*(\vec{x}_1, \dots, \vec{x}_j, \dots, \vec{x}_k, \dots, \vec{x}_n) \, \hat{A} \, \Psi(\vec{x}_1, \dots, \vec{x}_j, \dots, \vec{x}_k, \dots, \vec{x}_n)$$
$$= \int d^3x_1 \cdots \int d^3x_n \, \Psi^*(\vec{x}_1, \dots, \vec{x}_k, \dots, \vec{x}_j, \dots, \vec{x}_n) \, \hat{A} \, \Psi(\vec{x}_1, \dots, \vec{x}_k, \dots, \vec{x}_j, \dots, \vec{x}_n)$$

$\rightarrow$ characteristic properties of $\hat{A}$ and Ψ

$\hat{P}_{jk} \Psi(\vec{x}_1, \dots, \vec{x}_j, \dots, \vec{x}_k, \dots, \vec{x}_n) = \Psi(\vec{x}_1, \dots, \vec{x}_k, \dots, \vec{x}_j, \dots, \vec{x}_n)$ transposition

permutation: $\hat{P} = \prod \hat{P}_{jk}$

Note: $\hat{P}_{jk}^2 = 1$ (involutoric) $\Rightarrow$ $\hat{P}_{jk} = \hat{P}_{jk}^{-1}$

$$\hat{=} \; \langle \Psi | \hat{A} | \Psi \rangle = \langle \hat{P}_{jk} \Psi | \hat{A} | \hat{P}_{jk} \Psi \rangle = \langle \Psi | \hat{P}_{jk}^+ \hat{A} \hat{P}_{jk} | \Psi \rangle \quad (1)$$

trivial decomposition:

$$\langle \phi | \hat{A} | \Psi \rangle = \frac{1}{4} \{ \langle \phi + \Psi | \hat{A} | \phi + \Psi \rangle - \langle \phi - \Psi | \hat{A} | \phi - \Psi \rangle \quad (2)$$
$$+ i \langle \phi + i\Psi | \hat{A} | \phi + i\Psi \rangle - i \langle \phi - i\Psi | \hat{A} | \phi - i\Psi \rangle \}$$

(1) + (2): $\langle \phi | \hat{A} | \Psi \rangle = \langle \phi | \hat{P}_{jk}^+ \hat{A} \hat{P}_{jk} | \Psi \rangle$ for all $|\Psi\rangle$, $\langle \phi|$

operator identity: $\hat{A} = \hat{P}_{jk}^+ \hat{A} \hat{P}_{jk}$ (3)

special case: $\hat{A} = \hat{P}_{jk}$ $\Rightarrow$ $\hat{P}_{jk} = \hat{P}_{jk}^+ \underbrace{\hat{P}_{jk} \hat{P}_{jk}}_{=1}$ due to involutoric property $\Rightarrow$ $\hat{P}_{jk} = \hat{P}_{jk}^+$ (hermitian)

hermitian involutoric: $\hat{P}_{jk}^{-1} = \hat{P}_{jk}^+$ (4) $\Rightarrow$ unitary

(3) + (4): $\hat{A} = \hat{P}_{jk}^{-1} \hat{A} \hat{P}_{jk}$ $\Rightarrow$ $\hat{A} \hat{P}_{jk} - \hat{P}_{jk} \hat{A} = [\hat{A}, \hat{P}_{jk}]_- = 0$

special case: $\hat{A} = \hat{H}$ $\rightarrow$ $[\hat{H}, \hat{P}_{jk}]_- = 0$

There must exist states, which are eigenstates of both $\hat{H}$ and $\hat{P}_{jk}$:

$$\hat{H} |\Psi\rangle = E |\Psi\rangle, \qquad \hat{P}_{jk} |\Psi\rangle = \underline{P_{jk}} |\Psi\rangle$$

real due to $\hat{P}_{jk} = \hat{P}_{jk}^+$

involutoric: $(\hat{P}_{jk})^2 = 1$ $\Rightarrow$ $(P_{jk})^2 = 1$ $\Rightarrow$ $P_{jk} = \pm 1$

$\begin{cases} P_{jk} = +1: \text{bosons} \\ P_{jk} = -1: \text{fermions} \end{cases}$

Claim: $|\Psi\rangle$ has for all $\hat{P}_{jk}$ one and the same eigenvalue

$$\hat{P}_{1j} \hat{P}_{2k} \hat{P}_{12} \underbrace{\hat{P}_{2k} \hat{P}_{1j} \Psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_j, \dots, \vec{x}_k, \dots, \vec{x}_n)}$$
$$= \Psi(\vec{x}_j, \vec{x}_k, \dots, \vec{x}_1, \dots, \vec{x}_2, \dots, \vec{x}_n)$$
$$= \Psi(\vec{x}_k, \vec{x}_j, \dots, \vec{x}_1, \dots, \vec{x}_2, \dots, \vec{x}_n)$$
$$= \Psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_k, \dots, \vec{x}_j, \dots, \vec{x}_n) = \hat{P}_{jk} \Psi(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_j, \dots, \vec{x}_k, \dots, \vec{x}_n)$$

$\Rightarrow$ operator identity: $\hat{P}_{jk} = \hat{P}_{1j} \hat{P}_{2k} \hat{P}_{12} \hat{P}_{2k} \hat{P}_{1j}$

$\Rightarrow$ identity for eigenvalues: $P_{jk} = P_{1j} P_{2k} P_{12} P_{2k} P_{1j} = P_{12} \underbrace{(P_{1j})^2}_{=1} \underbrace{(P_{2k})^2}_{=1} = P_{12}$

irrespective of the transposition: always ± 1

symmetric wave function: $\varepsilon = +1$ $\rightarrow$ boson
anti – " " " : $\varepsilon = -1$ $\Rightarrow$ fermion
$\}$ $|\Psi^\varepsilon\rangle$, $\hat{P}_{jk} |\Psi^\varepsilon\rangle = \varepsilon |\Psi^\varepsilon\rangle$

Orthogonality:

$$\langle \Psi^- | \Psi^+ \rangle = \langle \Psi^- | \hat{P}_{jk} \Psi^+ \rangle = \langle \hat{P}_{jk}^+ \Psi^- | \Psi^+ \rangle = \langle \hat{P}_{jk} \Psi^- | \Psi^+ \rangle = - \langle \Psi^- | \Psi^+ \rangle \equiv 0$$

Symmetry character maintained through time evolution:

$$|\Psi^{\varepsilon_2}(t_2)\rangle = \hat{U}(t_2, t_1) |\Psi^{\varepsilon_1}(t_1)\rangle$$

$$\varepsilon_2 |\Psi^{\varepsilon_2}(t_2)\rangle = \hat{P}_{jk} |\Psi^{\varepsilon_2}(t_2)\rangle = \underbrace{\hat{P}_{jk} \hat{U}(t_2, t_1)}_{\hat{U}(t_2, t_1) \hat{P}_{jk}} |\Psi^{\varepsilon_1}(t_1)\rangle = \varepsilon_1 \underbrace{\hat{U}(t_2, t_1) \Psi^{\varepsilon_1}(t_1)\rangle}_{= |\Psi^{\varepsilon_2}(t_2)\rangle}$$

$[\hat{P}_{jk}, \hat{H}]_- = 0 \Rightarrow$

$\Rightarrow \varepsilon_2 = \varepsilon_1$

2.3 Non-Interacting Identical Particles

Taking into account (anti-)symmetry of many-body wave functions is quite cumbersome

example: $V_2(\vec{x}_\nu - \vec{x}_\mu) = 0$

$$\Rightarrow \sum_{\nu=1} \left\{ -\frac{\hbar^2}{2m} \Delta_\nu + V_1(\vec{x}_\nu) \right\} \Psi_E(\vec{x}_1, \dots, \vec{x}_n) = E \, \Psi_E(\vec{x}_1, \dots, \vec{x}_n)$$

Assumption: 1-particle problem is solved

$$\left\{-\frac{\hbar^2}{2m}\Delta + V_1(\vec{x})\right\}\psi_{E_\alpha}(\vec{x}) = E_\alpha \psi_{E_\alpha}(\vec{x}) \Rightarrow \alpha: \text{vector of eigenvalues}$$

orthonormality: $\int d^3x\, \psi^*_{E_\alpha}(\vec{x})\psi_{E_{\alpha'}}(\vec{x}) = \delta_{\alpha,\alpha'}$

completeness: $\sum_\alpha \psi^*_{E_\alpha}(\vec{x})\psi_{E_\alpha}(\vec{x}') = \delta(\vec{x}-\vec{x}')$

separation ansatz: $\psi_E(\vec{x}_1,\dots,\vec{x}_n) = \psi_{E_{\alpha_1}}(\vec{x}_1)\cdot\ldots\cdot\psi_{E_{\alpha_n}}(\vec{x}_n) = \psi_{E_{\alpha_1}\dots E_{\alpha_n}}(\vec{x}_1,\dots,\vec{x}_n)$

$\Rightarrow E = E_{\alpha_1}+\dots+E_{\alpha_n}$

orthonormality:

$$\int d^3x_1\dots\int d^3x_n\, \psi^*_{E_{\alpha_1}\dots E_{\alpha_n}}(\vec{x}_1,\dots,\vec{x}_n)\psi_{E_{\alpha'_1}\dots E_{\alpha'_n}}(\vec{x}_1,\dots,\vec{x}_n) = \delta_{\alpha_1,\alpha'_1}\dots\delta_{\alpha_n,\alpha'_n}$$

completeness:

$$\sum_{\alpha_1}\dots\sum_{\alpha_n}\psi^*_{E_{\alpha_1}\dots E_{\alpha_n}}(\vec{x}_1,\dots,\vec{x}_n)\psi_{E_{\alpha_1}\dots E_{\alpha_n}}(\vec{x}'_1,\dots,\vec{x}'_n) = \delta(\vec{x}_1-\vec{x}'_1)\dots\delta(\vec{x}_n-\vec{x}'_n)$$

(anti-)symmetrisation due to indistinguishability: $\hat{S}^\varepsilon = \sum_{\hat{P}}\varepsilon^P\hat{P}$

$\varepsilon = \pm 1$ number of transpositions for $\hat{P} = \prod \hat{P}_{jk}$

$$\psi^\varepsilon_{\{E_\alpha\}}(\vec{x}_1,\dots,\vec{x}_n) = N^\varepsilon_{\{E_\alpha\}}\hat{S}^\varepsilon\prod_{\nu=1}^n\psi_{E_{\alpha_\nu}}(\vec{x}_\nu)$$

concrete order of energy eigenvalues unimportant due to (anti-)symmetisation

check for symmetry:

$$\hat{P}_{jk}\hat{S}^\varepsilon = \sum_{\hat{P}}\varepsilon^P\underbrace{\hat{P}_{jk}\hat{P}}_{=\hat{P}'} \underset{P'=P\pm1}{=} \sum_{\hat{P}'}\varepsilon^{P'\mp1}\hat{P}' = \varepsilon\sum_{\hat{P}'}\varepsilon^{P'}\hat{P}' = \varepsilon\hat{S}^\varepsilon$$

$$\hat{P}_{jk}\psi^\varepsilon_{\{E_\alpha\}}(\vec{x}_1,\dots,\vec{x}_n) = \varepsilon\psi^\varepsilon_{\{E_\alpha\}}(\vec{x}_1,\dots,\vec{x}_n)$$

$$\hat{H}|\psi_E\rangle = E|\psi_E\rangle \Rightarrow \underbrace{\hat{S}^\varepsilon\hat{H}}_{=\hat{H}\hat{S}^\varepsilon}|\psi_E\rangle = E\hat{S}^\varepsilon|\psi_E\rangle \Rightarrow \hat{H}\left(\hat{S}^\varepsilon|\psi_E\rangle\right) = E\left(\hat{S}^\varepsilon|\psi_E\rangle\right)$$

$[\hat{H},\hat{P}_{jk}]=0 \Rightarrow$

(anti)-symmetrised wave function solves eigenvalue problem

special case: $\varepsilon = -1$ (fermion)

$$\psi^-_{\{E_\alpha\}}(\vec{x}_1,\dots,\vec{x}_n) = N^-_{\{E_\alpha\}}\sum_{\hat{P}}(-1)^P\psi_{E_{\alpha_1}}(\vec{x}_{P(1)})\cdot\ldots\cdot\psi_{E_{\alpha_n}}(\vec{x}_{P(n)})$$

slater determinant

$$= N^-_{\{E_\alpha\}}\begin{vmatrix}\psi_{E_{\alpha_1}}(\vec{x}_1) & \psi_{E_{\alpha_1}}(\vec{x}_2) & \dots & \psi_{E_{\alpha_1}}(\vec{x}_n)\\ \psi_{E_{\alpha_2}}(\vec{x}_1) & \psi_{E_{\alpha_2}}(\vec{x}_2) & \dots & \psi_{E_{\alpha_2}}(\vec{x}_n)\\ \vdots & \vdots & & \vdots\\ \psi_{E_{\alpha_n}}(\vec{x}_1) & \psi_{E_{\alpha_n}}(\vec{x}_2) & \dots & \psi_{E_{\alpha_n}}(\vec{x}_n)\end{vmatrix}$$

Equality of two rows, i.e. $\alpha_j = \alpha_k$ or of two columns, i.e. $x_j = x_k$, leads to a vanishing wave function $\Rightarrow$ Pauli exclusion principle: two fermions are not allowed either in the same state or at the same point

Note: no corresponding restriction occurs for bosons