Formelsammlung Quantenmechanik II

Postulates

I Observables $\to$ Hermitian operator A

II Measurement of A = selection of an eigenstate of A

III Probability to measure a for $A : P(a) = |\langle a|a\rangle|^2 = |c_a|^2$

IV Time evolution: $|\alpha, t\rangle = U|\alpha, 0\rangle$

V Observables of a system of N identical particles commute with all the permutations $\pi \in S_n$

Variance: $\Delta A = A - \langle A\rangle \mathbb{1}$

Uncertainty relation: $\left\langle \Delta A^2\right\rangle \left\langle \Delta B^2\right\rangle \geq \frac{1}{4}|\langle [A,B]\rangle|^2$

Schwarz inequality: $\langle a|a\rangle \langle b|b\rangle \geq |\langle a|b\rangle|^2$

Canonical commutator: $[x_i, p_i] = \mathrm{i}\hbar\delta_{ij}$

Baker-Hausdorff formula: A, B hermitian, $\lambda \in \mathbb{R}$
$\mathrm{e}^{\mathrm{i}\lambda B} A \mathrm{e}^{-\mathrm{i}\lambda B}$
$= A + \mathrm{i}\lambda[B,A] + \frac{(\mathrm{i}\lambda)^2}{2}[B,[B,A]] + \ldots + \frac{(\mathrm{i}\lambda)^n}{n!}[B,[B,\ldots[B,A]]]$

Baker-Campbell-Hausdorff formula:
$\exp(A \cdot B) = \exp(A)\exp(B)\exp\left(-\frac{[A,B]}{2}\right)$

Gaussian wave packet: $\Psi(x,t_0) = \frac{1}{\sqrt[4]{\pi d^2}}\exp\left(\mathrm{i}\frac{p_0 x}{\hbar}\right)\exp\left(-\frac{x^2}{2d^2}\right)$

Dynamics

Time evolution operator: $U(t,t_0) = \exp\left(-\frac{\mathrm{i}}{\hbar}H(t-t_0)\right)$ (time independent H)

$[H(t_1), H(t_2)] = 0 \Rightarrow U(t,t_0) = \exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}\tau\, H(\tau)\right)$

Dyson Series: (non-commuting $H(t)$)

$$U(t,t_0) = 1 + \sum_{n=1}^{\infty}\frac{(-\mathrm{i})^n}{\hbar}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\ldots\int_{t_0}^{t_{n-1}}\mathrm{d}t_n\, H(t_1)\ldots H(t_n)$$

Correlation amplitudes: $C(t) = \sum_a \exp\left(-\frac{\mathrm{i}}{\hbar}E_a t\right)|C_a|^2$

Schrödinger picture:
state $|\alpha\rangle \to U_t|\alpha\rangle$
observable A and eigenvalues a are time independent

Heisenberg picture:
observable $A \to A_H(t) = U_t^\dagger A_S U_t$ according to $\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}[A,H]$
state $|\alpha\rangle$ time independent, eigenstate $|a\rangle \to U^\dagger|\alpha\rangle$

Probability flux: $\boldsymbol{j} = \frac{\hbar}{m}\operatorname{Im}(\Psi^*\vec{\boldsymbol{\nabla}}\Psi)$

Continuity equation: $\dot{\rho} + \vec{\boldsymbol{\nabla}}\cdot\boldsymbol{j} = 0$ with $\rho = |\Psi|^2$

Hamilton-Jacobi: $-\frac{\partial S}{\partial t} = \frac{1}{2m}|\vec{\boldsymbol{\nabla}}S|^2 + V$ with $\Psi = \sqrt{\rho}\exp\left(\frac{\mathrm{i}}{\hbar}S\right)$

Propagator: $K(x,t,x',0) = \sum_a u_a(x)u_a^*(x)\exp\left(-\frac{\mathrm{i}}{\hbar}E_a t\right)$

$[x_i, F(\boldsymbol{p})] = \mathrm{i}\hbar\frac{\partial}{\partial p_i}F(\boldsymbol{p}), \qquad [p_i, G(\boldsymbol{x})] = -\mathrm{i}\hbar\frac{\partial}{\partial x_i}G(\boldsymbol{x})$

Ehrenfest theorem: $m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\boldsymbol{x}\rangle = -\left\langle\vec{\boldsymbol{\nabla}}V(\boldsymbol{x})\right\rangle$

Harmonic oscillator

Hamiltonian: $H = \frac{p^2}{2m} + \frac{m\omega^2x^2}{2} = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$

Ladder operator: $a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \mathrm{i}\frac{p}{m\omega}\right)$

$a^\dagger a = N, \quad [a, a^\dagger] = 1, [N, a^\dagger] = a^\dagger, [N, a] = -a$

$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \quad a|n\rangle = \sqrt{n}|n-1\rangle$

Electromagnetic fields

Lagrangian: $\mathcal{L}(\dot{\boldsymbol{x}}, \boldsymbol{x}) = \frac{1}{2}m\dot{\boldsymbol{x}}^2 + \frac{e}{c}\boldsymbol{A}\cdot\dot{\boldsymbol{x}} - e\phi$

Hamiltonian: $H = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2 + e\phi$

Gauge transformations: $\boldsymbol{A} \to \boldsymbol{A} + \vec{\boldsymbol{\nabla}}\Lambda \qquad \phi \to \phi - \frac{1}{c}\frac{\partial}{\partial t}\Lambda$

Minimal coupling: $H = \frac{p^2}{2m} + \phi$ with $p \to \boldsymbol{\Pi} := \boldsymbol{\pi} - \frac{e}{c}\boldsymbol{A}$

Symmetric gauge: $\boldsymbol{A} = \frac{B}{2}(-y, x, 0)$

Landau gauge: $\boldsymbol{A} = B(0, x, 0)$

Spin 1/2 systems

generic state: $|\alpha\rangle = \begin{pmatrix}1\\0\end{pmatrix}\langle +|\alpha\rangle + \begin{pmatrix}0\\1\end{pmatrix}\langle -|\alpha\rangle = \begin{pmatrix}c_+\\c_-\end{pmatrix}$

Pauli matrices= $\sigma_x = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}, \sigma_y = \begin{pmatrix}0 & -\mathrm{i}\\\mathrm{i} & 0\end{pmatrix}, \sigma_z = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$

$\sigma_k^2 = \mathbb{1}, \quad [\sigma_i, \sigma_j] = 2\mathrm{i}\varepsilon_{ijk}\sigma_k, \quad \{\sigma_i, \sigma_j\} = 2\delta_{ij}, \quad \sigma_i^\dagger = \sigma_i,$
$\det\sigma_i = 1, \quad \operatorname{Tr}\sigma_i = 0$

$S_x = \frac{\hbar}{2}(|+\rangle\langle -| + |-\rangle\langle +|), \quad |S_x;\pm\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm |-\rangle)$

$S_y = \frac{\mathrm{i}\hbar}{2}(|-\rangle\langle +| - |+\rangle\langle -|), \quad |S_y;\pm\rangle = \frac{1}{\sqrt{2}}(|+\rangle \pm \mathrm{i}\,|-\rangle)$

$S_z = \frac{\hbar}{2}(|+\rangle\langle +| + |-\rangle\langle -|), \quad |S_z;\pm\rangle = |\pm\rangle$

Angular momentum

Ladder operator: $J_\pm = J_x \pm \mathrm{i}J_y$

$[J^2, J_i] = 0, \quad [J_+, J_-] = 2\hbar J_z, \quad [J_z, J_\pm] = \pm\hbar J_\pm, \quad [J_\pm J^2] = 0$

$J^2 = J_+J_- + J_z(J_z - \hbar)$

Eigenvalues: $J^2|jm\rangle = \hbar^2 j(j+1)|jm\rangle, \quad J_z|jm\rangle = \hbar m|jm\rangle$

$\left\langle j'm'|J_\pm|jm\right\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}\hbar\delta_{jj'}\delta_{m'm+1}$

Two basis: $|j_1j_2m_1m_2\rangle$ and $|j_1j_2jm\rangle$

$$|j_1j_2jm\rangle = \sum_{m_1,m_2}|j_1j_2m_1m_2\rangle\underbrace{\langle j_1j_2m_1m_2|j_1j_2jm\rangle}_{\text{Clebsch-Gordan coeff.}}$$

$\langle j_1j_2m_1m_2|j_1j_2jm\rangle = 0$ unless $m = m_1 + m_2$

$\langle j_1j_2m_1m_2|j_1j_2m_1m_2\rangle = 0$ unless $|j_1 - j_2| \leq j \leq |j_1 + j_2|$

$$\sum_{j,m}\langle j_1j_2m_1m_2|j_1j_2jm\rangle\left\langle j_1j_2m_1'm_2'|j_1j_2jm\right\rangle = \delta_{m_1m_1'}\delta_{m_2m_2'}$$

Recursion relation to build CG-coefficients:
$\sqrt{(j\mp m)(j\pm m+1)}\langle m_1m_2|jm\pm 1\rangle =$
$\sqrt{(j_1\mp m_1+1)(j_1\pm m_1)}\langle m_1\mp 1, m_2|jm\rangle$
$+\sqrt{(j_2\mp m_2+1)(j_2\pm m_2)}\langle m_1, m_2\mp 1|jm\rangle$

Tensor operators

Spherical tensor components $T_q^{(k)}$ transform like $Y_{l=k,m=q}$

$$T_{i1,\dots,ik} = \sum_{q=-k}^{k} T_q^{(k)} Y_{i1,\dots,ik}^{(n_a)}$$

$[J_z, T_q^{(k)}] = \hbar q T_q^{(k)}$, Vector operator: $[V_a, J_b] = \mathrm{i}\varepsilon_{abc} V_c$

Wigner-Eckardt theorem:

$$\left\langle n', l', m' | R_q^{(k)} | n, l, m \right\rangle = \frac{\langle lk; mq | lk; l'm' \rangle \left\langle n'l' || R^{(1)} || nl \right\rangle}{\sqrt{2l+1}}$$

Time independent perturbation theory

Notation: $E_\lambda = E_0 + \sum_{k\geq 1} \lambda^k \delta_k, \quad |E_\lambda\rangle = |E_0\rangle + \sum_{k\geq 1} |\eta_k\rangle$

Recursion formula: $(H_0 - E_0)|E_\lambda\rangle = (E_\lambda - E_0)|E_\lambda\rangle - \lambda V |E_\lambda\rangle$

$$E_\lambda - E_0 = \lambda \frac{\langle E_0 | V | E_\lambda \rangle}{\langle E_0 | E_\lambda \rangle}$$

eigenvalue correction: $\delta_k = \langle E_0 | V | \eta_{k-1} \rangle, \qquad \delta_1 = \langle E_0 | V | E_0 \rangle$

eigenstate correction: $|\eta_k\rangle = R_0(E_0) \sum_j^{k-1} \delta_j |\eta_{k-1}\rangle - R_0(E_0) V |\eta_{k-1}\rangle$

Resolvent $R_0(E_0) = \begin{cases} (H_0 - E_0)^{-1} & H_0 \neq E_0 \\ 0 & H_0 = E_0 \end{cases}$

$$\begin{aligned} E_n &= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \mathcal{O}(\lambda^3) \\ &= E_n^{(0)} + \lambda \left\langle \Psi_n^{(0)} | V | \Psi_n^{(0)} \right\rangle + \lambda^2 \sum_{k\neq n} \frac{| \left\langle \Psi_k^{(0)} | V | \Psi_n^{(0)} \right\rangle |^2}{E_n^{(0)} - E_k^{(0)}} + \mathcal{O}(\lambda^3) \end{aligned}$$

$$\begin{aligned} |\Psi_n\rangle &= \left|\Psi_n^{(0)}\right\rangle + \lambda \left|\Psi_n^{(1)}\right\rangle + \mathcal{O}(\lambda^2) \\ &= \left|\Psi_n^{(0)}\right\rangle + \lambda \sum_{k\neq n} \frac{\left\langle \Psi_k^{(0)} | V | \Psi_n^{(0)} \right\rangle}{E_n^{(0)} - E_k^{(0)}} \left|\Psi_k^{(0)}\right\rangle + \mathcal{O}(\lambda^2) \end{aligned}$$

Feynmann-Hellmann theorem: $\left\langle n | \frac{\mathrm{d}H}{\mathrm{d}\alpha} | n \right\rangle = \frac{\mathrm{d}E_n}{\mathrm{d}\alpha}$

Virial theorem: $\left\langle \frac{p^2}{2m} \right\rangle = \left\langle \frac{\omega^2 q^2}{2} \right\rangle$

Degenerate case

1. Identify degenerate unperturbed eigenkets and construct the perturbation matrix V
2. Diagonalize the perturbation matrix by solving, as usual the appropriate secular equation.
3. Identify the roots with the first order energy shifts. The base kets that diagonalize the V matrix are the correct zeroth-order kets.
4. For higher orders use non-degenerate perturbation theory, excluding all contributions from the unperturbed kets in the degenerate subspace.

Relativistic correction: $H_{\mathrm{rel}} = -\frac{p^4}{8m^3c^2}$

$$\delta_1^{\mathrm{rel}} = -\frac{1}{2} mc^2 \frac{\alpha^4}{n^4} \left(-\frac{3}{4} + \frac{n}{l+1/2} \right)$$

Spin-orbit interaction: $H_{\mathrm{SO}} = -\boldsymbol{\mu} \cdot \boldsymbol{B} = \frac{\alpha\hbar^3}{2m^2c} \frac{1}{r^3} \boldsymbol{L} \cdot \boldsymbol{S}$

$$\delta_1^{\mathrm{SO}} = \frac{1}{2} mc^2 \frac{\alpha^4}{2\hbar^3 l(l+1)(l+1/2)} \begin{cases} l & j = l + 1/2 \\ -(l+1) & j = l - 1/2 \end{cases}$$

Time dependent perturbation theory

Interaction/Dirac picture:

$|\alpha, t\rangle_I = \exp\left(\frac{\mathrm{i}}{\hbar} H_0 t\right) |\alpha, t\rangle_S, \quad A_I(t) = \exp\left(\frac{\mathrm{i}}{\hbar} H_0 t\right) A_s \exp\left(-\frac{\mathrm{i}}{\hbar} H_0 t\right)$

Heisenberg time operation: $\frac{\mathrm{d}A_I}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}[A_I, H_0]$

Perturbative ansatz: $|\alpha\rangle_t = \sum_n c_n(t) \exp\left(-\frac{\mathrm{i}}{\hbar} E_n t\right) |n\rangle_0$

Transition frequencies: $\omega_{nm} = \frac{1}{\hbar}(E_n - E_m)$

Equation for $C_n(t)$: $\mathrm{i}\hbar \dot{C}_n(t) = \sum_m \mathrm{e}^{\mathrm{i}\omega_{mn} t} V_{nm} C_m(t)$

Perturbative ansatz: $C_n(t) = C_n^{(0)} + \lambda C_n^{(1)} + \lambda^2 C_n^{(2)}$

Time evolution in Dirac picture: $|\alpha, t\rangle_I = U_I(t, t_0) |\alpha, t_0\rangle_I$

$U_I(t, t_0) = \mathrm{e}^{\mathrm{i}/\hbar H_0 t} U(t, t_0) \mathrm{e}^{-\mathrm{i}/\hbar H_0 t}$

$$\begin{aligned} \mathcal{O}(\lambda^0) &: C_n^{(0)} = \langle n | \mathbb{1} | i \rangle = \delta_{ni} \\ \mathcal{O}(\lambda^1) &: C_n^{(1)} = -\frac{\mathrm{i}}{\hbar} \int \mathrm{d}\tau \, \langle n | V_I | i \rangle \\ &= -\frac{\mathrm{i}}{\hbar} \int \mathrm{d}\tau \, \mathrm{e}^{\mathrm{i}\omega_{ni}\tau} \langle n | V | i \rangle, \quad \omega_{ni} = \frac{E_n - E_i}{\hbar} \end{aligned}$$

Transition probability: $p(i \to n) = |\langle n | U_I | i \rangle|^2 = |C_n^{(0)} + \dots|^2$

Harmonic pert.: $C_n^{(1)} = A_{ni} \frac{1 - \mathrm{e}^{\mathrm{i}(\omega_{ni} - \omega)t}}{\hbar(\omega_{ni} - \omega)} + A_{ni}^\dagger \frac{1 - \mathrm{e}^{\mathrm{i}(\omega_{ni} + \omega)t}}{\hbar(\omega_{ni} + \omega)}$

Transition rate: $R(i \to n) := \lim_{t\to\infty} \frac{1}{t} P(i \to n)$

Fermis golden rule: $R(i \to n) = \frac{2\pi}{\hbar} |A_{ni}|^2 \delta(\hbar\omega - E_i + E_n)$

Detailed balance equation: $\frac{R(i \to n)}{\rho(E_n)} = \frac{R(n \to i)}{\rho(E_i)}$

Stimulated emission: $R(i \to f) = \frac{4\pi^2}{3} d_{fi}^2 \frac{u(\omega_{fi})}{\hbar^2}$

Spontaneous emission: $R(m \to n) = \frac{4}{3} \frac{\omega_{mn}^3}{\hbar c^3} d_{mn}^2$

Scattering processes

Generic compact potential between $-a \leq x \leq a$

$$\Psi(x) = \begin{cases} A\mathrm{e}^{\mathrm{i}kx} + B\mathrm{e}^{-\mathrm{i}kx} & x < -a \\ \Psi_{II}(x; C, D) & -a \leq x \leq a \\ F\mathrm{e}^{\mathrm{i}kx} + G\mathrm{e}^{-\mathrm{i}kx} & x > a \end{cases}$$

Transfermatrix: $\begin{pmatrix} F \\ G \end{pmatrix} = T \begin{pmatrix} A \\ B \end{pmatrix}, \qquad T = \begin{pmatrix} \xi & \eta \\ \eta^* & \xi^* \end{pmatrix} \in \mathrm{SU}(1,1)$

probability conservation: $|\rho|^2 + |\tau|^2 = 1$

S-matrix: $\begin{pmatrix} F \\ B \end{pmatrix} = S \begin{pmatrix} A \\ G \end{pmatrix}, \qquad S_{11} = \tau, S_{21} = \rho$ is unitary

Lippman-Schwinger: $\Psi(x) = \Psi_0(\boldsymbol{x}) + \int G(\boldsymbol{x} - \boldsymbol{x}') \chi_\Psi(\boldsymbol{x}) \, \mathrm{d}^3 x$

$|\Psi_\alpha\rangle = |\phi_\alpha\rangle + \int \mathrm{d}x_\beta \, \frac{1}{E - E_\beta \pm \mathrm{i}\varepsilon} |\phi_\beta\rangle \langle \phi_\beta | V | \Psi_\alpha \rangle$

Green Function of Helmholtz equation: $G_\pm(r) = -\frac{1}{4\pi} \frac{\mathrm{e}^{\pm \mathrm{i}kr}}{r}$

T-matrix: $T_{\beta\alpha} := \langle \phi_\beta | V | \Psi_\alpha \rangle, \quad T |\boldsymbol{k}\rangle = V \left| \Psi_+^{(k)} \right\rangle$

Born series: $T = V(1 - G \cdot V)^{-1}, \quad G = \dfrac{1}{E - H_0 + \mathrm{i}\varepsilon}$

$$f(k', k) = -\frac{2m}{2\pi\hbar^2}\left\langle k'|V|\Psi_+^{(k)}\right\rangle = -\frac{2m}{2\pi\hbar^2}\int \mathrm{d}^3x'\, \mathrm{e}^{-\mathrm{i}\boldsymbol{k'}\cdot\boldsymbol{x'}}\left\langle x'|V|\Psi_+^{(k)}\right\rangle$$

First order Born approximation ($\boldsymbol{q} := \boldsymbol{k} - \boldsymbol{k'}$)

$$f(k', k) = -\frac{2m}{2\pi\hbar^2}\left\langle k'|V|k\right\rangle = +\frac{2m}{q\hbar^2}\int_0^\infty r\sin(qr)V(r)\,\mathrm{d}r$$

Forward scattering: $q = |\boldsymbol{q}| = 2k\sin(\vartheta/2)$

Fermis rule for T-matrix: $R(i \to f) = \dfrac{2\pi}{\hbar}|T_{fi}|^2\delta(E_f - E_i)$

Cross section: $\dfrac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f|^2 \propto |T_{fi}|^2$

Coulomb scattering: $\dfrac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \dfrac{2mZZ'e^2}{\hbar^2}\dfrac{1}{16k^4\sin^4(\vartheta/2)}$

Partial waves

$$V(\boldsymbol{r}) = V(r) \Rightarrow \Psi(r,\vartheta) = \sum_{l=0}^{\infty} R_l(r)P_l(\cos\vartheta)$$

$$f(\vartheta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\vartheta)\underbrace{\frac{1}{2\mathrm{i}}(\mathrm{e}^{2\mathrm{i}\delta_l} - 1)}_{\mathrm{e}^{\mathrm{i}\delta_l}\sin(\delta_l)}$$

Total cross section: $\sigma = \dfrac{4\pi}{k}\sum_l (2l+1)\sin^2\delta_l$

Optical theorem $\sigma = \dfrac{4\pi}{k}\,\mathrm{Im}(f(\vartheta = 0))$

Determination of phase shift: Assume a potential with compact support, then apply junction conditions at the boundary

$R_l^{\text{out}} = c_l(j_l(kr)\cos\delta_l - n_l(kr)\sin\delta_l)$

Phase shift: $\tan\delta_l = \dfrac{kaj_l'(ka) - \beta_l j_l(ka)}{kan_l'(ka) - \beta_l j_l(ka)}, \quad \beta_l := \left.\dfrac{rR'}{R}\right|_a$

Statistical Quantum mechanics

Ensemble average: $\overline{A} := \sum_{i=1}^{N} w_i\langle\alpha_i|A|\alpha_i\rangle = \mathrm{Tr}(\rho A)$

Density operator: $\rho := \sum_i w_i|\alpha_i\rangle\langle\alpha_i|$

Properties: $\rho = \rho^\dagger, \mathrm{Tr}(\rho) = 1$

Pure ensemble: $\rho^2 = \rho, \mathrm{Tr}(\rho^2) = 1$, eigenvalues 1,0

Time evolution: $\mathrm{i}\hbar\partial_t\rho = -[\rho, H]$

Entropy: $\sigma := -\mathrm{Tr}(\rho\ln\rho) = -\sum_{k=1}^{N}\rho_{kk}\ln\rho_{kk}$

Many body systems

Heisenberg principle: Identical particles are indistinguishable

Permutation operator: $P_{12}|12\rangle = |21\rangle$
Properties: $P^2 = \mathbb{1}, P = P^{-1}, P = P^\dagger$, eigenvalues ± 1

Observables commute with the permutation operator $[A, P] = 0$

(Anti)symmetrizer operator: $P_\pm = \dfrac{1}{2}(\mathbb{1} \pm P)$

Slater determinant: $\Psi_-(x_1, x_2) = \dfrac{1}{\sqrt{2}}\det\begin{pmatrix}\Psi_1(x_1) & \Psi_2(x_1)\\ \Psi_1(x_2) & \Psi_2(x_2)\end{pmatrix}$

Transposition op.: $P_{ij}|a_1\dots a_i\dots a_j\dots a_n\rangle = |a_1\dots a_j\dots a_i\dots a_n\rangle$

Properties: $P_{ij} = (P_{ij})^\dagger, P_{ij} = (P_{ij})^{-1}, P_{ij}^2 = \mathbb{1}$,
$[P_{ij}, P_{kl}] = 0\ i \neq j \neq k \neq l, P_{ij}P_{ik} = P_{jk}P_{ij}\ j \neq k$

Total (anti)symmetrizer: $P_\xi = \dfrac{1}{N!}\sum_{\pi\in S_n}(\xi)^{n_\pi}P_\pi$

N-particle wave function: $\Psi_\xi = \dfrac{1}{\sqrt{N!}}\sum_{\pi\in S_n}\xi^{n_\pi}P_\pi\prod_{i=1}^{N}\Psi_i(x_{\pi_i})$

Spin statistic theorem: Particles with (semi-)integer spin are (Fermions) Bosons.

Wavefunction of two electron system:

$$\Psi(\boldsymbol{x}_1, \boldsymbol{x}_2) = \phi_{00}\chi_{00} + \sum_{m=-1}^{1}\phi_{1m}(\boldsymbol{x}_1, \boldsymbol{x}_2)\chi_{1m}$$

Variational method: Estimate the ground state of a Hamiltonian Guess $|\tilde{0}\rangle \approx |0\rangle$. Then an upper value for E_0 ist given by

$$\overline{H} := \langle\tilde{0}|H|\tilde{0}\rangle \geq E_0.$$

Supplementary

$$\mathcal{R}_{\hat{x}} = \begin{pmatrix}1 & 0 & 0\\ 0 & \cos\alpha & -\sin\alpha\\ 0 & \sin\alpha & \cos\alpha\end{pmatrix}, \qquad \mathcal{R}_{\hat{y}} = \begin{pmatrix}\cos\alpha & 0 & \sin\alpha\\ 0 & 1 & 0\\ -\sin\alpha & 0 & \cos\alpha\end{pmatrix}$$

$$\int_{-\infty}^{\infty}\mathrm{d}x\,\mathrm{e}^{-ax^2+bx+c} = \sqrt{\frac{\pi}{a}}\exp\left(\frac{b^2}{4a} + c\right)$$

$$\int_{-\infty}^{\infty}\mathrm{d}x\,x^2\mathrm{e}^{-ax^2+bx+c} = \frac{1}{4}\sqrt{\frac{\pi}{a^5}}(b^2 + 2a)\exp\left(\frac{b^2}{4a} + c\right)$$

$$\int_{-\infty}^{\infty}\mathrm{d}x\,x^2\mathrm{e}^{-ax^2} = \frac{1}{2}\sqrt{\frac{\pi}{a^3}}, \qquad \int_{-\infty}^{\infty}\mathrm{d}x\,x^4\mathrm{e}^{-ax^2} = \frac{3}{4}\sqrt{\frac{\pi}{a^5}}$$

$$\sin^2\alpha = \frac{1 - \cos(2\alpha)}{2}, \quad \cos^2\alpha = \frac{1 + \cos(2\alpha)}{2}$$

$$\int\mathrm{d}x\sin^2(x) = \frac{1}{2}(x - \sin x\cos x), \qquad \int\mathrm{d}x\cos^2(x) = \frac{1}{2}(x + \sin x\cos x)$$

$$\Psi_{100} = \sqrt{\frac{4Z^3}{a_0^3}}\exp\left(-\frac{Zr}{a_0}\right)\sqrt{\frac{1}{4\pi}}$$

$$\Psi_{200} = \sqrt{\frac{Z^3}{8a_0^3}}\left(-\frac{Zr}{a_0} + 2\right)\exp\left(-\frac{Zr}{2a_0}\right)\sqrt{\frac{1}{4\pi}}$$

$$\Psi_{210} = \sqrt{\frac{Z^3}{8a_0^3}}\left(\frac{Zr}{a_0}\right)\exp\left(-\frac{Zr}{2a_0}\right)\sqrt{\frac{1}{4\pi}}\cos\vartheta.$$

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}\left(\sin\vartheta\frac{\partial}{\partial\vartheta}\right) + \frac{1}{r^2\sin^2\vartheta}\frac{\partial^2}{\partial\varphi^2}$$

Y_{lm}	$l = 0$	$l = 1$	$l = 2$
$m = 1$		$-\sqrt{\frac{3}{8\pi}}\sin\vartheta\mathrm{e}^{+\mathrm{i}\varphi}$	$-\sqrt{\frac{15}{8\pi}}\sin\vartheta\cos\vartheta\mathrm{e}^{+\mathrm{i}\varphi}$
$m = 0$	$\frac{1}{\sqrt{4\pi}}$	$\sqrt{\frac{3}{4\pi}}\cos\vartheta$	$\sqrt{\frac{5}{16\pi}}(3\cos^2\vartheta - 1)$
$m = -1$		$\sqrt{\frac{3}{8\pi}}\sin\vartheta\mathrm{e}^{-\mathrm{i}\varphi}$	$\sqrt{\frac{15}{8\pi}}\sin\vartheta\cos\vartheta\mathrm{e}^{-\mathrm{i}\varphi}$