Many-particle systems

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many particle wavefunction

- many particle wavefunction

$$\psi_T\left(x_1, x_2, x_3, \cdots, x_N\right)$$

- normalization condition

$$\int\int\cdots\int dx_1\, dx_2 \cdots dx_N \left|\psi_T\left(x_1, x_2, x_3, \cdots, x_N\right)\right|^2 = 1$$

- time evolution

$$i\hbar\frac{\partial}{\partial t}\psi_T\left(x_1, x_2, x_3, \cdots, x_N\right) = H\psi_T\left(x_1, x_2, x_3, \cdots, x_N\right)$$

hamiltonian

- many-particle hamiltonian

$$H = \sum_j \frac{p_j^2}{2m_j} + V\left(x_1, x_2, x_3, \cdots, x_N\right)$$

$$H = -\hbar^2 \left(\frac{1}{2m_1}\frac{\partial^2}{\partial x_1^2} + \frac{1}{2m_2}\frac{\partial^2}{\partial x_2^2} + \cdots \frac{1}{2m_N}\frac{\partial^2}{\partial x_N^2} \right) + V\left(x_1, x_2, x_3, \cdots, x_N\right)$$

- energy eigenvalue

$$-\hbar^2 \left(\frac{1}{2m_1}\frac{\partial^2}{\partial x_1^2} + \frac{1}{2m_2}\frac{\partial^2}{\partial x_2^2} + \cdots \frac{1}{2m_N}\frac{\partial^2}{\partial x_N^2} \right)\psi_T + V\left(x_1, x_2, x_3, \cdots, x_N\right)\psi_T = E\psi_T$$

N-noninteracting particles

- For non-interacting particles

$$V(x_1, x_2, x_3, \cdots, x_N) = V(x_1) + V(x_2) + \cdots V(x_N)$$

- Hamiltonian is separable

$$H = \sum_j H_j$$

$$H_j = \frac{p_j^2}{2m} + V(x_j)$$

2-particle wavefunction

- wavefunctions are separable

$$H\psi_{\alpha}(1,2,\cdots,N)=E_{\alpha}\psi_{\alpha}(1,2,\cdots,N)$$

- for 2-particles, the following are the solutions to the Schrodinger equations

$$\psi_{E}(1,2)=\psi_{\alpha}(x_1)\psi_{\beta}(x_2) \qquad \psi_{E}(1,2)=\psi_{\alpha}(x_2)\psi_{\beta}(x_1)$$

- energy is additive

$$E=E_{\alpha}+E_{\beta}$$

identical particles

- the particles are indistinguishable
- Probability density should be invariant under index interchange

$$\psi_E^*(1,2)\psi_E(1,2)=\psi_E^*(2,1)\psi_E(2,1)$$

$$\psi_\alpha(x_1)\psi_\beta(x_2)\leftrightarrow\psi_\alpha(x_2)\psi_\beta(x_1)$$

- The possible choices of 2-particle wave functions are

$$\psi_S=\frac{1}{\sqrt{2}}\left[\psi_\alpha(x_1)\psi_\beta(x_2)+\psi_\beta(x_1)\psi_\alpha(x_2)\right]$$

$$\psi_A=\frac{1}{\sqrt{2}}\left[\psi_\alpha(x_1)\psi_\beta(x_2)-\psi_\beta(x_1)\psi_\alpha(x_2)\right]$$

index exchange

- For symmetric wavefunction

$$\psi_S \xrightarrow[1\leftrightarrow 2]{} \frac{1}{\sqrt{2}}\left[\psi_\alpha(x_1)\psi_\beta(x_2)+\psi_\beta(x_1)\psi_\alpha(x_2)\right]=\psi_S$$

$$\psi_S^*\psi_S \xrightarrow[1\leftrightarrow 2]{} \psi_S^*\psi_S$$

- For anti-symmetric wavefunction

$$\psi_A \xrightarrow[1\leftrightarrow 2]{} \frac{1}{\sqrt{2}}\left[\psi_\alpha(x_2)\psi_\beta(x_1)-\psi_\beta(x_2)\psi_\alpha(x_1)\right]=-\psi_A$$

$$\psi_A^*\psi_A \xrightarrow[1\leftrightarrow 2]{} (-1)^2\,\psi_A^*\psi_A$$

Pauli principle

- Fermions: systems consisting identical particles of half-odd-integral spin are described by anti-symmetric wave functions
- Bosons: systems consisting identical particles of integral spin are described by symmetric wave functions
- Anyons $\psi_\alpha(x_1)\psi_\beta(x_2) \xrightarrow[1\leftrightarrow 2]{} e^{i\theta}\psi_\beta(x_1)\psi_\alpha(x_2)$

Pauli principle

- Fermions: no more than one fermion can be in the same quantum state.
- Why?

$$\psi_A = \frac{1}{\sqrt{2}}\left[\psi_\alpha(x_1)\psi_\alpha(x_2) - \psi_\alpha(x_1)\psi_\alpha(x_2)\right] = 0$$

Slater determinant

- For many particles, we can express the answer using the determinant

change state

change position →

$$\psi_A(1,2,\cdots,N)=\frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_\alpha(x_1) & \psi_\alpha(x_2) & \cdots & \psi_\alpha(x_N) \\ \psi_\beta(x_1) & \psi_\beta(x_2) & & \\ \vdots & & \ddots & \\ \psi_\rho(x_1) & & & \psi_\rho(x_N) \end{vmatrix} \downarrow$$

antisymmetrized wavefunction

- For Fermions, the 2-particle wavefunction has to be anti-symmetrized

$$u_A(1,2)=\frac{1}{\sqrt{2}}\left[u_{E_1}(x_1)u_{E_2}(x_2)-u_{E_1}(x_2)u_{E_2}(x_1)\right]$$

example: 2 particles in a infinite well

$$\frac{1}{\sqrt{2}}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right)-\sin\left(\frac{\pi x_2}{a}\right)\sin\left(\frac{2\pi x_1}{a}\right)\right]$$

- 3-particle case

$$\psi_A(1,2,3)=\frac{1}{\sqrt{3!}}\left[\psi(1,2,3)-\psi(2,1,3)+\psi(2,3,1)\right.$$
$$\left.-\psi(3,2,1)+\psi(3,1,2)-\psi(1,3,2)\right]$$

the necessity for (anti-)symmertization

$$\psi_{S,A}(x_1,x_2)=\frac{1}{\sqrt{2}}\left[\psi_a(x_1)\psi_b(x_2)\pm\psi_a(x_2)\psi_b(x_1)\right]$$

- When two particles are close.
- How close? calculate the overlapping probability

$$\int\psi_a^*(x)\psi_b(x)dx$$

- If it is very small, we can treat them separably

Probability property

- Consider the probability for the particles are close $x_1 \sim x_2$

$$
\begin{aligned}
\psi_A &= \frac{1}{\sqrt{2}}\left[\psi_\alpha(x_1)\psi_\beta(x_2) - \psi_\beta(x_1)\psi_\alpha(x_2)\right] \\
&\sim \frac{1}{\sqrt{2}}\left[\psi_\alpha(x_1)\psi_\beta(x_1) - \psi_\beta(x_1)\psi_\alpha(x_1)\right] \\
&\sim 0
\end{aligned}
$$

$$
\begin{aligned}
\psi_S &= \frac{1}{\sqrt{2}}\left[\psi_\alpha(x_1)\psi_\beta(x_2) + \psi_\beta(x_1)\psi_\alpha(x_2)\right] \\
&\sim \frac{1}{\sqrt{2}}\left[\psi_\alpha(x_1)\psi_\beta(x_1) + \psi_\beta(x_1)\psi_\alpha(x_1)\right] \\
&\sim \sqrt{2}\psi_\alpha(x_1)\psi_\beta(x_1)
\end{aligned}
$$

Comparison with the distinguishable case

- Distinguishable at same position

$$\psi = \psi_{\alpha}(x_1)\psi_{\beta}(x_1) \qquad \psi^{*}\psi = \psi_{\alpha}^{*}(x_1)\psi_{\alpha}(x_1)\psi_{\beta}^{*}(x_1)\psi_{\beta}(x_1)$$

- Antisymmetric $\qquad \psi_A^{*}\psi_A = 0$

particles are more separated

- Symmetric $\qquad \psi_S^{*}\psi_S = 2\psi^{*}\psi$

particles are more closed to each other

spin wavefunction

- The spin states:
- singlet is anti-symmetric under interchange

$$\frac{1}{\sqrt{2}}\left(\chi_+^{(1)}\chi_-^{(2)} - \chi_-^{(1)}\chi_+^{(2)}\right)$$

- triplet is symmetric under interchange

$$\chi_+^{(1)}\chi_+^{(2)}$$

$$\frac{1}{\sqrt{2}}\left(\chi_+^{(1)}\chi_-^{(2)} + \chi_-^{(1)}\chi_+^{(2)}\right)$$

$$\chi_-^{(1)}\chi_-^{(2)}$$

Exchange force

- spatial wavefunction

$$\psi_S = \frac{1}{\sqrt{2}}\left[\psi_\alpha(x_1)\psi_\beta(x_2)+\psi_\beta(x_1)\psi_\alpha(x_2)\right]$$

$$\psi_A = \frac{1}{\sqrt{2}}\left[\psi_\alpha(x_1)\psi_\beta(x_2)-\psi_\beta(x_1)\psi_\alpha(x_2)\right]$$

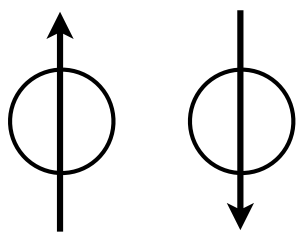
- Combining spin part together

spatial	spin	total
sym	asym(singlet)	asym
asym	sym(triplet)	asym

spatial-spin wavefunctions

- The probability density for $x_1 \sim x_2$ is very small for spin triplet.

- The probability density for $x_1 \sim x_2$ is slightly higher for spin singlet.



Coulomb interaction

- V for interparticle interaction is positive (same polarity)
- To reduce potential energy, separated particles are favored
- The spatial wavefunction is antisymmetric and the spin part is symmetric
- Called “exchange” interaction

Hartree theory

- To deal with the electron-electron interaction in a muliti-electron atom
- The effect is included in a local potential generated by all electrons
- The potential should obeys the properties

$$V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r}$$

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$$

$r \to 0$

$r \to \infty$

Procedures I

- With the guessed/modified V(r), one numerically solve all eigenstates $\psi_\alpha, \psi_\beta, \psi_\gamma$ and associated eigenenergies $E_\alpha, E_\beta, E_\gamma$
- Use Pauli exclusive principle to assign total wavefunction without considering particle interactions(but not antisymmetrized)
- Electron charge distributions are obtained from $|\psi_\alpha|^2, |\psi_\beta|^2, |\psi_\gamma|^2$

Procedures 2

- With charge distribution, the potential satisfies

$$\nabla^2 V = \frac{\rho}{\varepsilon_0} \qquad \rho = \rho_0 - e n_e$$

- Go back to step 1 with the modified V and recursively to obtain a converged V and

$\psi_\alpha, \psi_\beta, \psi_\gamma$

Bose system

- Bosons obey symmetrized wave functions

$$\psi_S = \frac{1}{\sqrt{2}}\left[\psi_\alpha(x_1)\psi_\beta(x_2) + \psi_\beta(x_1)\psi_\alpha(x_2)\right]$$

- We may put them in the same state $\alpha = \beta$

$$\psi_S = \frac{1}{\sqrt{2}}\left[\psi_\beta(x_1)\psi_\beta(x_2) + \psi_\beta(x_1)\psi_\beta(x_2)\right]$$

$$= \sqrt{2}\psi_\beta(x_1)\psi_\beta(x_2)$$

- The probability density

$$\psi_S^*\psi_S = 2\psi_\beta^*(x_1)\psi_\beta^*(x_2)\psi_\beta(x_1)\psi_\beta(x_2)$$

Distinguishable case

- For distinguishable particles, the wavefunction is

$$\psi = \psi_\alpha(x_1)\psi_\beta(x_2) = \psi_\beta(x_1)\psi_\beta(x_2)$$

- The probability density is

$$\psi^*\psi = \psi_\beta^*(x_1)\psi_\beta^*(x_2)\psi_\beta(x_1)\psi_\beta(x_2)$$

- Indistinguashability increases the probability

$$\psi_S^*\psi_S = 2\psi^*\psi$$

N-particle case

- Symmetrized N-particle wavefuncitons

$$\psi_S = \frac{1}{\sqrt{N!}}(N!)\psi_\beta(x_1)\psi_\beta(x_2)\cdots\psi_\beta(x_N)$$

- Probability density

$$\psi_S^*\psi_S = (N!)\psi_\beta^*(x_1)\psi_\beta^*(x_2)\cdots\psi_\beta^*(x_N)\psi_\beta(x_1)\psi_\beta(x_2)\cdots\psi_\beta(x_N)$$

- Enhancement in probability

$$\psi_S^*\psi_S = (N!)\psi^*\psi$$

Probability Enhancement

- For 1-particle $P_1 = \psi_\beta^* \psi_\beta$

- For N-particle $P_N = N!P_1^N = N!\left(\psi_\beta^* \psi_\beta\right)^N$

- For N+1 particle
$$P_{N+1} = (N+1)!P_1^{N+1} = (N+1)N!P_1^N P_1$$
$$= (N+1)P_N P_1$$

- The probability for more bosons joining together is enhanced