PHYS 4410

Quantum Mechanics 2

Spring 2023

Lecture 21

Exchange interactions

March 10

1 lecture 20: variational principle.

for any state $|\psi\rangle$

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0 .$$

Strategy: look for $|\psi\rangle$ out of some set ... w/ lowest E.

Qualitative ground state.

Today: 2 interacting spin-1/2 electrons in potential well.
whether spin singlet or triplet has lower energy.

(HW 7: Problem 3)

Our model: $H = \underset{\substack{\uparrow \\ \text{first particle}}}{H_1} + \underset{\substack{\uparrow \\ \text{second particle}}}{\overset{(p_2^2/2m)}{H_2}} + \underbrace{V_{int}}_{\text{interaction potential}}$

$\boxed{2}$ Review lecture 8: if $H = H_1 + H_2$

$$= \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \begin{cases} 0 & 0 \le x_1, x_2 \le L \\ \infty & \text{else} \end{cases}$$

$$\psi_1(x) = \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}$$

What's ground state?

$$|0\rangle = |\overset{n_1 n_2}{1\ 1}\rangle \otimes \frac{|\overset{s_1 s_2}{\uparrow\downarrow}\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$$

spin-1/2 $\to$ fermion

$$P_{12} |\psi\rangle = -|\psi\rangle$$

$\uparrow$ particle exchange

First excited state 4-fold degeneracy:

(singlet)

$$|S\rangle = \frac{|12\rangle + |21\rangle}{\sqrt{2}} \otimes \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} \quad \Big\}\ j=0$$

(triplet)

$$|t_1\rangle = \frac{|12\rangle - |21\rangle}{\sqrt{2}} \otimes |\uparrow\uparrow\rangle$$

$$|t_0\rangle = \frac{|12\rangle - |21\rangle}{\sqrt{2}} \otimes \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \quad \Bigg\}\ j=1$$

$$|t_{-1}\rangle = \frac{|12\rangle - |21\rangle}{\sqrt{2}} \otimes |\downarrow\downarrow\rangle.$$

$|\psi\rangle = |\text{position}\rangle \otimes |\text{spin}\rangle$

odd = even $\otimes$ odd

odd $\otimes$ even

$\boxed{3}$ Turn on interaction: $H = H_1 + H_2 + V_{int}$

$$V_{int} = U(|x_1 - x_2|)$$

Variational principle: $|0\rangle$, $|s\rangle$, $|t_1\rangle$ as "trial g.s. wave functions".

$$E_n = \frac{n^2\hbar^2\pi^2}{2mL^2}$$

$$\langle 0|H|0\rangle = \langle 0|H_1 + H_2 + V_{int}|0\rangle$$

$$= 2E_{n=1} + \langle 0|V_{int}|0\rangle = \frac{\hbar^2\pi^2}{mL^2} + \langle 0|V_{int}|0\rangle$$

$$\langle s|H|s\rangle = E_1 + E_2 + \langle s|V_{int}|s\rangle = \frac{5\hbar^2\pi^2}{2mL^2} + \langle s|V_{int}|s\rangle$$

$$\langle t_1|H|t_1\rangle = \frac{5}{2}\frac{\hbar^2\pi^2}{mL^2} + \langle t_1|V_{int}|t_1\rangle$$

$\boxed{4}$ If $|\psi\rangle = |\text{position}\rangle \otimes |\text{spin}\rangle$, then

$$\langle\psi|V_{int}|\psi\rangle = \langle\psi|\, U(x_1-x_2) \otimes \mathbb{1}\, |\psi\rangle$$

$$= \langle pos|U|pos\rangle \otimes \underbrace{\langle spin|\cancel{\mathbb{1}}|spin\rangle}_{1}$$

$$= \int_0^L dx_1 \int_0^L dx_2 \;\; U(x_1-x_2)\, |\psi(x_1,x_2)|^2 .$$

$$\langle 0|V_{int}|0\rangle = \langle \overset{n_1\, n_2}{1\,1}|\, U \,|1\,1\rangle = \int dx_1 dx_2 \;\; U(x_1-x_2) \Bigg| \underbrace{\frac{2}{L} \sin\frac{\pi x_1}{L} \sin\frac{\pi x_2}{L}}_{|\varphi_1(x_1)\varphi_1(x_2)|^2} \Bigg|^2$$

$$= \int dx_1\, dx_2 \;\; U(x_1-x_2) \underbrace{|\varphi_1(x_1)|^2}_{\text{prob. } x_1} \underbrace{|\varphi_1(x_2)|^2}_{\text{prob. } x_2}$$

$$= J_{11}$$ (direct interaction)

$\boxed{5}$ $\langle s | V_{int} | s \rangle = \int dx_1 dx_2 \, U(x_1 - x_2) \left| \frac{\psi_1(x_1)\psi_2(x_2) + \psi_2(x_1)\psi_1(x_2)}{\sqrt{2}} \right|^2$

$= 2 \cdot \int dx_1 dx_2 \, \frac{1}{2} |\psi_1(x_1)|^2 |\psi_2(x_2)|^2 U(x_1 - x_2) \Big\} J_{12}$ (direct int.)

$+ 2 \int dx_1 dx_2 \frac{1}{2} \psi_1(x_1)^* \psi_2(x_2)^* \psi_2(x_1) \psi_1(x_2) U(x_1 - x_2) \Big\} K_{12}$ ("exchange interaction")

$\langle s | H | s \rangle = \frac{5\hbar^2\pi^2}{2mL^2} + J_{12} + K_{12}$

What happens for $|t_1\rangle$?

$\psi_{t_1}(x_1, x_2) = \frac{\psi_1(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2)}{\sqrt{2}}$

$\langle t_1 | H | t_1 \rangle = \frac{5\hbar^2\pi^2}{2mL^2} + J_{12} - K_{12}$

6 Concrete example: "contact interaction"

$$V(x_1-x_2) = \alpha\, \underbrace{\delta(x_1-x_2)}$$

Dirac δ:

$$\delta(x) = \begin{cases} \infty & x=0 \\ 0 & x\neq 0 \end{cases}$$

$$\int_{-\infty}^{\infty} dx\, \delta(x) f(x) = f(0).$$

$$J_{nm} = \int_0^L dx_1 \int_0^L dx_2\, |\psi_n(x_1)|^2 |\psi_m(x_2)| \cdot \alpha\,\delta(x_1-x_2)$$

$$= \alpha \int_0^L dx_1\, |\psi_n(x_1)|^2 |\psi_m(x_1)|^2.$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}.$$

Explicit calc:

$$J_{11} = \frac{3\alpha}{2L}$$

$$J_{12} = \frac{\alpha}{L}.$$

Claim: $K_{12} = \frac{\alpha}{L}$. Why?

so $J_{12} - K_{12} = 0.$

In $|t_1\rangle$: $\psi_{t_1}(x_1, x_2) = -\psi_{t_1}(x_2, x_1)$; $\psi_{t_1}(x, x) = 0.$

$$\langle t_1 | V_{int} | t_1 \rangle = \alpha \int dx\, \cancelto{0}{|\psi_{t_1}(x,x)|^2} = 0.$$

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Summarize:

$$\langle 0|H|0\rangle = \frac{\pi^2\hbar^2}{mL^2} + \frac{3}{2}\frac{\alpha}{L}$$

$$\langle s|H|s\rangle = \frac{5}{2}\frac{\pi^2\hbar^2}{mL^2} + \frac{\alpha}{L}$$

$$\langle t_1|H|t_1\rangle = \frac{5}{2}\frac{\pi^2\hbar^2}{mL^2}$$

What's ground state?

(based on trial)

"g.s." $\alpha < 0$.

$\alpha > 0$

$E_t < E_s$

$$\frac{\pi^2\hbar^2}{mL^2} + \frac{3}{2}\frac{\alpha}{L} > \frac{5}{2}\frac{\pi^2\hbar^2}{mL^2}$$

or $\alpha > \frac{\pi^2\hbar^2}{mL}$,

$E_t < E_0$,

expect g.s. is $j=1$ (magnetic)

Punchline: "exchange interactions" can favor $|t\rangle$ over $|0\rangle$.

- atom/molecules: Hund's rule
- ferromagnetism.