

PHYS 2170
General Physics 3 for Majors
Fall 2021

Lecture 39

The independent particle approximation

December 3

1

Review bosons and fermions.

2 types of indistinguishable particles in QM:

boson

spin

$$s=0, 1, 2, 3, \dots$$

$$\vec{S}^2 = \hbar^2 s(s+1)$$

no restrictions
on # of bosons
in a state

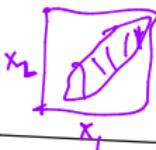
Symmetric:

$$\Psi(1, 2) = \Psi(2, 1)$$

$$\Psi(x_1, x_2) = \psi(x_1)\phi(x_2) + \psi(x_2)\phi(x_1)$$

"apparent
interaction"

$$|\Psi|^2$$



fermions

spin

$$s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots$$

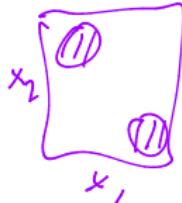
Pauli exclusion:
no 2 fermions
occupy same state

antisymmetric

$$\Psi(1, 2) = -\Psi(2, 1)$$

$$\Psi(x_1, x_2) = \psi(x_1)\phi(x_2) - \psi(x_2)\phi(x_1)$$

"repulsion"



2 What is the independent particle approximation?

$$E = K_1 + \dots + K_N - \frac{(Ne)e}{4\pi\epsilon_0 r_1} - \dots - \frac{Ne^2}{4\pi\epsilon_0 r_N}$$

\downarrow
 $\frac{p_1^2}{2M}$ (kinetic)

"Unwanted"

$$\begin{aligned}
 &+ \frac{e^2}{4\pi\epsilon_0 |r_1 - r_2|} \\
 &+ \dots + \frac{e^2}{4\pi\epsilon_0 |r_{N-1} - r_N|}
 \end{aligned}$$

\otimes nucleus

N

Z (or N) electrons

- begin by ignore interactions btwn electrons

$$E = \underbrace{\left[\frac{p_1^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0 r_1} \right]}_{E_1} + \underbrace{\left[\frac{p_2^2}{2m} - \frac{Ze^2}{4\pi\epsilon_0 r_2} \right]}_{E_2} + \dots$$

- if we know allowed E's of 1 particle,

$$E_{\text{total}} = E_{\#1} + E_{\#2} + \dots$$

Caveat:
if fermions,
Pauli exclusion
must be obeyed.

3

A quantum system has single-particle energy levels $\epsilon, 2\epsilon, 3\epsilon, \dots$. What is the ground state energy of 5 particles of spin $\frac{1}{2}$, 1, or $\frac{3}{2}$?

spin - $\frac{1}{2}$

fermions:

$$\begin{aligned} \text{total: } & \epsilon + \epsilon + 2\epsilon + 2\epsilon \\ & + 3\epsilon = 9\epsilon \\ & \vdots \end{aligned}$$



$$\begin{aligned} \epsilon & \xrightarrow{\uparrow} \quad \downarrow \\ S_z = +\frac{\hbar}{2} & \quad S_z = -\frac{\hbar}{2} \end{aligned}$$

Spin 1

$$\begin{aligned} \text{total energy} &= 5\epsilon \\ \text{bosons} & \end{aligned}$$

⋮



$$\begin{aligned} \epsilon & \xrightarrow{\downarrow} \text{any spin} \\ \epsilon & \xrightarrow{\downarrow} \text{any spin} \end{aligned}$$

$$\begin{aligned} \text{Spin } \frac{3}{2} & . \\ \text{total energy} &= 6\epsilon \end{aligned}$$

⋮

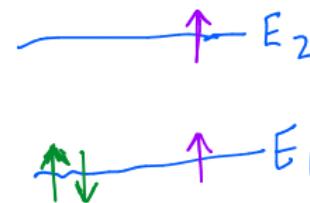
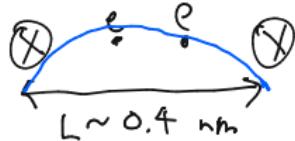


$$\begin{aligned} 2\epsilon & \xrightarrow{\downarrow} \text{any spin} \\ 2\epsilon & \end{aligned}$$

$$\begin{aligned} \epsilon & \xrightarrow{\uparrow} \quad \uparrow \quad \uparrow \quad \uparrow \\ S_z = -\frac{3}{2}\hbar, -\frac{1}{2}\hbar, \frac{1}{2}\hbar, \frac{3}{2}\hbar & \end{aligned}$$

4

Consider 2 electrons of mass $m \approx 10^{-30}$ kg in a solid between two atoms separated by $L \approx 4 \times 10^{-10}$ m. Suppose the electrons are modeled well by a “particle in a box” of length L . What is the ground state energy if the electrons have opposite/same spin?



$$\text{quantum "particle in a box" of length } L:$$

$$k_n = \frac{n\pi}{L} \quad (\rho = \hbar k) \quad \text{allowed wavelengths: } \lambda_n = \frac{2L}{n} \quad n=1, 2, 3, \dots$$

$$E_n = \frac{\rho^2}{2m} = \frac{\hbar^2}{2m} k_n^2 = \frac{\hbar^2 \pi^2}{2m L^2} n^2$$

$$\begin{aligned} \text{Opposite } S_z: E_{\min} &= 2E_1 = 2 \frac{\hbar^2 \pi^2}{2m L^2} \\ \text{Same } S_z: E_{\min} &= E_1 + 4E_1 \\ &= 5 \frac{\hbar^2 \pi^2}{2m L^2} \end{aligned}$$

Do you think the electrons will be closer or farther in the state with the same spin, or in the state with opposite spin?

Spatial wave function is antisym if both \uparrow : apparent repulsion
 $|\Delta x_{12}| \sim L/2$

opp spin: Sym spatial wave function; $|\Delta x_{12}| \sim L/4$

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Using that

$$\frac{e^2}{4\pi\epsilon_0} \sim 2 \times 10^{-28} \text{ J} \cdot \text{m}, \quad L \sim 4 \times 10^{-10} \text{ m}$$

estimate the *loss* in potential energy ΔU if the electrons are in the same-spin state, and the *gain* in kinetic energy. Which one wins out?

$$\begin{aligned}\Delta U &= V_{\text{same}} - V_{\text{opp}} = \underbrace{\frac{e^2}{4\pi\epsilon_0 |\Delta x_{\text{same}}|}}_{\text{Same-Spin}} - \underbrace{\frac{e^2}{4\pi\epsilon_0 |\Delta x_{\text{opp}}|}}_{\text{Opposite-Spin}} \\ &= \frac{e^2}{4\pi\epsilon_0} \left[\frac{1}{L_2} - \frac{1}{L_4} \right] \approx -\frac{2}{\sum} \frac{e^2}{4\pi\epsilon_0} \sim -1 \times 10^{-18} \text{ J}\end{aligned}$$

$$\Delta K = K_{\text{same}} - K_{\text{opp}} \sim 0.9 \times 10^{-18} \text{ J} \sim 3 \cdot \underbrace{\frac{\hbar^2 \pi^2}{2mL^2}}_{0.3 \times 10^{-18}}$$

$$(\Delta U + \Delta K) = -10^{-19} \text{ J} \quad : \quad \begin{array}{l} \text{Spontaneous aligned spin} \\ \downarrow \\ \text{magnetism in iron...} \end{array}$$

($\approx 5000 \text{ K}$)