

* Last week of classes!

SFF's!!

- * HW #13 : - Maybe some changes
- You can collaborate
- I will grade it

Today: Identical Particles

aka Intro to "Quantum Field Theory"

Fundamental Problem! Deserves much more time
than we can devote to it.

"Fermions" vs "Bosons": Relativistic Quantum Fields!

("half-integer spin")

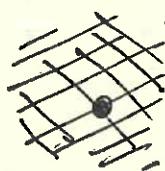
e.g. Spin-1/2

"Electrons"

"integer spin" e.g. spin-0, spin-1

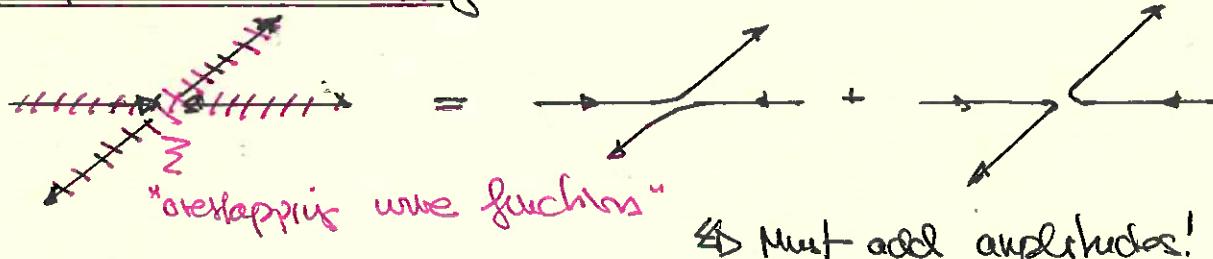
"photons" "photon"

Example: Helium Atom



→ two electrons. Completely overlapping
probability distributions.
Can't tell which is which!

Example: Rutherford Scattering



↳ Must add amplitudes!

We need a formalism to deal with this!

nb. There are choices for the formalism!

Permutation Symmetry: Wannier - The Notation & Intuition

Let $|a\rangle$ and $|b\rangle$ be "single particle states"

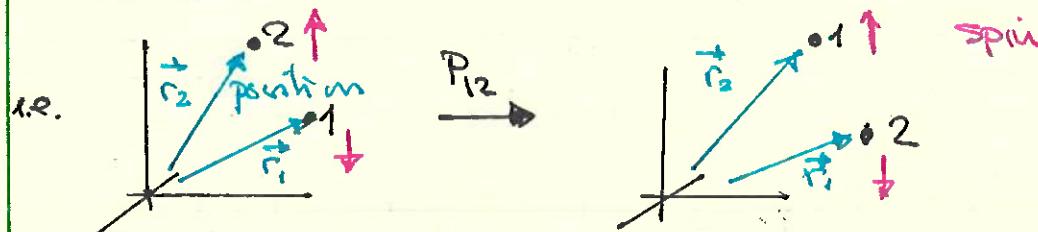
[aka "orbitals" to chemists]

$$\Leftrightarrow |a,b\rangle = |a\rangle \otimes |b\rangle = |a\rangle_1 |b\rangle_2$$

is a two particle state with #1 in $|a\rangle$ and #2 in $|b\rangle$

Exchange Operator P_{12}

$$P_{12} |a,b\rangle = |b,a\rangle \quad \text{i.e. } P_{12} (|a\rangle_1 |b\rangle_2) = |b\rangle_1 |a\rangle_2$$



Let $|\psi\rangle$ be an arbitrary two-particle state

Must have $P_{12}|\psi\rangle = e^{i\delta}|\psi\rangle$ so $|\psi\rangle$ is physical!

Also $P_{12}^2|\psi\rangle = e^{2i\delta}|\psi\rangle = |\psi\rangle$ Cancels: Anyons in 2D!!

$$\Leftrightarrow 2i\delta = 2\pi i \times n \Rightarrow \delta = n\pi \Rightarrow P_{12}|\psi\rangle = \pm |\psi\rangle$$

"Exchange Degeneracy"

$$|\psi_S\rangle = \frac{1}{\sqrt{2}}(|a,b\rangle + |b,a\rangle) \Rightarrow P_{12}|\psi_S\rangle = +|\psi_S\rangle$$

$$|\psi_A\rangle = \frac{1}{\sqrt{2}}(|a,b\rangle - |b,a\rangle) \Rightarrow P_{12}|\psi_A\rangle = -|\psi_A\rangle$$

Must be one or the other. But which one??

Note to the reader: Bosons and Fermions

nb. Need Relativistic Quantum Field Theory to "Prove"!!

Spin $S = 0, 1/2, \dots \Rightarrow |q\rangle = |q_s\rangle$ "Boson"

$S = 1/2, 3/2, 5/2, \dots \Rightarrow |q\rangle = |q_A\rangle$ "Fermion"

Note: $|a\rangle = |b\rangle \Rightarrow |q_A\rangle = 0$ "Pauli Exclusion Principle"

NOT TRUE FOR BOSONS! \Rightarrow "Superfluid Helium"

"Bose-Einstein Condensate"

Helium Atom: Good Problem to Work Through!

$$H = \frac{\vec{p}_1^2}{2m} + \frac{\vec{p}_2^2}{2m} - \frac{ze^2}{r_1} - \frac{ze^2}{r_2} + \frac{e^2}{|r_1 - r_2|}$$

"the Hard Part"

- Post-Hartree's Variational HIGM2c See 12.2
HGM3c See 7.4

- Density Functional Theory MOLSE See 7.6

Two Fermions*: Same Spatial State *Take spin-1/2

$$\text{let } |\alpha\rangle = |n; +\frac{1}{2}\rangle = |n\rangle |+\frac{1}{2}\rangle = |n; +\rangle = |n\rangle |+\rangle$$

$$|\beta\rangle = |n; -\frac{1}{2}\rangle = |n; -\rangle \text{ etc...}$$

We consciously say "one spin up the other down"
but this is inaccurate!

$$\begin{aligned} \text{Must have } |q\rangle &= |q_A\rangle = \frac{1}{\sqrt{2}} [|\alpha\rangle_1 |\beta\rangle_2 - |\beta\rangle_1 |\alpha\rangle_2] \\ &= |n\rangle \frac{1}{\sqrt{2}} [|+\rangle_1 |-\rangle_2 - |-\rangle_1 |+\rangle_2] \end{aligned}$$

Recall: Total spin = 0 state!!

Two Fermions: Arbitrary single particle states

"Slater Determinant"

* $2! = 2$ permutations

$$|\psi\rangle = \frac{1}{\sqrt{2}} \begin{vmatrix} |\alpha\rangle_1 & |\beta\rangle_1 \\ |\alpha\rangle_2 & |\beta\rangle_2 \end{vmatrix} = \frac{1}{\sqrt{2}} \left[|\alpha\rangle_1 |\beta\rangle_2 - |\beta\rangle_1 |\alpha\rangle_2 \right]$$

orthogonal!

Note: P_{12} reverses rows $\Rightarrow (-)$ sign is automatic!

Also $|\beta\rangle = |\alpha\rangle \Rightarrow$ Two identical columns $\Rightarrow \underline{\text{Zero!}}$

N Fermions: Orbital Generalization

$$|\psi\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} |\alpha\rangle_1 & |\beta\rangle_1 & |\gamma\rangle_1 & \dots \\ |\alpha\rangle_2 & |\beta\rangle_2 & |\gamma\rangle_2 & \dots \\ \vdots & \vdots & \vdots & \ddots \\ |\alpha\rangle_N & |\beta\rangle_N & |\gamma\rangle_N & \dots \end{vmatrix} \Rightarrow \underline{\text{Atoms!!}}$$

Second Quantization (i.e. Quantum Fields)

A Different Approach to multiparticle quantum mechanics

"The Bible": Quantum Theory of Many Particle Systems

Fetter & Waleckas McGraw-Hill (1971) \Rightarrow Dover

... and the "Bible" of Feynman & Drell.

Fock Space

Given eigenstates $|\alpha_1\rangle, |\alpha_2\rangle, \dots, |\alpha_i\rangle, \dots$

$\Leftrightarrow |\psi\rangle = (n_1, n_2, \dots, n_i, \dots) \rangle \quad n_i = \# \text{ of particles in } |\alpha_i\rangle$

$|0, 0, \dots, 0, \dots\rangle = |0\rangle$ "Vacuum"

$|0, 0, \dots, 1, \dots\rangle = |\alpha_i\rangle$ "Single particle state"

"Field operator" $a_i^+ |n_1, n_2, \dots, n_i, \dots\rangle \rightarrow |n_1, n_2, \dots, n_i + 1, \dots\rangle$

proportionality const TBD

Postulate that $a_i^+ |0\rangle = |\alpha_i\rangle$

$$\Leftarrow 1 = \langle \alpha_i | \alpha_i \rangle = [\langle 0 | a_i] [a_i^+ | 0 \rangle] = \langle 0 | a_i | \alpha_i \rangle$$

i.e. Need $a_i | \alpha_i \rangle = | 0 \rangle$

" a_i^+ and a_i behave like creation and annihilation"

Also postulate that $a_i | \alpha_j \rangle = 0$ if $i \neq j$

$$\Leftarrow a_i | \alpha_j \rangle = \delta_{ij} | 0 \rangle$$

Now $a_i^+ a_j^+ | 0 \rangle$ means "#1 in i, #2 in j"

$$\Leftarrow a_i^+ a_j^+ | 0 \rangle = \pm a_j^+ a_i^+ | 0 \rangle \quad \text{for Bosons/Fermions}$$

Generalize to multiparticle states:

$$a_i^+ a_j^+ - a_j^+ a_i^+ = 0 = [a_i^+, a_j^+] \quad \text{Bosons}$$

$$a_i^+ a_j^+ + a_j^+ a_i^+ = 0 = \{a_i^+, a_j^+\} \quad \text{Fermions}$$

Adjoint: $[a_i, a_j] = 0$ Bosons $\{a_i, a_j\} = 0$ Fermions

Number Operator $N_i = a_i^+ a_i$

$$\Leftarrow N = \sum_i N_i = \sum_i a_i^+ a_i$$

\Leftarrow Easy to make an "additive" single particle operator into a field operator!

e.g. k_i = kinetic energy in state $|\alpha_i\rangle$

$$\Leftarrow K = \sum_i k_i N_i = \sum_i k_i a_i^+ a_i$$

\Leftarrow Different bases, two-body operators, etc..

Applications of Second Quantization

RSW Chaps. 1

1) Degenerate Electron Gas (use Sec. 7.7.3)

$$H = H_{\text{el}} + H_b + H_{\text{el-b}} \quad \text{electrons w/ positive background}$$

$$\sum_i \frac{\vec{p}_i^2}{2m} + \sum_{ij} \frac{e^2}{4\pi \epsilon_0 r_{ij}}$$

"positive background" \Rightarrow uniform

FERMIONS!

Convert to momentum basis in second quantization
 ↳ Good model for an alkali metal like sodium!

2) Electromagnetic Field (use Sec. 7.8)

BOSONS!

"Big Box" solution of Maxwell's Equations

$$\hat{A}(\vec{r}, t) = \sum_{\vec{k}, \lambda} \hat{e}_{\vec{k}, \lambda} A_{\vec{k}, \lambda}(\vec{r}, t)$$

Individual solutions to wave equations

Not proportional to quantum fields!

$$\text{↪ } H = \sum_{\vec{k}, \lambda} \hbar \omega_k a_{\vec{k}, \lambda}^\dagger a_{\vec{k}, \lambda} + E_0 \quad \text{"vacuum energy"}$$

3) Klein-Gordon Field (use Sec. 8.1.5)

Thursday!

"the Negative Energy Problem Vanishes"