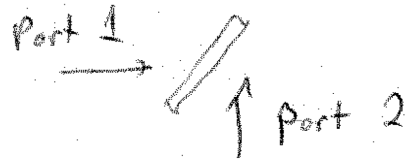
Physics 492 - Quantum II

Problem Set #8 Solutions

Problem 1: Identical particles on beam splitter

The beam splitter performs the following transformation on the single particle



$$|1\rangle \Longrightarrow \frac{1}{\sqrt{2}}\left(|1\rangle + i\,|2\rangle\right)$$

$$|2\rangle \Longrightarrow \frac{1}{\sqrt{2}}\left(|2\rangle + i\,|1\rangle\right)$$

Consider now 2 particles, A and B, A incident in port 1 and particle B in port 2

$$|1\rangle_A |2\rangle_B \rightarrow \left(\frac{|1\rangle_A + i\,|2\rangle_A}{\sqrt{2}}\right) \otimes \left(\frac{|2\rangle_B + i\,|1\rangle_B}{\sqrt{2}}\right)$$

$$= \frac{1}{2}\Big(\underbrace{|1\rangle_A |2\rangle_B}_{\text{(i)}} - \underbrace{|2\rangle_A |1\rangle_B}_{\text{(ii)}} + \underbrace{i\,|1\rangle_A |1\rangle_B}_{\text{(iii)}} + \underbrace{i\,|2\rangle_A |2\rangle_B}_{\text{(iv)}} \Big)$$

Process (i) (ii) (iii) (iv)

If these are identical particles, we must consider the exchanged case (B in 1, A in 2)

$$|2\rangle_A |1\rangle_B \rightarrow \frac{1}{2}\Big(\underset{(i)}{|2\rangle_A |1\rangle_B} - \underset{(ii)}{|1\rangle_A |2\rangle_B} + \underset{(iii)}{i|1\rangle_A |1\rangle_B} + \underset{(iv)}{i|2\rangle_A |2\rangle_B} \Big)$$

- For bosons (in same spin state) we must have a symmetric spatial wave function

$$\Rightarrow |\Psi\rangle_{in} = \frac{|1\rangle_A |2\rangle_B + |2\rangle_A |1\rangle_B}{\sqrt{2}} \Rightarrow \frac{i}{\sqrt{2}}\left(|1\rangle_A |1\rangle_B + |2\rangle_A |2\rangle_B \right)$$

Processes (i) and (ii) destructively interfere for bosons. They "bunch", both coming out together in the same port.

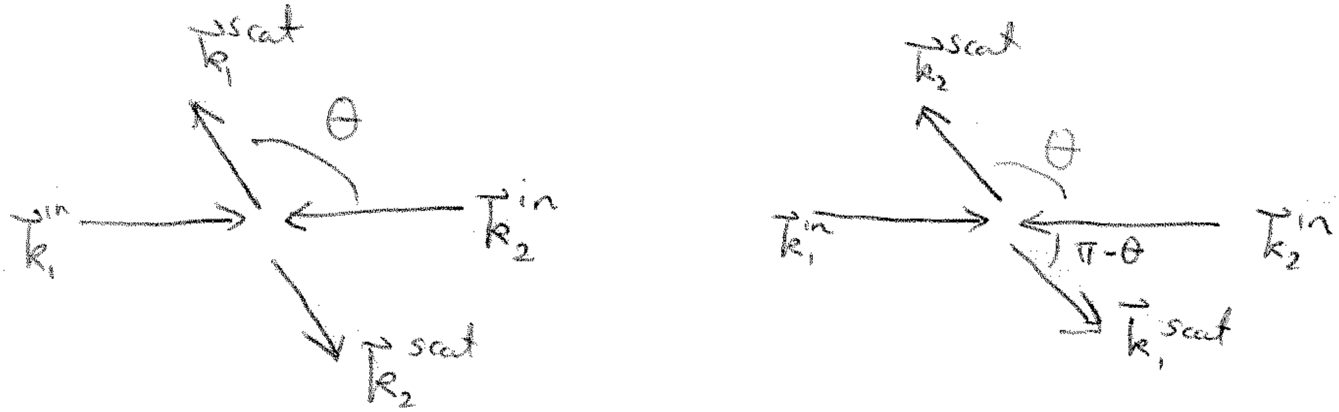
- For fermions, antisymmetric case

$$|\Psi_{in}\rangle = \frac{|1\rangle_A |2\rangle_B - |2\rangle_A |1\rangle_B}{\sqrt{2}} \Rightarrow \frac{1}{\sqrt{2}}\left(|1\rangle_A |2\rangle_B - |2\rangle_A |1\rangle_B \right)$$

Processes (iii) + (iv) destructive interfere for Fermions they "anti-bunch", never coming out in same port.

Now scattering in free space,

Two indistinguishable processes



The scattering amplitudes must be symmetrized or antisymmetrized depending upon whether the two particles are identical bosons or fermions.

Recall

$$\frac{d\sigma}{d\Omega} = \left| f(\vec{k}^{inc} \to \vec{k}^{scat}) \right|^2$$

where $\vec{k} = \vec{k}_1 - \vec{k}_2$ = relative momentum

Under exchange $\vec{k}_1 \leftrightarrow \vec{k}_2 \implies \vec{k}_{scat} \to -\vec{k}_{scat}$

$\implies$ For bosons / fermions

$$\boxed{\frac{d\sigma}{d\Omega} = \left| f(\vec{k}^{inc} \to \vec{k}^{scat}) \pm f(\vec{k}^{inc} \to -\vec{k}_{scat}) \right|^2}$$

(b) for spherical symmetry, $f(\vec{k}) = f(k, \theta)$

$$\underset{\text{scattered direction}}{\vec{k}}$$

$$\Rightarrow \quad \frac{d\sigma}{d\Omega} = \big| f(\underset{\vec{k}_s}{k,\theta}) \pm f(\underset{-\vec{k}_s}{k, \pi-\theta}) \big|^2$$

$$\Rightarrow \quad \boxed{\begin{aligned} \frac{d\sigma}{d\Omega} = {} & |f(k,\theta)|^2 + |f(k, \pi-\theta)|^2 \\ & \pm \big(\underbrace{f(k,\theta) f^*(k, \pi-\theta) + f^*(k,\theta) f(k, \pi-\theta)}_{= 2\mathrm{Re}\,(f(k,\theta) f^*(k, \pi-\theta))} \big) \end{aligned}}$$

(c) <u>Cancelled</u>: <u>Error in assignment</u>

Coulomb scattering (unsymmetrized)

$$f(k, \theta) = \frac{\gamma\, e^{2i\gamma \ln(\sin\frac{\theta}{2})}}{2k \sin^2(\theta/2)} \quad \text{where} \quad \gamma = \frac{me^2}{\hbar^2 k}$$

(Rutherford cross section

$$\frac{d\sigma}{d\Omega} = |f(k,\theta)|^2 = \frac{m^2 e^4}{4(\hbar k)^4} \frac{1}{\sin^4\frac{\theta}{2}}$$
)

→ Electrons in triplet state ⇒ Antisymmetric spatial

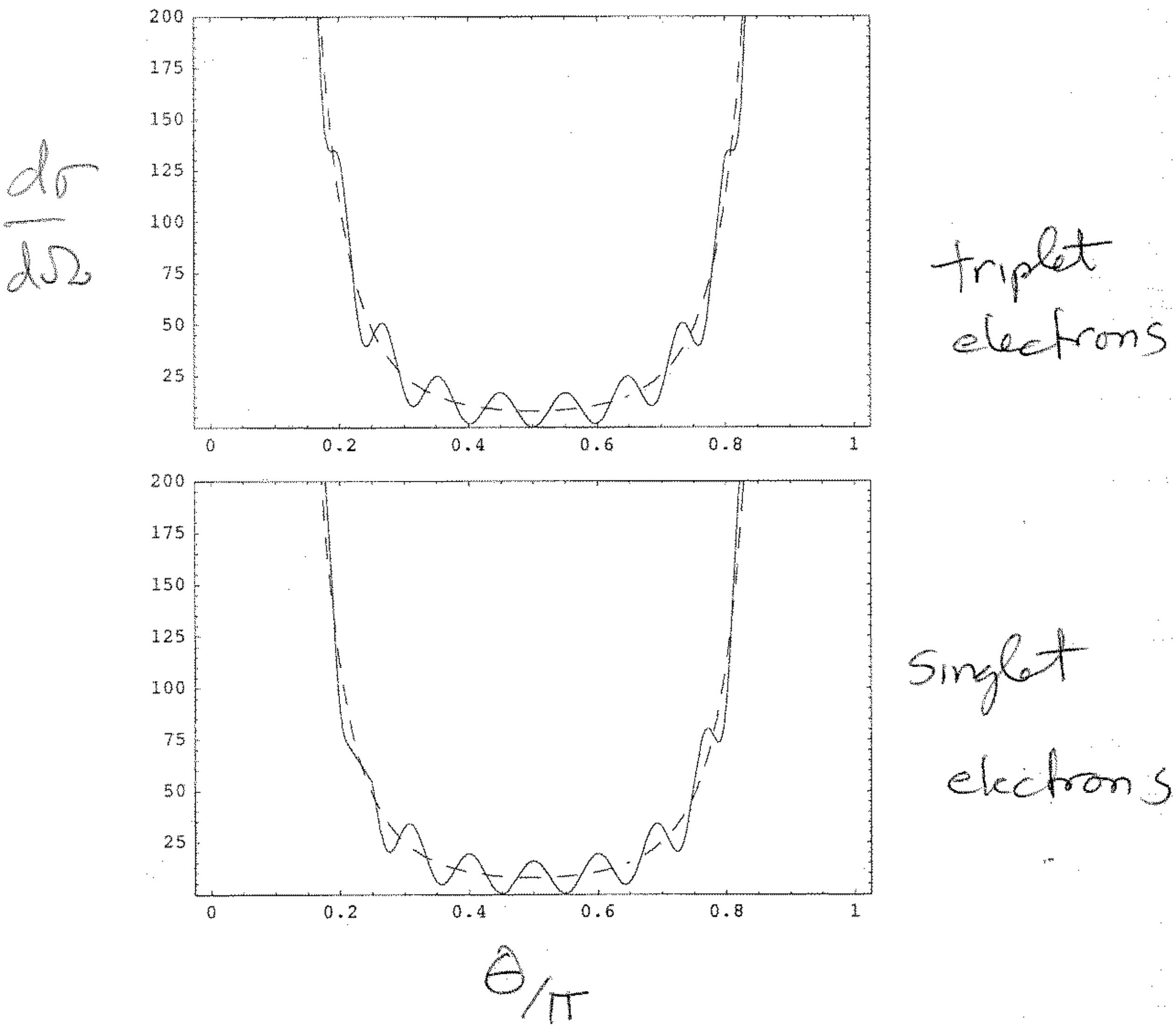
Electrons in singlet state ⇒ Symmetric spatial

$$\Rightarrow \boxed{\left.\frac{d\sigma}{d\Omega}\right|_{\substack{trip \\ sing}} = \frac{m^2 e^4}{4(\hbar k)^4}\left\{\frac{1}{\sin^4(\frac{\theta}{2})} + \frac{1}{\cos^4(\frac{\theta}{2})} \pm \frac{2\cos(2\gamma \ln(\tan^2\frac{\theta}{2}))}{(\sin\frac{\theta}{2}\cos\frac{\theta}{2})^2}\right\}}$$

Note: If the particles are <u>distinguishable</u>, the scattering cross-section for one particle to go into $\vec{k}_1$ and the other into $\vec{k}_2$ is the sum of $|f(k,\theta)|^2$ and $|f(k,\pi-\theta)|^2$

$$\Rightarrow \left.\frac{d\sigma}{d\Omega}\right| = \frac{m^2 e^4}{4(\hbar k)^4}\left\{\frac{1}{\sin^4(\frac{\theta}{2})} + \frac{1}{\cos^4(\frac{\theta}{2})}\right\}$$

The effect of the quantum statistics is <u>interference</u> between the two processes



The dashed curves shown $\frac{d\sigma}{d\Omega}$ if the particles are distinguishable. The interference effects due to exchange are shown. They can enhance and diminish the scattering probability into different directions.

Problem 2: Covalent bonds

(a) Classically, in order to bond two protons together, one must have the maximum negative charge density between them

"Bounding configuration"

Of course, this is not a stable configuration classically. One cannot bound a molecule solely with classical electrostatic force

The maximum repulsion occurs when the two electrons are farest away from each other

"Antibounding"

(b) We consider diatomic a Hydrogen molecule. The nuclei move in presence of the electron density associated with fixed orbitals (Born-Oppenheimer approximation). We approximate these as products of atomic orbitals, properly symmetrized.

$$\Rightarrow |\Psi_{12}\rangle = \left(\frac{|\phi_A\rangle_1 |\phi_B\rangle_2 \pm |\phi_B\rangle_1 |\phi_A\rangle_2}{\sqrt{2}} \right) \otimes |\chi\rangle$$

where $|\phi_A\rangle \doteq \phi_{1s}(\vec{r} + \frac{\vec{R}}{2})$ (1s orbital centered @ nucleus A)

$|\phi_B\rangle \doteq \phi_{1s}(\vec{r} - \frac{\vec{R}}{2})$ (1s orbital at nucleus B)

$|\chi\rangle$ = Spin state (singlet or triplet)

singlet $\to$ symmetric space

triplet $\to$ anti-symmetric space

The joint probability density for the two electrons to be half way between the two nuclei (the origin)

$$|\Psi_{12}(\vec{r}_1 = 0, \vec{r}_2 = 0)|^2$$

$$= \underbrace{|\phi_A(0)||\phi_B(0)|^2}_{\text{direct term}} \pm \underbrace{|\phi_A(0)|^2 \, |\phi_B(0)|^2}_{\text{exchange term}}.$$

$\Rightarrow$ • Singlet, constructive interference
electrons bunch together at origin
$\rightarrow$ Binding configuration

• Triplet, destructive interference
electrons maximally anti-bunched
$\Longrightarrow$ Anti binding configuration

(C) Sketch: Potential energy seen by nuclei as a function of R

- Small R → repulsive coulomb $\frac{e^2}{R}$
- $R \to \infty$ two atoms, no interaction
- Large but not infinite R, two configurations
  - singlet, lower energy
  - triplet, higher energy