

Assignment 2: Question 1

Wednesday, 30 March 2022 6:33 am

(1) Time-dependent Schrödinger Eqn for electron in hydrogen atom:

$$i\hbar \frac{\partial \psi(\underline{r}, t)}{\partial t} = \left[\frac{1}{2m} (\underline{p} + \frac{e}{c} \underline{A}(\underline{r}, t))^2 - \frac{e^2}{r} \right] \psi(\underline{r}, t)$$

In the dipole approximation, its spatial dependence is neglected. $\underline{A}(\underline{r}, t) \rightarrow \underline{A}(t)$. Want to show that the above equation can be transformed to:

$$i\hbar \frac{\partial \psi(\underline{r}, t)}{\partial t} = \left[\frac{\underline{p}^2}{2m} - \frac{e^2}{r} + e \underline{r} \cdot \vec{E}(t) \right] \psi(\underline{r}, t)$$

Solution:

$$i\hbar \frac{\partial \psi(\underline{r}, t)}{\partial t} = \left[\frac{1}{2m} \left[\underline{p}^2 + \frac{e^2}{c^2} \vec{A}^2 + 2 \frac{e \underline{p} \cdot \vec{A}}{c} \right] - \frac{e^2}{r} \right] \psi(\underline{r}, t)$$

$$i\hbar \frac{\partial \psi(\underline{r}, t)}{\partial t} = \left[\frac{\underline{p}^2}{2m} + \frac{e^2}{2mc^2} \vec{A}^2 + \frac{e \underline{p} \cdot \vec{A}}{mc} - \frac{e^2}{r} \right] \psi(\underline{r}, t)$$

It is known that the TDSE is invariant under gauge transformations of the type:

$$\begin{aligned} \vec{A} &\rightarrow \vec{A}' = \vec{A} + \nabla \phi \\ \phi &\rightarrow \phi' = \phi - \partial_t f \\ \psi &\rightarrow \psi' = e^{-i\phi'/\hbar} \psi \end{aligned} \quad \left. \begin{array}{l} \text{scalar function of choice} \\ \text{ } \end{array} \right\}$$

In order to obtain the desired form, (i.e. one that does not involve $\vec{A}(t)$), one can make a gauge transformation to the length gauge choosing:

$$f = -\vec{A}(t) \cdot \underline{r} \Rightarrow \vec{A}' = \vec{A} - \vec{A} = \underline{0}$$

$$\phi' = \phi - \partial_t f = \phi - \frac{\partial \vec{A} \cdot \underline{r}}{\partial t} = -\vec{E}(t) \cdot \underline{r} \quad (\text{in this case } \phi' \text{ can be chosen to be } \frac{e}{2mc} \vec{A}^2)$$

Hence, the TDSE in the length gauge is given by:

$$i\hbar \frac{\partial \psi(\underline{r}, t)}{\partial t} = \left(\frac{\underline{p}^2}{2m} - \frac{e^2}{r} + \vec{E}(t) \cdot \underline{r} \right) \psi(\underline{r}, t)$$

Assignment 2: Question 2

Wednesday, 30 March 2022 8:32 am

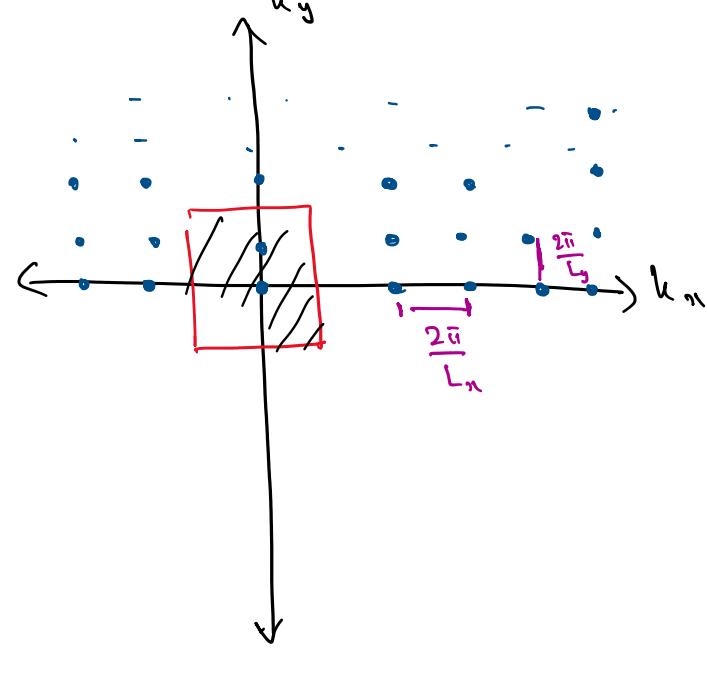
- a. Semiconductor quantum wells host 2D electron gas with conventional dispersion relation: $\epsilon_2 = \frac{p^2}{2m}$. Seek to compute the electronic density of states and compare its energy dependence with 3D case.

- b. Low energy electrons - gapless linear relativistic-like electronic spectrum ϵ_{sp} . It mimics dispersion for relativistic massless particles but with velocity $v=10^6 \text{ m/s}$ instead of c . \pm - conduction and valence bands which touch at $\mathbf{k}=\mathbf{0}$. Seek to compute electronic density of states and compare energy dependence with that for 2D electrons with quadratic dispersion

Solution:

- a. Density of states = number of states corresponding to a given energy (no. of states per unit energy)

$$d(E) = \frac{dN}{dE} \xrightarrow{\substack{\text{number of states} \\ \text{unit energy}}}$$



- Smallest reciprocal area A_i occupied by a single state:

$$A_i = \frac{(2\pi)^2}{A}$$

A = area of real 2D lattice

- Since states are close to each other, one can approximate the reciprocal area A_N occupied by states N^{2d} by a circular area. Each circle inside this circular area is a line of constant energy (since distance from origin to all k values on the circle line is given by the radius k). Area of circle enclosing the N^{2d} states:

$$A_N = \pi k^2$$

- ∴ To find N (no. of states), one can determine $\frac{A_N}{A_i} = \frac{\pi k^2}{(2\pi)^2} = \pi k^2 \cdot \frac{A}{4\pi^2} = \frac{k^2 A}{4\pi}$

- One must multiply the above by 2 in order to account for electron spin states:

$$N^{2d} = \frac{2 A k^2}{4\pi} = \frac{A k^2}{2\pi} = N^{2d}(k)$$

- Applying the dispersion relation, $\epsilon_{\text{sp}} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = E_p$,

$$\therefore E_p = \frac{\hbar^2 k^2}{2m} \Rightarrow k = \sqrt{\frac{2m E_p}{\hbar^2}}$$

$$\therefore N^{2d} = \frac{A m E}{\pi \hbar^2}$$

- ∴ $\frac{dN}{dE} = \frac{A m}{\pi \hbar^2}$ = density of states for a 2D-free electron gas

- One can compare the above result to the 3D case, wherein the density of states, $\frac{dN}{dE}$ is given by:

$$\frac{dN}{dE}_{(3D)} = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{E}$$

- One can note that the density of states for the 2D electron gas differs from the 3D analog in that the former is independent of the energy (i.e. it is constant with respect to the energy), while the latter exhibits an energy dependence $\frac{dN}{dE}_{(3D)} \propto E^{1/2} = \sqrt{E}$

- b. Seek to calculate the electronic density of states for low energy electrons in graphene. with The sum over all states \sum_p becomes an integral in momentum space as follows

$$\sum_p \rightarrow \int \frac{dp}{(2\pi\hbar)^2} \quad (\text{as we are working in two dimensions})$$

- The number of states N is given by:

$$N = A g_s \frac{\pi p_F^2}{(2\pi\hbar)^2} \Rightarrow n = \frac{N}{A} = \frac{2\pi p_F^2}{(2\pi\hbar)^2} \quad (*)$$

spin degeneracy = 2 for electrons

- Noting that $\epsilon_F = \pm p_F v$, one can observe that $\frac{\epsilon_F}{v} = p_F$. Substituting this for p_F into (*) yields:

$$\frac{\pm 2\pi \epsilon_F^2}{4\pi^2 \hbar^2 v} = n \Rightarrow n = \frac{\pm \epsilon_F^2}{2\pi \hbar^2} \Rightarrow \frac{dn}{dE} = \frac{\pm 2\epsilon_F}{2\pi \hbar^2} = \frac{\pm \epsilon_F}{\pi \hbar^2}$$

While the density of states for the 2D electron gas with the quadratic dispersion was independent of ϵ_F , the expression varies linearly with ϵ_F in the case of the low energy electrons in graphene.

Assignment 2: Question 3

Friday, 1 April 2022 1:46 pm

- Hamiltonian describing a coupling between two bosonic modes (with ladder operators a_p and b_p):

$$H = \sum_p [\epsilon_p^a a_p^\dagger a_p + \epsilon_p^b b_p^\dagger b_p + g_p a_p^\dagger b_p + g_p b_p^\dagger a_p]$$

ϵ_p^a and ϵ_p^b = dispersion relations and g_p parametrises the coupling strength:

- Consider:

$$u_p = \cos(\theta_p) a_p + \sin(\theta_p) b_p, \quad v_p = -\sin(\theta_p) a_p + \cos(\theta_p) b_p$$

- Seek to argue that u_p and v_p are also bosonic

- Wish to demonstrate that the transformation diagonalises the Hamiltonian H : if θ_p is given by:

$$\cos(2\theta_p) = \frac{\epsilon_p^a}{\Delta_p}, \quad \sin(2\theta_p) = \frac{g_p}{\Delta_p}$$

$$\epsilon_p^{av} = (\epsilon_p^a \pm \epsilon_p^b)/2 \quad \text{and} \quad \Delta_p = \sqrt{\epsilon_p^{av^2} + g_p^2}$$

- Seek to determine the spectrum of novel modes (u_p and v_p). Required to sketch it assuming $\epsilon_p^a = \frac{p^2}{2m}$ and $\epsilon_p^b = \delta$ (with $\delta > 0$)

Solution:

- Want to show that u_p and v_p are bosonic.
(i.e. they obey bosonic commutation relations):

Claim:

$$\textcircled{1} \quad [u_p, u_q] = [u_p^\dagger, u_q^\dagger] = 0 \quad \textcircled{2} \quad [v_p, v_q] = [v_p^\dagger, v_q^\dagger] = 0$$

$$\textcircled{3} \quad [u_p, u_q^\dagger] = \delta_{pq} \quad \textcircled{4} \quad [v_p, v_q^\dagger] = \delta_{pq}$$

$$\begin{aligned} \textcircled{1} \quad [u_p, u_q] &= [\cos(\theta_p) a_p + \sin(\theta_p) b_p, \cos(\theta_q) a_q + \sin(\theta_q) b_q] \\ &= [\cos(\theta_p) a_p, \cos(\theta_q) a_q] + [\cos(\theta_p) a_p, \sin(\theta_q) a_q] + [\sin(\theta_p) b_p, \cos(\theta_q) a_q] + [\sin(\theta_p) b_p, \sin(\theta_q) b_q] \\ &= \cos(\theta_p) \cos(\theta_q) [a_p, a_q] + \cos(\theta_p) \sin(\theta_q) [a_p, a_q] + \sin(\theta_p) \cos(\theta_q) [b_p, a_q] + \sin(\theta_p) \sin(\theta_q) [b_p, b_q] \\ &\Rightarrow [u_p, u_q] = 0 \quad ([u_p^\dagger, u_q^\dagger] = 0 \text{ by similar arguments}) \end{aligned}$$

$$\textcircled{2} \quad [u_p, u_q^\dagger] = \delta_{pq} : \text{Claim:}$$

$$\begin{aligned} &[\cos(\theta_p) a_p + \sin(\theta_p) b_p, \cos(\theta_q) a_q^\dagger + \sin(\theta_q) b_q^\dagger] \\ &= [\cos(\theta_p) a_p, \cos(\theta_q) a_q^\dagger] + [\cos(\theta_p) a_p, \sin(\theta_q) b_q^\dagger] + [\sin(\theta_p) b_p, \cos(\theta_q) a_q^\dagger] + [\sin(\theta_p) b_p, \sin(\theta_q) b_q^\dagger] \\ &= \cos(\theta_p) \cos(\theta_q) [a_p, a_q^\dagger] + \cos(\theta_p) \sin(\theta_q) [a_p, b_q^\dagger] + \sin(\theta_p) \cos(\theta_q) [b_p, a_q^\dagger] + \sin(\theta_p) \sin(\theta_q) [b_p, b_q^\dagger] \\ &= \cos(\theta_p) \cos(\theta_q) \delta_{pq} + \sin(\theta_p) \sin(\theta_q) \delta_{pq} = \delta_{pq} \end{aligned}$$

$$\textcircled{3} \quad [v_p, v_q] = 0 : \text{Claim:}$$

$$\begin{aligned} &[-\sin(\theta_p) a_p + \cos(\theta_p) b_p, -\sin(\theta_q) a_q + \cos(\theta_q) b_q] \\ &= [-\sin(\theta_p) a_p, -\sin(\theta_q) a_q] + [-\sin(\theta_p) a_p, \cos(\theta_q) b_q] + [\cos(\theta_p) b_p, -\sin(\theta_q) a_q] + [\cos(\theta_p) b_p, \cos(\theta_q) b_q] \\ &= \sin(\theta_p) \sin(\theta_q) [a_p, a_q] - \sin(\theta_p) \cos(\theta_q) [a_p, b_q] - \cos(\theta_p) \sin(\theta_q) [b_p, a_q] + \cos(\theta_p) \cos(\theta_q) [b_p, b_q] = 0 \\ &\Rightarrow [v_p^\dagger, v_q^\dagger] = 0 \text{ by similar arguments} \end{aligned}$$

$$\textcircled{4} \quad [v_p, v_q^\dagger] = \delta_{pq} : \text{Claim:}$$

$$\begin{aligned} &[-\sin(\theta_p) a_p + \cos(\theta_p) b_p, -\sin(\theta_q) a_q^\dagger + \cos(\theta_q) b_q^\dagger] \\ &= \sin(\theta_p) \sin(\theta_q) [a_p, a_q^\dagger] - \sin(\theta_p) \cos(\theta_q) [a_p, b_q^\dagger] - \cos(\theta_p) \sin(\theta_q) [b_p, a_q^\dagger] + \cos(\theta_p) \cos(\theta_q) [b_p, b_q^\dagger] \\ &= \sin(\theta_p) \sin(\theta_q) \delta_{pq} + \cos(\theta_p) \cos(\theta_q) \delta_{pq} \\ &= \delta_{pq} \end{aligned}$$

Hence, since the operators u_p and v_p obey the bosonic commutation relations listed above, they are bosonic in nature.

- One can attempt to diagonalise the Hamiltonian by first constructing a coefficient matrix H as follows:

$$H = \begin{bmatrix} \epsilon_p^a & g \\ g & \epsilon_p^b \end{bmatrix}$$

- One can then define the transformation matrix P as:

$$P = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \Rightarrow P^{-1} = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix}$$

- In order to diagonalise a matrix A , one must be able to write it in the form: $A = P D P^{-1}$

- In order to diagonalise H , one must first determine D . This can be done by computing:

$$\therefore D = P^{-1} H P = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix} \begin{bmatrix} \epsilon_a & g \\ g & \epsilon_b \end{bmatrix} \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

$$\therefore D = \begin{bmatrix} \frac{1}{2}(\epsilon_a + \epsilon_b) + (\epsilon_a - \epsilon_b) \cos(2\theta) + 2g \sin(\theta) & g \cos(2\theta) + (\epsilon_b - \epsilon_a) \sin(2\theta) \\ g \cos(2\theta) + (\epsilon_b - \epsilon_a) \sin(2\theta) & \frac{1}{2}(\epsilon_a + \epsilon_b) + (\epsilon_b - \epsilon_a) \cos(2\theta) - 2g \sin(2\theta) \end{bmatrix}$$

- One can substitute $\sin(2\theta) = \frac{g}{\Delta} = \frac{g}{\sqrt{\frac{1}{4}(\epsilon_a - \epsilon_b)^2 + g^2}}$ and $\cos(2\theta) = \frac{(\epsilon_a - \epsilon_b)}{\sqrt{\frac{1}{4}(\epsilon_a - \epsilon_b)^2 + g^2}}$

$$\therefore \cos(2\theta) = \frac{\epsilon_a - \epsilon_b}{2\sqrt{\frac{1}{4}(\epsilon_a - \epsilon_b)^2 + g^2}} \quad \text{and} \quad \sin(2\theta) = \frac{g}{2\sqrt{\frac{1}{4}(\epsilon_a - \epsilon_b)^2 + g^2}}$$

- Substituting these expressions into the off diagonal elements (both of which are equal to each other), one obtains:

$$\frac{g(\epsilon_a - \epsilon_b)}{2\sqrt{\frac{1}{4}(\epsilon_a - \epsilon_b)^2 + g^2}} \rightarrow \frac{(-\epsilon_a + \epsilon_b)g}{2\sqrt{\frac{1}{4}(\epsilon_a - \epsilon_b)^2 + g^2}} = 0$$

Since the off diagonal elements are equal to zero, one can conclude that D is indeed a diagonal matrix and hence, H is diagonalisable with the given values of $\cos(2\theta)$ and $\sin(2\theta)$.

- One can substitute the above expressions for $\cos(2\theta)$ and $\sin(2\theta)$ into the diagonal elements of the matrix D , which correspond to the eigenvalues of the Hamiltonian (i.e. the spectrum). Substituting and simplifying the expressions using Mathematica yields:

$$\epsilon_p^a = \frac{1}{2}(\epsilon_a + \epsilon_b) + \sqrt{g^2 + \left(\frac{1}{2}(\epsilon_a - \epsilon_b)\right)^2}$$

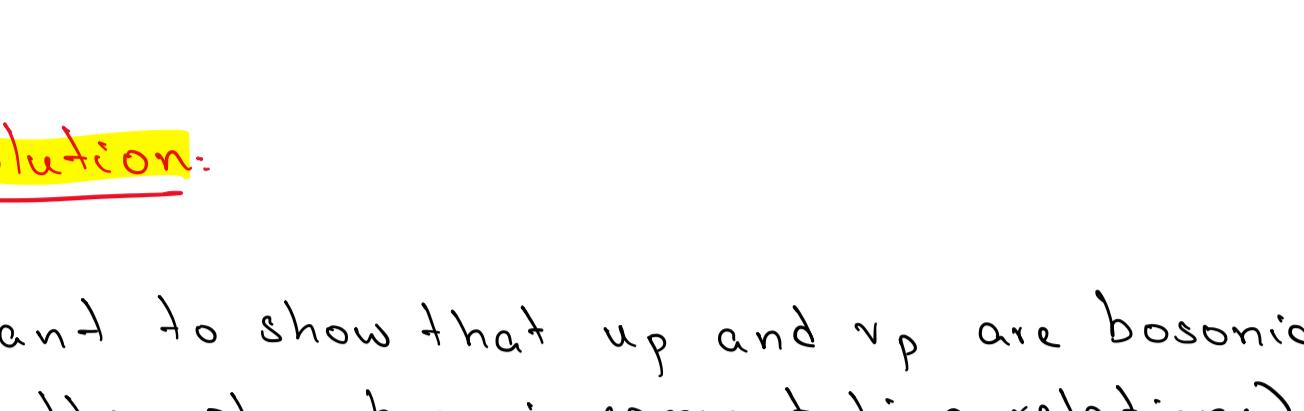
$$\epsilon_p^b = \frac{1}{2}(\epsilon_b - \epsilon_a) - \sqrt{g^2 + \left(\frac{1}{2}(\epsilon_a - \epsilon_b)\right)^2}$$

$$\epsilon_p^a = \epsilon_p^b \pm \Delta_p$$

- Substituting $\epsilon_a = \frac{p^2}{2m}$ and $\epsilon_b = \delta$ ($\delta > 0$) yields:

$$\epsilon_p^a = \frac{1}{2}\left(\delta + \frac{p^2}{2m}\right) \pm \sqrt{g^2 + \left(\frac{1}{2}\left(\frac{p^2}{2m} - \delta\right)\right)^2}$$

- Sketching the spectrum for the modes u and v (setting $\delta = 0.001$ and $g = 1$) results in the following:



Assignment 2: Question 4

Sunday, 3 April 2022 9:22 am

(4) a. By the conservation of energy:

$$\begin{aligned} E_f &= E_i \\ \therefore \frac{(p - q)^2}{2m} &= \frac{p^2}{2m} - cq \end{aligned}$$

$$\Rightarrow \frac{p^2}{2m} - \frac{2pq\cos(\theta)}{2m} + \frac{q^2}{2m} = \frac{p^2}{2m} - cq$$

$$\therefore -2\frac{pq\cos(\theta)}{2m} + \frac{q^2}{2m} = -cq$$

Take $q = |q|$ since LHS = and RHS must both be scalars

$$\therefore -2\frac{pq\cos(\theta)}{2m} + \frac{q^2}{2m} = -cq \Rightarrow -c = -2\frac{pq\cos(\theta)}{2m} + \frac{q}{2m}$$

From the above expression, it is evident that a phonon, which can only be emitted when its momentum $q > 0$, will be emitted when $v_0 > c$

$$b. P = \frac{2\pi}{\hbar} \sum_q |\langle b_q | H_{e-p} | i \rangle|^2 \delta(E_i - E_f)$$

$|i\rangle = e_{p_0}^\dagger |0\rangle$ and $|f\rangle = a_q^\dagger e_{p_0-q}^\dagger |0\rangle$ are the states before and after the phonon emission

- Seek to evaluate the angular distribution $I(\theta, \phi)$ of the phonon emission.

$$P = \int_0^{2\pi} \int_0^\pi \sin(\theta) d\theta d\phi I(\theta, \phi)$$

- One can first evaluate:

$$P = \frac{2\pi}{\hbar} \sum_q |\langle b_q | H_{e-p} | i \rangle|^2 \delta(E_f - E_i)$$

- Evaluating the matrix element above as follows yields:

$$\sum_q \langle 0 | a_q e_{p_0-q} \cdot \sum_{q'} g \sqrt{\frac{\hbar \omega_q}{2V}} e_{p_0-q'}^\dagger e_p (a_{q'}^\dagger + a_{-q'}) e_{p_0}^\dagger | 0 \rangle$$

$$= g \sqrt{\frac{\hbar}{2V}} \sum_q \langle 0 | a_q e_{p_0-q} \sum_{q'} \sqrt{\hbar \omega_{q'}} e_{p_0-q'}^\dagger e_p (a_{q'}^\dagger + a_{-q'}) e_{p_0}^\dagger | 0 \rangle$$

$$= g \sqrt{\frac{\hbar}{2V}} \sum_q \langle 0 | a_q e_{p_0-q} \underbrace{\left(\text{lowers phonon with momentum } q \right)}_{\substack{\text{lowers } e \\ \text{with } p_0-q}} \underbrace{\left(\text{raises } e \right)}_{\substack{\text{raises } e \\ \text{with } p_0-q}} \underbrace{\left(\text{lowers } e \text{ with } p_0 \right)}_{\substack{\text{lowers } e \\ \text{with } p_0}} \underbrace{\left(\text{raises } e \text{ with } p_0 \right)}_{\substack{\text{raises } e \\ \text{with } p_0}} \underbrace{\left(a_{q'}^\dagger + a_{-q'} \right)}_{\substack{\text{cannot act on } |0\rangle \\ (\text{cannot lower this any further})}} e_{p_0}^\dagger | 0 \rangle$$

$$\therefore \sum_q |\langle b_q | H_{e-p} | i \rangle|^2 = g^2 c \sum_q q \quad \left(\text{where } \omega_q = \frac{q c}{\hbar} \right)$$

$$\therefore P = \frac{2\pi}{\hbar} \cdot \frac{g^2 c}{2V} \sum_q q \delta(E_f - E_i)$$

- One can convert the sum into an integral as follows:

$$\sum_q \rightarrow V \int \frac{dq}{(2\pi\hbar)^3}$$

- Hence:

$$P = \frac{2\pi}{\hbar} \cdot \frac{g^2 c}{2V} \cdot \frac{V}{(2\pi\hbar)^3} \int q^2 dq \delta(E_f - E_i)$$

$$\therefore P = \frac{g^2 c}{2(2\pi)^2 \hbar^4} \int_0^{2\pi} \int_0^\pi \int_0^\infty q^2 \sin(\theta) dq d\theta d\phi \delta(E_f - E_i)$$

- Hence, by comparing the given expression for P with the one obtained above, it is clear that:

$$I(\theta, \phi) = \int_0^\infty q^2 \delta(E_f - E_i) dq$$

- One can write the Dirac Delta in terms of q as follows:

$$E_f = \frac{1}{2m} (p - q)^2 + qc$$

$$E_i = \frac{p^2}{2m}$$

$$\therefore E_f - E_i = \left(\frac{p^2}{2m} - \frac{2pq\cos(\theta)}{2m} + \frac{q^2}{2m} - \frac{p^2}{2m} \right) + qc - \frac{2pq\cos(\theta)}{2m} + \frac{q^2}{2m} - qc$$

$$= \frac{q}{2m} (-2p\cos(\theta) + q + 2mc)$$

$$\therefore \delta(E_f - E_i) = \delta \left(\frac{q}{2m} (-2p\cos(\theta) + q) \right) = \frac{1}{2m} \delta(q(-2p\cos(\theta) + q))$$

- Using the property that $\delta(dx) = \frac{1}{\alpha} \delta(x)$ for a scalar α , one can write

$$= \int_0^\infty \frac{2m}{q} \delta(q - (2p\cos(\theta) - 2mc)) q^3 dq = 2m (2p\cos(\theta) - 2mc)^2 k \quad \left(\text{where } k = \frac{g^2 c}{2(2\pi)^2 \hbar^4} \right)$$

- $I(\theta, \phi) = 2m (2m v_0 \cos(\theta) - mc)^2$. This varies quadratically with v_0

$$P = k \int_0^{2\pi} \int_0^\pi \sin(\theta) (2m (2m v_0 \cos(\theta) - mc)^2) d\theta d\phi$$

- Evaluating the above integral by Mathematica yields

$$P = \frac{8cq^2 m^3}{3\pi\hbar} (3c^2 + v_0^2)$$

- Hence it is evident that the probability P is a quadratic function of v_0 , however, there is no angular dependence