QM1 - Selected Problems for the Exam 2017 - Suggested Solutions

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Question

Discuss possible (pure and mixed) states of spin 1/2 “pointing” along a given direction.

Full Question (2014, 1)

a. Find the density matrix of a spin 1/2 state “pointing” along (θ, φ) direction. Is this a pure state. Repeat the above but for a (mixed) state having probability w_1 to have the spin along this direction. What happens for $w_1 = 1/2$?

b. Consider two orthonormal states $|\psi_1\rangle$ and $|\psi_2\rangle$. You are asked to compare a linear combination $|\psi\rangle = a\,|\psi_1\rangle + b\,|\psi_2\rangle$ with the density matrix $\rho = w_1\,|\psi_1\rangle\,\langle\psi_1| + w_2\,|\psi_2\rangle\,\langle\psi_2|$ with $w_1 = |a|^2$ and $w_2 = |b|^2$. Do they describe the same state? What are the similarities? The differences? Explain in as many details as you can.

c. Think roughly of ”coherence” as sensitivity to phases. In this understanding which are the above two states? Are they totally coherent? Are they totally incoherent? Argument your answer.

d. In a general $N \times N$ density matrix one often calls the off diagonal matrix elements ρ_{ij} $(i \neq j)$ by names ”coherences”. Does this mean that when all coherences vanish one has an incoherent state? When in your understanding a density matrix describes a totally incoherent state?

e. Give arguments for why one needs a bilocal $\rho\,(x, x_0)$ and can not get away with just $\rho\,(x, x)$.

Solution Outline

a

1. Write a general form of the density matrix: $\rho = \frac{1}{2}\left(1 + \boldsymbol{P} \cdot \boldsymbol{\sigma}\right)$, $P\left(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta\right)$.
2. $\mathrm{Tr}\left[\rho^2\right]$ to check pure/mixed state.
3. Rotate the spin to z direction and write $\rho = \begin{pmatrix} w_1 & 0 \\ 0 & w_2 \end{pmatrix}$.

Solution

a

We can write the density matrix, using Pauli matrices, as follows

$$\rho = \frac{1}{2}\left(1 + \boldsymbol{P}\cdot\boldsymbol{\sigma}\right) \tag{1.1}$$

where $\boldsymbol{P} = \langle\boldsymbol{\sigma}\rangle$ is the polarization vector. $\boldsymbol{P}$ can be written as

$$\boldsymbol{P} = |\boldsymbol{P}|\,\hat{P} = P\left(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta\right) \tag{1.2}$$

and therefore we can write ρ as follows,

$$\begin{aligned}
\rho &= \frac{1}{2}\left(1 + P\hat{P}\cdot\boldsymbol{\sigma}\right)\\
&= \frac{1}{2}\left[1 + P\left(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta\right)\cdot\left(\sigma_x, \sigma_y, \sigma_z\right)\right]\\
&= \frac{1}{2}\left[1\cdot\mathbb{I} + P\left(\sin\theta\cos\varphi\sigma_x + \sin\theta\sin\varphi\sigma_y + \cos\theta\sigma_z\right)\right]\\
&= \frac{1}{2}\left[\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} + P\left(\sin\theta\cos\varphi\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} + \sin\theta\sin\varphi\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} + \cos\theta\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right)\right]\\
&= \frac{1}{2}\begin{pmatrix}1 + P\cos\theta & P\sin\theta\cos\varphi - iP\sin\theta\sin\varphi\\ P\sin\theta\cos\varphi + iP\sin\theta\sin\varphi & 1 - P\cos\theta\end{pmatrix}\\
&= \frac{1}{2}\begin{pmatrix}1 + P\cos\theta & P\sin\theta\left(\cos\varphi - i\sin\varphi\right)\\ P\sin\theta\left(\cos\varphi + i\sin\varphi\right) & 1 - P\cos\theta\end{pmatrix}\\
&= \frac{1}{2}\begin{pmatrix}1 + P\cos\theta & P\sin\theta e^{-i\varphi}\\ P\sin\theta e^{i\varphi} & 1 - P\cos\theta\end{pmatrix}
\end{aligned} \tag{1.3}$$

In order to check whether this is in a pure state, we will check if $\mathrm{Tr}\left[\rho^2\right] = 1$. So first,

$$\begin{aligned}
\rho^2 &= \frac{1}{4}\begin{pmatrix}1 + P\cos\theta & P\sin\theta e^{-i\varphi}\\ P\sin\theta e^{i\varphi} & 1 - P\cos\theta\end{pmatrix}\begin{pmatrix}1 + P\cos\theta & P\sin\theta e^{-i\varphi}\\ P\sin\theta e^{i\varphi} & 1 - P\cos\theta\end{pmatrix}\\
&= \frac{1}{4}\begin{pmatrix}\left(1 + P\cos\theta\right)^2 + P^2\sin^2\theta & \left(1 + P\cos\theta\right)P\sin\theta e^{-i\varphi} + \left(1 - P\cos\theta\right)P\sin\theta e^{-i\varphi}\\ \left(1 + P\cos\theta\right)P\sin\theta e^{i\varphi} + \left(1 - P\cos\theta\right)P\sin\theta e^{i\varphi} & \left(1 - P\cos\theta\right)^2 + P^2\sin^2\theta\end{pmatrix}\\
&= \frac{1}{4}\begin{pmatrix}\left(1 + P\cos\theta\right)^2 + P^2\sin^2\theta & 2P\sin\theta e^{-i\varphi}\\ 2P\sin\theta e^{i\varphi} & \left(1 - P\cos\theta\right)^2 + P^2\sin^2\theta\end{pmatrix}
\end{aligned} \tag{1.4}$$

and the trace is

$$\begin{aligned}
\mathrm{Tr}\left[\rho^2\right] &= \frac{1}{4}\left[\left(1 + P\cos\theta\right)^2 + P^2\sin^2\theta + \left(1 - P\cos\theta\right)^2 + P^2\sin^2\theta\right]\\
&= \frac{1}{4}\left[1 + 2P\cos\theta + P^2 + 1 - 2P\cos\theta + P^2\right]\\
&= \frac{1}{2}\left[1 + P^2\right]
\end{aligned} \tag{1.5}$$

which means that it will be a pure state only if $P = \pm 1$, namely when the spin is fully polarized. If the spin is polarized in (θ, φ) direction, we can rotate the axis where it is polarized in z direction, where $\varphi = 0$ and $\theta = 0$. So we get

$$\rho = \frac{1}{2}\begin{pmatrix}1 + P & 0\\ 0 & 1 - P\end{pmatrix} \equiv \begin{pmatrix}w_1 & 0\\ 0 & w_2\end{pmatrix} \tag{1.6}$$

For a mixed state, as we already mentioned, $|P| < 1$ and therefore,

$$0 < w_1 < 1 \tag{1.7}$$
$$0 < w_2 < 1 \tag{1.8}$$

For $w_1 = 1/2$ we get

$$\rho = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} = \frac{1}{2} \cdot \mathbb{I} \tag{1.9}$$

and therefore it is a maximally mixed state, in which we will get equal probability for every direction (no matter the basis).

b

<u>The first case:</u>

$$|\psi\rangle = a\,|\psi_1\rangle + b\,|\psi_2\rangle \tag{1.10}$$

therefore the density matrix is

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} a \\ b \end{pmatrix} \begin{pmatrix} a^* & b^* \end{pmatrix} = \begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix} \tag{1.11}$$

and by normalization, $\langle\psi|\psi\rangle = 1$ so

$$|a|^2 + |b|^2 = w_1 + w_2 = 1 \tag{1.12}$$

Is this a pure state?

$$\begin{aligned} \mathrm{Tr}\left[\rho^2\right] &= \mathrm{Tr}\left[\begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix}\begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix}\right] \\ &= \mathrm{Tr}\left[\begin{pmatrix} |a|^4 + |a|^2|b|^2 & ab^*\left(|a|^2 + |b|^2\right) \\ a^*b\left(|a|^2 + |b|^2\right) & |b|^4 + |a|^2|b|^2 \end{pmatrix}\right] \\ &= |a|^4 + |b|^4 + 2|a|^2|b|^2 \\ &= \left(|a|^2 + |b|^2\right)^2 \\ &= (w_1 + w_2)^2 \\ &= 1 \end{aligned} \tag{1.13}$$

hence this is a pure state.

<u>The second case:</u>
The density matrix is

$$\rho = w_1\,|\psi_1\rangle\langle\psi_1| + w_2\,|\psi_2\rangle\langle\psi_2| = \begin{pmatrix} w_1 & 0 \\ 0 & w_2 \end{pmatrix} = \begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix} \tag{1.14}$$

and has no information about the phase. Is this a pure state?

$$\mathrm{Tr}\left[\rho^2\right] = \mathrm{Tr}\left[\begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix}\begin{pmatrix} |a|^2 & 0 \\ 0 & |b|^2 \end{pmatrix}\right] = |a|^4 + |b|^4 < 1 \tag{1.15}$$

hence this is a mixed state.

Both cases have the same probability $w_1 = |a|^2$ of finding the system in state $|\psi_1\rangle$, and the same probability $w_2 = |b|^2$ for state $|\psi_2\rangle$. The difference is the off-diagonal terms which tell about the phase of each state, or more precisely the difference between their phases.

c

The second case is a mixed state and thus it lacks some information about the phases. If $w_1 = w_2 = 1/2$ (maximally mixed state), $\rho \propto \mathbb{I}$ and therefore it is diagonal in any basis and have no phase information at all. Therefore, this state is incoherent and in the case of maximally pure state it will be fully incoherent. The first case describes a pure state. It has the full description as a linear sum of states, and therefore the density matrix has all the information about the relative phase between $|\psi_1\rangle$ and $|\psi_2\rangle$. Therefore, this state is coherent.

d

Not necessarily. If the density matrix is not in a maximally mixed state, we can rotate it such that we will have off-diagonal elements ("coherences"), and therefore it will (apparently) not describe a totally incoherent state. However, if the density matrix is in a maximally mixed state ($\rho \propto \mathbb{I}$), the state will be totally incoherent. A fully coherent state will be where we have all the information about the phases, namely a pure state.

e

Let us take an orthonormal basis $\{\phi_n(x)\}$ and expand $\rho(x, x')$ as follows,

$$\rho(x, x') = \langle x| \rho |x'\rangle = \sum_{nm} \langle x|m\rangle \langle m| \rho |n\rangle \langle n|x'\rangle = \sum_{nm} \rho_{mn} \phi_m(x) \phi_n^*(x') \tag{1.16}$$

Therefore,

$$\rho_{mn} = \int dx \int dx'\, \phi_m^*(x) \phi_n(x') \rho(x, x') \tag{1.17}$$

So in order to have a full description of the density matrix, including the coherences ($m \neq n$), one must use $\rho(x, x')$ and can not get away with just $\rho(x, x)$.

2

Question

Consider the energy levels of a (spinless) charged particle moving in the (x, y) plane in a magnetic field of an infinitely long cylinder of radius R placed parallel to the z axis with a uniform magnetic field inside and zero field outside. Disregard any other forces apart of those coming from the magnetic field of the cylinder.

Solution Outline

1. Get $\boldsymbol{A}$ from the magnetic field $\boldsymbol{B}$. Get $\boldsymbol{A} \parallel \hat{\varphi}$ and $H = \frac{\boldsymbol{p}^2}{2M} - \frac{e}{2Mc}\left(p_\varphi A_\varphi + A_\varphi p_\varphi\right) + \frac{e^2 A_\varphi^2}{2Mc^2}$. Write H_{in} and H_{out}.
2. Guess $\psi(r, \varphi) = \chi(r)\, e^{im\varphi}$ where $\chi(r) = u(r)\, r^n$, get $n = -1/2$.
3. Rearrange $H_{\text{in}}\chi(\boldsymbol{r}) = E\chi(\boldsymbol{r})$ to $H_{\text{in}}u(\boldsymbol{r}) = Eu(\boldsymbol{r})$ and write the Hamiltonian as $H_{\text{in}} = H_0 + V_{\text{in}}^{\text{eff}}(\boldsymbol{r})$. Do the same for H_{out}.
4. Find minimum for each region, and find the conditions for bound states.

Solution

The Hamiltonian is

$$H = \frac{\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2}{2M} + eA_0 \tag{2.1}$$

The magnetic field is

$$\boldsymbol{B} = \begin{cases} B_0\hat{z} & r \le R \\ 0 & r > R \end{cases} \tag{2.2}$$

Finding A inside $(r \le R)$:

$$\text{flux} = \pi r^2 B_0 = \iint \boldsymbol{B} d\boldsymbol{s} = \iint (\nabla \times \boldsymbol{A})\, d\boldsymbol{s} \overset{\text{Stokes}}{=} \oint \boldsymbol{A} d\boldsymbol{l} = A_\varphi \cdot 2\pi r \qquad \Longrightarrow \qquad A_\varphi = \frac{B_0 r}{2} \tag{2.3}$$

Finding A inside $(r > R)$:

$$\text{flux} = \pi R^2 B_0 = \iint \boldsymbol{B} d\boldsymbol{s} = \iint (\nabla \times \boldsymbol{A})\, d\boldsymbol{s} \overset{\text{Stokes}}{=} \oint \boldsymbol{A} d\boldsymbol{l} = A_\varphi \cdot 2\pi r \qquad \Longrightarrow \qquad A_\varphi = \frac{B_0 R^2}{2r} \tag{2.4}$$

Therefore the vector potential is

$$\boldsymbol{A} = A_\varphi \hat{\varphi} = \begin{cases} \frac{B_0 r}{2}\hat{\varphi} & r \le R \\ \frac{B_0 R^2}{2r}\hat{\varphi} & r > R \end{cases} \tag{2.5}$$

Inserting $\boldsymbol{A}$ into the Hamiltonian will give

$$\begin{aligned} H &= \frac{\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2}{2M} + e\cancelto{0}{A_0} \\ &= \frac{\boldsymbol{p}^2}{2M} - \frac{e}{2Mc}\left(\boldsymbol{p}\boldsymbol{A} + \boldsymbol{A}\boldsymbol{p}\right) + \frac{e^2 \boldsymbol{A}^2}{2Mc^2} \\ &= \frac{\boldsymbol{p}^2}{2M} - \frac{e}{2Mc}\left(p_\varphi A_\varphi + A_\varphi p_\varphi\right) + \frac{e^2 A_\varphi^2}{2Mc^2} \end{aligned} \tag{2.6}$$

Let us focus on Hamiltonian in two different regions

$$H = \begin{cases} H_{\text{in}} & r \leq R \\ H_{\text{out}} & r > R \end{cases} \tag{2.7}$$

For the region $r \leq R$ we get

$$H_{\text{in}} = \frac{\boldsymbol{p}^2}{2M} - \frac{eB_0}{4Mc}\left(p_\varphi r + rp_\varphi\right) + \frac{e^2B_0^2r^2}{8Mc^2} = \frac{\boldsymbol{p}^2}{2M} - \frac{eB_0L_z}{2Mc} + \frac{e^2B_0^2r^2}{8Mc^2} \tag{2.8}$$

Denoting $\omega_c = \frac{eB_0}{2Mc}$, and ignoring the non interesting solution for z dimension (free particle),

$$H_{\text{in}} = \frac{p_r^2}{2M} + \frac{p_\varphi^2}{2M} - \omega_c L_z + \frac{1}{2}M\omega_c^2r^2 \tag{2.9}$$

Guessing a separable solution of the form

$$\psi\left(r,\varphi\right) = \chi\left(r\right)e^{im\varphi} \tag{2.10}$$

By the Sch. equation,

$$\begin{aligned} E\psi &= H\psi \\ &= \left[\frac{p_r^2}{2M} + \frac{p_\varphi^2}{2M} - \omega_c L_z + \frac{1}{2}M\omega_c^2r^2\right]\chi\left(r\right)e^{im\varphi} \\ &= \left[-\frac{\hbar^2}{2M}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)\right) - \frac{\hbar^2}{2M}\left(\frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}\right) - \omega_c\hbar m + \frac{1}{2}M\omega_c^2r^2\right]\chi\left(r\right)e^{im\varphi} \\ &= \left[-\frac{\hbar^2}{2M}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)\right) + \frac{\hbar^2m^2}{2Mr^2} - \omega_c\hbar m + \frac{1}{2}M\omega_c^2r^2\right]\chi\left(r\right)e^{im\varphi} \end{aligned} \tag{2.11}$$

We will write $\chi\left(r\right)$ in the standard form $\chi\left(r\right) = u\left(r\right)r^n$, and let us find n as follows,

$$\begin{aligned} \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\chi\left(r\right)}{\partial r}\right) &= \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\left(u\left(r\right)r^n\right)\right) \\ &= \frac{1}{r}\frac{\partial}{\partial r}\left(\frac{\partial u\left(r\right)}{\partial r}r^{n+1} + nu\left(r\right)r^n\right) \\ &= \frac{1}{r}\left(\frac{\partial^2u\left(r\right)}{\partial r^2}r^{n+1} + \left(n+1\right)\frac{\partial u\left(r\right)}{\partial r}r^n + n\frac{\partial u\left(r\right)}{\partial r}r^n + n^2u\left(r\right)r^{n-1}\right) \\ &= \frac{\partial^2u\left(r\right)}{\partial r^2}r^n + \left(2n+1\right)\frac{\partial u\left(r\right)}{\partial r}r^{n-1} + n^2u\left(r\right)r^{n-2} \end{aligned} \tag{2.12}$$

Our objective is to reach to a Sch. equation of the form $Hu\left(r\right) = -\frac{\hbar^2}{2M}\frac{\partial^2u(r)}{\partial r^2} + V^{\text{eff}}\left(r\right)u\left(r\right)$, so we cannot have a first derivative of $u\left(r\right)$. Therefore, we will demand that the middle term will be zero (for every r), so,

$$\left(2n+1\right)\frac{\partial u\left(r\right)}{\partial r}r^{n-1} = 0 \quad\Longrightarrow\quad n = -\frac{1}{2} \tag{2.13}$$

Hence $\chi(r) = u(r)/\sqrt{r}$, and therefore

$$H_{\text{in}} \frac{u(r)}{\sqrt{r}} = -\frac{\hbar^2}{2M}\left(\frac{1}{\sqrt{r}}\frac{\partial^2 u(r)}{\partial r^2} + \frac{1}{4}\frac{u(r)}{r^{5/2}}\right) + \left[\frac{\hbar^2 m^2}{2Mr^2} - \omega_c \hbar m + \frac{1}{2}M\omega_c^2 r^2\right]\frac{u(r)}{\sqrt{r}}$$

$$H_{\text{in}} u(r) = -\frac{\hbar^2}{2M}\frac{\partial^2 u(r)}{\partial r^2} + \left[-\frac{\hbar^2}{8Mr^2} + \frac{\hbar^2 m^2}{2Mr^2} - \omega_c \hbar m + \frac{1}{2}M\omega_c^2 r^2\right] u(r)$$

$$H_{\text{in}} u(r) = -\frac{\hbar^2}{2M}\frac{\partial^2 u(r)}{\partial r^2} + \underbrace{\left[\frac{\hbar^2}{2Mr^2}\left(m^2 - \frac{1}{4}\right) - \omega_c \hbar m + \frac{1}{2}M\omega_c^2 r^2\right]}_{V_{\text{in}}^{\text{eff}}(r)} u(r) \tag{2.14}$$

For the region $r > R$ we get

$$\begin{aligned} H_{\text{out}} &= \frac{\boldsymbol{p}^2}{2M} - \frac{eB_0R^2}{4Mc}\left(p_\varphi \frac{1}{r} + \frac{1}{r}p_\varphi\right) + \frac{e^2B_0^2R^4}{8Mc^2r^2} \\ &= \frac{\boldsymbol{p}^2}{2M} - \frac{eB_0R^2 L_z}{2Mcr^2} + \frac{e^2B_0^2R^4}{8Mc^2r^2} \\ &= \frac{\boldsymbol{p}^2}{2M} - \frac{\omega_c R^2}{r^2}L_z + \frac{1}{2}M\omega_c^2\frac{R^4}{r^2} \end{aligned} \tag{2.15}$$

Which gives similar calculation that results in

$$H_{\text{out}} u(r) = -\frac{\hbar^2}{2M}\frac{\partial^2 u(r)}{\partial r^2} + \left[\frac{\hbar^2}{2Mr^2}\left(m^2 - \frac{1}{4}\right) - \frac{\omega_c R^2 \hbar m}{r^2} + \frac{1}{2}M\omega_c^2\frac{R^4}{r^2}\right] u(r)$$

$$H_{\text{out}} u(r) = -\frac{\hbar^2}{2M}\frac{\partial^2 u(r)}{\partial r^2} + \underbrace{\frac{1}{r^2}\left[\frac{\hbar^2}{2M}\left(m^2 - \frac{1}{4}\right) - \omega_c R^2 \hbar m + \frac{1}{2}M\omega_c^2 R^4\right]}_{V_{\text{out}}^{\text{eff}}(r)} u(r) \tag{2.16}$$

Hence we got the following effective potential in the two regions:

$$V_{\text{in}}^{\text{eff}}(r) = \frac{\hbar^2}{2Mr^2}\left(m^2 - \frac{1}{4}\right) - \omega_c \hbar m + \frac{1}{2}M\omega_c^2 r^2 \tag{2.17}$$

$$V_{\text{out}}^{\text{eff}}(r) = \frac{1}{r^2}\left[\frac{\hbar^2}{2M}\left(m^2 - \frac{1}{4}\right) - \omega_c R^2 \hbar m + \frac{1}{2}M\omega_c^2 R^4\right] \tag{2.18}$$

Inside: Let us find minimum of $V_{\text{in}}^{\text{eff}}(r)$,

$$0 = \left.\frac{\partial V_{\text{in}}^{\text{eff}}(r)}{\partial r}\right|_{r_{\text{m}}} = -\frac{\hbar^2}{Mr_{\text{m}}^3}\left(m^2 - \frac{1}{4}\right) + M\omega_c^2 r_{\text{m}} \tag{2.19}$$

$$r_{\text{m}} = \left[\frac{\hbar^2}{M^2\omega_c^2}\left(m^2 - \frac{1}{4}\right)\right]^{1/4} \tag{2.20}$$

which means that there will be a minimum if $m^2 > 1/4$, therefore $m \neq 0$ (since m is an integer). Moreover, in this region we have the condition $r_{\text{m}} < R$, which also gives

$$m^2 < \frac{M^2\omega_c^2 R^4}{\hbar^2} + \frac{1}{4} \tag{2.21}$$

The ground level energy (at r_{m}) will be,

$$\begin{aligned}
V_{\mathrm{in}}^{\mathrm{eff}}\left(r_{\mathrm{m}}\right) &= \frac{\hbar^2}{2Mr_{\mathrm{m}}^2}\left(m^2-\frac{1}{4}\right)-\omega_c\hbar m+\frac{1}{2}M\omega_c^2 r_{\mathrm{m}}^2 \\
&= \frac{1}{2}\hbar\omega_c\sqrt{m^2-\frac{1}{4}}-\omega_c\hbar m+\frac{1}{2}\hbar\omega_c\sqrt{m^2-\frac{1}{4}} \\
&= \hbar\omega_c\left(\sqrt{m^2-\frac{1}{4}}-m\right)
\end{aligned} \tag{2.22}$$

therefore for every $m>0$ we get $V_{\mathrm{in}}^{\mathrm{eff}}\left(r_{\mathrm{m}}\right)<0$ (the condition demands $m>1/4$ but m is an integer so we get $m>0$, or equivalently $m\geq 1$).

Outside: The outer effective potential $V_{\mathrm{out}}^{\mathrm{eff}}\left(r\right)$ will be repulsive if $V_{\mathrm{out}}^{\mathrm{eff}}\left(r\right)>0$, namely, the critical point where $V_{\mathrm{out}}^{\mathrm{eff}}\left(r\right)=0$ is

$$\begin{aligned}
\frac{1}{r^2}\left[\frac{\hbar^2}{2M}\left(m^2-\frac{1}{4}\right)-\omega_c R^2\hbar m+\frac{1}{2}M\omega_c^2 R^4\right] &= 0 \\
m^2-\frac{2M\omega_c R^2 m}{\hbar}+\frac{M^2\omega_c^2 R^4}{\hbar^2}-\frac{1}{4} &= 0 \\
m &= \frac{\frac{2M\omega_c R^2}{\hbar}\pm\sqrt{\frac{4M^2\omega_c^2R^4}{\hbar^2}-\frac{4M^2\omega_c^2R^4}{\hbar^2}+1}}{2} \\
m &= \frac{M\omega_c R^2}{\hbar}\pm\frac{1}{2}
\end{aligned} \tag{2.23}$$

Hence, $V_{\mathrm{out}}^{\mathrm{eff}}\left(r\right)>0$ where $m>\frac{M\omega_c R^2}{\hbar}+\frac{1}{2}$ or $m<\frac{M\omega_c R^2}{\hbar}-\frac{1}{2}$. Namely,

$$\left|m-\frac{M\omega_c R^2}{\hbar}\right|>\frac{1}{2} \tag{2.24}$$

Conclusions

To summarize,

$$\begin{cases}
m^2>\frac{M^2\omega_c^2R^4}{\hbar^2}+\frac{1}{4} & \left(r_{\mathrm{m}}>R\right) & \text{no bound state} \\
m^2<\frac{M^2\omega_c^2R^4}{\hbar^2}+\frac{1}{4}, \quad m>0 & \left(V_{\mathrm{in}}^{\mathrm{eff}}\left(r_{\mathrm{m}}\right)<0\right) & \text{bound state} \\
m^2<\frac{M^2\omega_c^2R^4}{\hbar^2}+\frac{1}{4}, \quad m<0 & \left(V_{\mathrm{in}}^{\mathrm{eff}}\left(r_{\mathrm{m}}\right)>0\right) & \text{decaying to continuum}
\end{cases} \tag{2.25}$$

In the case of $R\to\infty$, we get $r<R$ for every r, meaning that there is only one region of the effective potential, that for large r ($r\gg\sqrt{\frac{\hbar}{M\omega_c}}$),

$$V_{\mathrm{in}}^{\mathrm{eff}}\left(r\right)\propto r^2 \tag{2.26}$$

so there is no decaying to continuum and there are only bound states. The degeneracy must appear since we moved from a continuum energy spectrum to a discrete one. In any case there is also a degeneracy in z direction.

3

Question

Assume that the a potential $V(x)$ in a form of a barrier is added to the Landau levels problem. Discuss what will happen. What will an added uniform electric field do to your results?

Solution Outline

1. Choose the gauge $\boldsymbol{A} = (0, Bx, 0)$ since it is convenient choose it so that we have only one dimension (x, where the potential exists).

2. Discuss about the symmetry breaking for translations. The potential will lift the degeneracy of states (of a free particle).

3. If $V(x)$ is generally given, explore different cases of the shape and the location of the potential. Draw how it will affect the energy spectrum.

Solution

In this problem we will ignore the solutions in the z direction since in any case we have this degree of freedom. Let us first consider an Hamiltonian with the absence a potential $V(x)$, and use the gauge $\boldsymbol{A} = (0, Bx, 0)$. Thus, the Hamiltonian will be

$$H = \frac{p_x^2}{2M} + \frac{1}{2}M\omega_c^2 (x - x_0)^2 \tag{3.1}$$

where $\omega_c = \frac{eB}{Mc}$ and $x_0 = \frac{\hbar k_y}{M\omega_c}$. The energy is $E_n = \hbar\omega_c (n + 1/2)$ and depends only in one quantum number n and not in k_y. However we are still dealing with two degrees of freedom on the $x-y$ plane, so therefore we have a degeneracy of states. For each Landau level n we have infinite states with the quantum number k_y of the same energy. The choice of the gauge is arbitrary (as long as it produces the same magnetic field), so it does not have to be k_y, but in any choice there will be only one relevant quantum number.

Uniform electric field

Adding a uniform electric field, $V(x) = -eEx$, will give the following Hamiltonian

$$H = \frac{p_x^2}{2M} + \frac{1}{2}M\omega_c^2 (x - x_0)^2 - eEx \tag{3.2}$$

which can be written as follows,

$$\begin{aligned}
H &= \frac{p_x^2}{2M} + \frac{1}{2}M\omega_c^2 x^2 - M\omega_c^2 x x_0 + \frac{1}{2}M\omega_c^2 x_0^2 - eEx \\
&= \frac{p_x^2}{2M} + \frac{1}{2}M\omega_c^2 x^2 - x\left(M\omega_c^2 x_0 + eE\right) + \frac{1}{2}M\omega_c^2 x_0^2 \\
&= \frac{p_x^2}{2M} + \frac{1}{2}M\omega_c^2 \left(x - \left(x_0 + \frac{eE}{M\omega_c^2}\right)\right)^2 - \frac{1}{2}M\omega_c^2 \left(x_0 + \frac{eE}{M\omega_c^2}\right)^2 + \frac{1}{2}M\omega_c^2 x_0^2 - \frac{1}{2}\frac{e^2E^2}{M\omega_c^2} \\
&= \frac{p_x^2}{2M} + \frac{1}{2}M\omega_c^2 \left(x - \left(x_0 + \frac{eE}{M\omega_c^2}\right)\right)^2 - eEx_0 - \frac{1}{2}\frac{e^2E^2}{M\omega_c^2} - \frac{1}{2}\frac{e^2E^2}{M\omega_c^2} \\
&= \frac{p_x^2}{2M} + \frac{1}{2}M\omega_c^2 \left(x - \underbrace{\left(x_0 + \frac{eE}{M\omega_c^2}\right)}_{\tilde{x}_0}\right)^2 - eEx_0 - \underbrace{\frac{e^2E^2}{M\omega_c^2}}_{\text{const}}
\end{aligned}$$

Denoting $\tilde{x}_0 = x_0 + \frac{eE}{M\omega_c^2}$,

$$H = \underbrace{\frac{p_x^2}{2M} + \frac{1}{2}M\omega_c^2 \left(x - \tilde{x}_0\right)^2}_{H_{\text{HO}}} - eEx_0 \tag{3.3}$$

and therefore the energies are

$$E_{n,k_y} = \hbar\omega_c \left(n + \frac{1}{2}\right) - \frac{\hbar eEk_y}{m\omega_c^2} = \hbar\omega_c \left(n + \frac{1}{2}\right) - \frac{cE\hbar k_y}{B} \tag{3.4}$$

Now the energies depend on two quantum numbers. The potential $V\left(x\right) = -eEx$ lifts the degeneracy of the Landau levels, and break the symmetry for translations in x.

4

Question

In this problem you are asked to make a connection between the Hilbert space of photon states and the real space. As an example consider a one photon state which at some moment of time is localized at a point $\boldsymbol{r} = \boldsymbol{r}_0$. Understand what "localized" may mean. Discuss other examples of building photon states with a given "presence" in the real space (say a wave packet, etc).

Solution Outline

1. Write a general single photon state: $|\psi\rangle = \int d^3k\, \phi(\boldsymbol{k})\, a^\dagger_{\boldsymbol{k}} |0\rangle$.
2. Write the electric field operator. Show that $\langle E(\boldsymbol{r})\rangle = 0$ and find $\left\langle E^2(\boldsymbol{r})\right\rangle$.
3. Show that if setting $\phi(\boldsymbol{k}) = e^{-i\boldsymbol{k}\boldsymbol{r}_0}/\sqrt{k}$, we get localization by getting $\left\langle E^2(\boldsymbol{r})\right\rangle \sim \delta(\boldsymbol{r} - \boldsymbol{r}_0)$.
4. For time dependence use the Heisenberg picture, $a^\dagger_{\boldsymbol{k}}(t) = a^\dagger_{\boldsymbol{k}} e^{-i\omega t}$.
5. For a moving photon change the distribution of $\phi(\boldsymbol{k})$ from isotropic to anisotropic in $\boldsymbol{k}$ direction. $\phi(\boldsymbol{k}) \sim \frac{e^{i\boldsymbol{k}\boldsymbol{r}_0}}{\sqrt{k}} e^{-(\boldsymbol{k}-\boldsymbol{k}_0)^2}$.

Solution

The most general single photon state (ignoring polarization) can be written as follows,

$$|\psi\rangle = \int d^3k\, \phi(\boldsymbol{k})\, a^\dagger_{\boldsymbol{k}} |0\rangle \tag{4.1}$$

where $\int d^3k\, |\phi(\boldsymbol{k})|^2 = 1$, by normalization. The electric field operator is

$$E(\boldsymbol{r}) \sim i \int d^3k\, \sqrt{k} \left(a_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{r}} - a^\dagger_{\boldsymbol{k}} e^{-i\boldsymbol{k}\boldsymbol{r}} \right) \tag{4.2}$$

The first moment of the electric field:

$$\begin{aligned}
\langle E(\boldsymbol{r})\rangle &= \langle\psi|E(\boldsymbol{r})|\psi\rangle \\
&\sim i \int d^3q \int d^3q' \int d^3k\, \langle 0|\, \phi^*(\boldsymbol{q})\, a_{\boldsymbol{q}} \sqrt{k} \left(a_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{r}} - a^\dagger_{\boldsymbol{k}} e^{-i\boldsymbol{k}\boldsymbol{r}} \right) \phi(\boldsymbol{q}')\, a^\dagger_{\boldsymbol{q}'} |0\rangle \\
&\sim i \int d^3q \int d^3q' \int d^3k\, \sqrt{k} \phi^*(\boldsymbol{q})\, \phi(\boldsymbol{q}') \left[e^{i\boldsymbol{k}\boldsymbol{r}} \underbrace{\langle 0|\, a_{\boldsymbol{q}} a_{\boldsymbol{k}} a^\dagger_{\boldsymbol{q}'} |0\rangle}_{0} - e^{-i\boldsymbol{k}\boldsymbol{r}} \underbrace{\langle 0|\, a_{\boldsymbol{q}} a^\dagger_{\boldsymbol{k}} a^\dagger_{\boldsymbol{q}'} |0\rangle}_{0} \right] \\
&= 0
\end{aligned} \tag{4.3}$$

The second moment of the electric field:

$$\begin{aligned}
\left\langle E^2(\boldsymbol{r})\right\rangle &= \langle\psi|E^2(\boldsymbol{r})|\psi\rangle \\
&\sim - \int d^3q \int d^3q' \int d^3k \int d^3k'\, \langle 0|\, \phi^*(\boldsymbol{q})\, a_{\boldsymbol{q}} \sqrt{kk'} \left(a_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{r}} - a^\dagger_{\boldsymbol{k}} e^{-i\boldsymbol{k}\boldsymbol{r}} \right) \left(a_{\boldsymbol{k}'} e^{i\boldsymbol{k}'\boldsymbol{r}} - a^\dagger_{\boldsymbol{k}'} e^{-i\boldsymbol{k}'\boldsymbol{r}} \right) \phi(\boldsymbol{q}')\, a^\dagger_{\boldsymbol{q}'} |0\rangle \\
&\sim - \int d^3q \int d^3q' \int d^3k \int d^3k'\, \sqrt{kk'} \phi^*(\boldsymbol{q})\, \phi(\boldsymbol{q}') \left[\langle 0|\, a_{\boldsymbol{q}} \left(a_{\boldsymbol{k}} e^{i\boldsymbol{k}\boldsymbol{r}} - a^\dagger_{\boldsymbol{k}} e^{-i\boldsymbol{k}\boldsymbol{r}} \right) \left(a_{\boldsymbol{k}'} e^{i\boldsymbol{k}'\boldsymbol{r}} - a^\dagger_{\boldsymbol{k}'} e^{-i\boldsymbol{k}'\boldsymbol{r}} \right) a^\dagger_{\boldsymbol{q}'} |0\rangle \right]
\end{aligned} \tag{4.4}$$

Keeping only the terms that consist of equal number of creation and annihilation operators (the rest will be zero),

$$\begin{aligned}
\left\langle E^2\left(\boldsymbol{r}\right)\right\rangle &\sim \int d^3q\int d^3q'\int d^3k\int d^3k'\,\sqrt{kk'}\phi^*\left(\boldsymbol{q}\right)\phi\left(\boldsymbol{q}'\right)\left[e^{i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}}\left\langle 0\right| a_{\boldsymbol{q}}a_{\boldsymbol{k}}a^\dagger_{\boldsymbol{k}'}a^\dagger_{\boldsymbol{q}'}\left|0\right\rangle + e^{-i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}}\left\langle 0\right| a_{\boldsymbol{q}}a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}'}a^\dagger_{\boldsymbol{q}'}\left|0\right\rangle\right]\\
&\sim \int d^3q\int d^3q'\int d^3k\int d^3k'\,\sqrt{kk'}\phi^*\left(\boldsymbol{q}\right)\phi\left(\boldsymbol{q}'\right)\left[e^{i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}}\left(\delta\left(\boldsymbol{q}-\boldsymbol{k}'\right)\delta\left(\boldsymbol{q}'-\boldsymbol{k}\right)+\delta\left(\boldsymbol{q}-\boldsymbol{q}'\right)\delta\left(\boldsymbol{k}-\boldsymbol{k}'\right)\right)\right.\\
&\quad\left.+e^{-i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}}\delta\left(\boldsymbol{q}-\boldsymbol{k}\right)\delta\left(\boldsymbol{q}'-\boldsymbol{k}'\right)\right]\\
&\sim \int d^3q\int d^3k\int d^3k'\,\sqrt{kk'}\left[e^{i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}}\left(\phi^*\left(\boldsymbol{q}\right)\phi\left(\boldsymbol{k}\right)\delta\left(\boldsymbol{q}-\boldsymbol{k}'\right)+\phi^*\left(\boldsymbol{q}\right)\phi\left(\boldsymbol{q}\right)\delta\left(\boldsymbol{k}-\boldsymbol{k}'\right)\right)\right.\\
&\quad\left.+\phi^*\left(\boldsymbol{q}\right)\phi\left(\boldsymbol{k}'\right)e^{-i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}}\delta\left(\boldsymbol{q}-\boldsymbol{k}\right)\right]\\
&\sim \int d^3k\int d^3k'\,\sqrt{kk'}\phi^*\left(\boldsymbol{k}'\right)\phi\left(\boldsymbol{k}\right)e^{i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}}+\int d^3q\int d^3k\,k\left|\phi\left(\boldsymbol{q}\right)\right|^2+\int d^3k\int d^3k'\,\sqrt{kk'}\phi^*\left(\boldsymbol{k}\right)\phi\left(\boldsymbol{k}'\right)e^{-i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}}\\
&\sim \underbrace{\int d^3q\int d^3k\,k\left|\phi\left(\boldsymbol{q}\right)\right|^2}_{\left\langle 0\right|E\left(\boldsymbol{r}\right)\left|0\right\rangle}+2\int d^3k\int d^3k'\,\sqrt{kk'}\phi^*\left(\boldsymbol{k}\right)\phi\left(\boldsymbol{k}'\right)e^{-i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}} \qquad (4.5)
\end{aligned}$$

The first term is related to the vacuum energy and has no dependence on $\boldsymbol{r}$, therefore it can be ignored. Hence,

$$\left\langle E^2\left(\boldsymbol{r}\right)\right\rangle \sim \int d^3k\int d^3k'\,\sqrt{kk'}\phi^*\left(\boldsymbol{k}\right)\phi\left(\boldsymbol{k}'\right)e^{-i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}} \qquad (4.6)$$

For $\phi\left(\boldsymbol{k}\right)=e^{-i\boldsymbol{k}\boldsymbol{r}_0}/\sqrt{k}$, we will get,

$$\begin{aligned}
\left\langle E^2\left(\boldsymbol{r}\right)\right\rangle &\sim \int d^3k\int d^3k'\,\sqrt{kk'}\frac{e^{i\boldsymbol{k}\boldsymbol{r}_0}}{\sqrt{k}}\frac{e^{-i\boldsymbol{k}'\boldsymbol{r}_0}}{\sqrt{k'}}e^{-i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}}\\
&\sim \int d^3k\int d^3k'\,e^{i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}_0}e^{-i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}}\\
&\sim \int d^3k\int d^3k'\,e^{-i\boldsymbol{k}\left(\boldsymbol{r}-\boldsymbol{r}_0\right)}e^{i\boldsymbol{k}'\left(\boldsymbol{r}-\boldsymbol{r}_0\right)}\\
&\sim \delta^2\left(\boldsymbol{r}-\boldsymbol{r}_0\right) \qquad (4.7)
\end{aligned}$$

Therefore $\sqrt{\left\langle E^2\left(\boldsymbol{r}\right)\right\rangle}\sim\delta\left(\boldsymbol{r}-\boldsymbol{r}_0\right)$, meaning that in this case the intensity of the photon is localized at the point $\boldsymbol{r}=\boldsymbol{r}_0$.

How does this state develop in time?

In the Heisenberg picture

$$a^\dagger_{\boldsymbol{k}}\left(t\right)=a^\dagger_{\boldsymbol{k}}e^{-i\omega t} \qquad (4.8)$$

where $\omega=ck$. Therefore,

$$\left|\psi\left(t\right)\right\rangle=\int d^3k\,\phi\left(\boldsymbol{k}\right)a^\dagger_{\boldsymbol{k}}e^{-i\omega t}\left|0\right\rangle=\int d^3k\,\frac{1}{\sqrt{k}}e^{-i\left(\boldsymbol{k}\boldsymbol{r}_0+\omega t\right)}a^\dagger_{\boldsymbol{k}}\left|0\right\rangle \qquad (4.9)$$

How would you make it move in a certain direction?

In order to make the photon move we need to change $\phi\left(\boldsymbol{k}\right)$ to a function which will be anisotropic (in the direction of $\boldsymbol{k}$), which means preferring some direction over the others. Generally we can choose

$$\phi\left(\boldsymbol{k}\right)=\frac{e^{-\left(\boldsymbol{k}-\boldsymbol{k}_0\right)^2-i\boldsymbol{k}\boldsymbol{r}_0}}{\sqrt{k}} \qquad (4.10)$$

5

Question

Two charged particles of equal masses M are attached to the ends of a massless rod of length L which can freely rotate in a plane around its midpoint. Discuss the interaction of this system with radiation.

Solution Outline

1. Write the Hamiltonian as $H = H_{\text{matter}} + H_{\text{rad}} + H_{\text{int}}$.
2. Solve the "matter" part, and get the eigenstates and energies.
3. In order to calculate the Fermi golden rule, we need to find the initial, the final state and the condition for the energy conservation.
   (a) For absorption:
      i. The initial state: $|i\rangle = \overbrace{|m_i\rangle}^{\text{matter}} \overbrace{|N_{\boldsymbol{k},\alpha}\rangle}^{\text{rad}}$
      ii. The final state: $|f\rangle = |m_f\rangle |N_{\boldsymbol{k},\alpha} - 1\rangle$
      iii. The energy condition: $\delta\left(E_{m_f} - (E_{m_i} + \hbar\omega)\right)$
   (b) For emission:
      i. The initial state: $|i\rangle = |m_i\rangle |N_{\boldsymbol{k},\alpha}\rangle$
      ii. The final state: $|f\rangle = |m_f\rangle |N_{\boldsymbol{k},\alpha} + 1\rangle$
      iii. The energy condition: $\delta\left(E_{m_f} + \hbar\omega - E_{m_i}\right)$
4. Get $\Gamma_{\boldsymbol{k},\alpha} \sim \left| \underbrace{\langle m_f| \boldsymbol{\lambda}_{\boldsymbol{k},\alpha} \boldsymbol{j}_{-\boldsymbol{k}} |m_i\rangle}_{\text{interaction}} \underbrace{\langle N_{\boldsymbol{k},\alpha} - 1| a_{\boldsymbol{k},\alpha} |N_{\boldsymbol{k},\alpha}\rangle}_{\text{rad}} \right|^2 \delta\left(E_{m_f} - (E_{m_i} + \hbar\omega)\right)$, e.g. for absorption.
5. The "radiation" term (after the square) will be $N_{\boldsymbol{k},\alpha}$ in absorption or $N_{\boldsymbol{k},\alpha} + 1$ in emission.
6. The "interaction" term:
   (a) Calculate $\boldsymbol{j}_{-\boldsymbol{k}} = \int d^3r\, e^{i\boldsymbol{k}\boldsymbol{r}} \boldsymbol{j}(\boldsymbol{r})$.
   (b) Write parametrization for $\boldsymbol{k}, \boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2$ (dependence on θ, φ). $\boldsymbol{\lambda}_{\boldsymbol{k},\alpha} = \boldsymbol{\lambda}_1 \cos\alpha + \boldsymbol{\lambda}_2 \sin\alpha$.
   (c) Calculate the term and get expression (dependence on θ, φ, α), with delta functions as conditions on m_i, m_f (selection rules).
7. The power per unit solid angle in a given direction and for a given polarization is $\frac{dP_\alpha}{d\gamma} = \int \frac{\Omega\omega^2 d\omega}{(2\pi c)^3} \hbar\omega\Gamma_{\boldsymbol{k},\alpha}$. Can also use $\frac{dP_{\boldsymbol{\lambda}}}{d\gamma} = \frac{\omega^2 e^2}{2\pi c^3} |\langle f| \boldsymbol{j}_{\boldsymbol{k}} \cdot \boldsymbol{\lambda}^* |i\rangle|^2$.

Solution

In this kind of problems we want to get to a total Hamiltonian of the form

$$H = H_{\text{matter}} + H_{\text{rad}} + H_{\text{int}} \tag{5.1}$$

We can do it by writing the Hamiltonian as follow,

$$H = \sum_i \frac{\left(\boldsymbol{p}_i - \frac{q_i}{c}\boldsymbol{A}\right)^2}{2M} + H_{\text{rad}} = \underbrace{\sum_i \frac{\boldsymbol{p}_i^2}{2M}}_{H_{\text{matter}}} \underbrace{- \sum_i \frac{q_i}{2Mc}\left(\boldsymbol{p}_i\boldsymbol{A} + \boldsymbol{A}\boldsymbol{p}_i\right)}_{H_{\text{int}}} + \overbrace{\cancel{\sum_i \frac{q_i^2}{2Mc^2}}}^{\text{quadratic}}\boldsymbol{A}^2 + H_{\text{rad}} \tag{5.2}$$

Matter

The Hamiltonian can be written as

$$H_{\text{matter}} = \frac{L_z^2}{2I} \tag{5.3}$$

where $L_z = -i\hbar\partial_\varphi$ is the angular momentum operator in z direction and I is the moment of inertia given by

$$I = \sum_{i=1,2} M r_i^2 = \sum_{i=1,2} M \left(\frac{L}{2}\right)^2 = \frac{ML^2}{2} \tag{5.4}$$

The solution is for this Hamiltonian is $|m\rangle = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$. Using the Sch. equation,

$$H_{\text{matter}} |m\rangle = \frac{L_z^2}{ML^2} |m\rangle = \frac{-\hbar^2\partial_\varphi^2}{ML^2} |m\rangle = \frac{\hbar^2 m^2}{ML^2} |m\rangle \tag{5.5}$$

therefore the energies are

$$E_m = \frac{\hbar^2 m^2}{ML^2} \tag{5.6}$$

Matter-radiation interaction

$$A(\boldsymbol{r}) = \sum_{\boldsymbol{k},\alpha} \sqrt{\frac{\hbar c^2}{\omega\Omega}} \left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha} a_{\boldsymbol{k},\alpha} e^{i\boldsymbol{kr}} + \boldsymbol{\lambda}^*_{\boldsymbol{k},\alpha} a^\dagger_{\boldsymbol{k},\alpha} e^{-i\boldsymbol{kr}}\right] \tag{5.7}$$

The interaction Hamiltonian is

$$\begin{aligned}
H_{\text{int}} &= -\frac{1}{c}\int d^3r\, \boldsymbol{j}(\boldsymbol{r})\, \boldsymbol{A}(\boldsymbol{r}) \\
&= -\frac{1}{c}\int d^3r\, \boldsymbol{j}(\boldsymbol{r}) \sum_{\boldsymbol{k},\alpha} \sqrt{\frac{\hbar c^2}{\omega\Omega}} \left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha} a_{\boldsymbol{k},\alpha} e^{i\boldsymbol{kr}} + \boldsymbol{\lambda}^*_{\boldsymbol{k},\alpha} a^\dagger_{\boldsymbol{k},\alpha} e^{-i\boldsymbol{kr}}\right] \\
&= -\sum_{\boldsymbol{k},\alpha} \sqrt{\frac{\hbar}{\omega\Omega}} \left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha} a_{\boldsymbol{k},\alpha} \int d^3r\, \boldsymbol{j}(\boldsymbol{r})\, e^{i\boldsymbol{kr}} + \boldsymbol{\lambda}^*_{\boldsymbol{k},\alpha} a^\dagger_{\boldsymbol{k},\alpha} \int d^3r\, \boldsymbol{j}(\boldsymbol{r})\, e^{-i\boldsymbol{kr}}\right] \\
&= -\sum_{\boldsymbol{k},\alpha} \sqrt{\frac{\hbar}{\omega\Omega}} \left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha} \boldsymbol{j}_{-\boldsymbol{k}} a_{\boldsymbol{k},\alpha} + a^\dagger_{\boldsymbol{k},\alpha} \boldsymbol{\lambda}^*_{\boldsymbol{k},\alpha} \boldsymbol{j}_{\boldsymbol{k}}\right]
\end{aligned} \tag{5.8}$$

The current density is

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{1}{2}\sum_a \left[\frac{\boldsymbol{p}_a}{M} q_a \delta(\boldsymbol{r} - \boldsymbol{r}_a(t)) + q_a \delta(\boldsymbol{r} - \boldsymbol{r}_a(t)) \frac{\boldsymbol{p}_a}{M}\right] \tag{5.9}$$

therefore,

$$\begin{aligned}
\boldsymbol{j}_{-\boldsymbol{k}} &= \int d^3r\, \boldsymbol{j}(\boldsymbol{r})\, e^{i\boldsymbol{kr}} \\
&= \int d^3r\, \frac{1}{2}\sum_a \left[\frac{\boldsymbol{p}_a}{M} q_a \delta(\boldsymbol{r} - \boldsymbol{r}_a(t)) + q_a \delta(\boldsymbol{r} - \boldsymbol{r}_a(t)) \frac{\boldsymbol{p}_a}{M}\right] e^{i\boldsymbol{kr}} \\
&= \sum_a \frac{q_a}{2M} \left[\boldsymbol{p}_a e^{i\boldsymbol{kr}_a(t)} + e^{i\boldsymbol{kr}_a(t)} \boldsymbol{p}_a\right]
\end{aligned} \tag{5.10}$$

In our problem, from geometrical reasons,

$$\boldsymbol{p}_1 = -\boldsymbol{p}_2 \equiv \boldsymbol{p} \tag{5.11}$$
$$\boldsymbol{r}_1 = -\boldsymbol{r}_2 \tag{5.12}$$

and for simplicity we will assume $|q_1| = |q_2| = q$, or equivalently w.l.o.g. $q = q_1 = \pm q_2$. Therefore,

$$\begin{aligned}
\boldsymbol{j}_{-\boldsymbol{k}} &= \frac{q_1}{2M}\left[\boldsymbol{p}_1 e^{i\boldsymbol{k}\boldsymbol{r}_1} + e^{i\boldsymbol{k}\boldsymbol{r}_1}\boldsymbol{p}_1\right] + \frac{q_2}{2M}\left[\boldsymbol{p}_2 e^{i\boldsymbol{k}\boldsymbol{r}_2} + e^{i\boldsymbol{k}\boldsymbol{r}_2}\boldsymbol{p}_2\right] \\
&= \frac{q_1}{2M}\left[\boldsymbol{p} e^{i\boldsymbol{k}\boldsymbol{r}_1} + e^{i\boldsymbol{k}\boldsymbol{r}_1}\boldsymbol{p}\right] - \frac{q_2}{2M}\left[\boldsymbol{p} e^{-i\boldsymbol{k}\boldsymbol{r}_1} + e^{-i\boldsymbol{k}\boldsymbol{r}_1}\boldsymbol{p}\right] \\
&= \frac{q}{2M}\left[\boldsymbol{p} e^{i\boldsymbol{k}\boldsymbol{r}_1} + e^{i\boldsymbol{k}\boldsymbol{r}_1}\boldsymbol{p}\right] \mp \frac{q}{2M}\left[\boldsymbol{p} e^{-i\boldsymbol{k}\boldsymbol{r}_1} + e^{-i\boldsymbol{k}\boldsymbol{r}_1}\boldsymbol{p}\right] \\
&= \frac{q}{2M}\left[\boldsymbol{p} e^{i\boldsymbol{k}\boldsymbol{r}_1} + e^{i\boldsymbol{k}\boldsymbol{r}_1}\boldsymbol{p} \mp \left(\boldsymbol{p} e^{-i\boldsymbol{k}\boldsymbol{r}_1} + e^{-i\boldsymbol{k}\boldsymbol{r}_1}\boldsymbol{p}\right)\right] \\
&= \frac{q}{2M}\left[\boldsymbol{p}\left(e^{i\boldsymbol{k}\boldsymbol{r}_1} \mp e^{-i\boldsymbol{k}\boldsymbol{r}_1}\right) + \left(e^{i\boldsymbol{k}\boldsymbol{r}_1} \mp e^{-i\boldsymbol{k}\boldsymbol{r}_1}\right)\boldsymbol{p}\right] \\
&= \hat{\varphi}\frac{q}{2MR}\left[L_z\left(e^{i\boldsymbol{k}\boldsymbol{r}_1} \mp e^{-i\boldsymbol{k}\boldsymbol{r}_1}\right) + \left(e^{i\boldsymbol{k}\boldsymbol{r}_1} \mp e^{-i\boldsymbol{k}\boldsymbol{r}_1}\right)L_z\right]
\end{aligned}$$

Let us explore the absorption rate of a photon with momentum $\boldsymbol{k}$ and polarization $\boldsymbol{\lambda}$. The initial and final states:

$$|i\rangle = \overbrace{|m_i\rangle}^{\text{matter}}\overbrace{\left|N^i_{\boldsymbol{k},\alpha}\right\rangle}^{\text{rad}} = |m_i\rangle\,|N_{\boldsymbol{k},\alpha}\rangle \tag{5.13}$$
$$|f\rangle = |m_f\rangle\left|N^f_{\boldsymbol{k},\alpha}\right\rangle = |m_f\rangle\,|N_{\boldsymbol{k},\alpha} - 1\rangle \tag{5.14}$$

Moreover, there is only one degree of freedom of the position of the particles, which is the angle φ_1. Therefore,

$$\boldsymbol{j}_{-\boldsymbol{k}} = \hat{\varphi}\frac{q}{2MR}\left[L_z\left(e^{ikR\cos\varphi_1} \mp e^{-ikR\cos\varphi_1}\right) + \left(e^{ikR\cos\varphi_1} \mp e^{-ikR\cos\varphi_1}\right)L_z\right] \tag{5.15}$$

The reason $\boldsymbol{k}\boldsymbol{r} = kR\cos(\varphi_1)$ is because that there will be not φ dependence in the photon direction (absorption/emission), since there is an angular symmetry ($[H_{\text{matter}}, L_z] = 0$). Therefore, we can conduct the calculations just for a photon in one direction (in that case we chose $\boldsymbol{k} \parallel \hat{x}$). The energies:

$$E_i = E_{m_f} = \frac{\hbar^2 m_i^2}{ML^2} \tag{5.16}$$
$$E_f = \overbrace{E_{m_i}}^{\text{matter}} + \overbrace{\hbar\omega}^{\text{rad}} = \frac{\hbar^2 m_f^2}{ML^2} + \hbar\omega \tag{5.17}$$

Let us calculate the transition rate using Fermi's golden rule,

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}\left|\langle f|\, H_{\text{int}}\,|i\rangle\right|^2 \delta\left(E_i - E_f\right) \tag{5.18}$$

Calculating

$$
\begin{aligned}
\left|\langle f| H_{\text{int}} |i\rangle\right|^2 &= \left| \langle m_f| \left\langle N^f_{\boldsymbol{k},\alpha}\right| \left\{ -\sqrt{\frac{\hbar}{\omega\Omega}} \left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha} \boldsymbol{j}_{-\boldsymbol{k}} a_{\boldsymbol{k},\alpha} + a^\dagger_{\boldsymbol{k},\alpha} \boldsymbol{\lambda}^*_{\boldsymbol{k},\alpha} \boldsymbol{j}_{\boldsymbol{k}} \right] \right\} |m_i\rangle \left| N^i_{\boldsymbol{k},\alpha} \right\rangle \right|^2 \\
&= \frac{\hbar}{\omega\Omega} \left| \underbrace{\langle m_f| \boldsymbol{\lambda}_{\boldsymbol{k},\alpha} \boldsymbol{j}_{-\boldsymbol{k}} |m_i\rangle}_{\text{matter}} \underbrace{\langle N_{\boldsymbol{k},\alpha} - 1| a_{\boldsymbol{k},\alpha} |N_{\boldsymbol{k},\alpha}\rangle}_{\text{rad}} + \cancelto{0}{\langle N_{\boldsymbol{k},\alpha} - 1| a^\dagger_{\boldsymbol{k},\alpha} |N_{\boldsymbol{k},\alpha}\rangle} \langle m_f| \boldsymbol{\lambda}^*_{\boldsymbol{k},\alpha} \boldsymbol{j}_{\boldsymbol{k}} |m_i\rangle \right|^2 \\
&= \frac{\hbar}{\omega\Omega} \left| \langle m_f| \boldsymbol{\lambda}_{\boldsymbol{k},\alpha} \boldsymbol{j}_{-\boldsymbol{k}} |m_i\rangle \sqrt{N_{\boldsymbol{k},\alpha}} \langle N_{\boldsymbol{k},\alpha} - 1 | N_{\boldsymbol{k},\alpha} - 1\rangle \right|^2 \\
&= \frac{\hbar N_{\boldsymbol{k},\alpha}}{\omega\Omega} \left| \langle m_f| \boldsymbol{\lambda}_{\boldsymbol{k},\alpha} \boldsymbol{j}_{-\boldsymbol{k}} |m_i\rangle \right|^2 \qquad (5.19)
\end{aligned}
$$

Parametrization:

$$
\begin{aligned}
\boldsymbol{k} &= k\left(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta\right) && (5.20)\\
\boldsymbol{\lambda}_1 &= \left(\cos\theta\cos\varphi, \cos\theta\sin\varphi, -\sin\theta\right) && (5.21)\\
\boldsymbol{\lambda}_2 &= \left(\sin\varphi, -\cos\varphi, 0\right) && (5.22)
\end{aligned}
$$

$$
\begin{aligned}
\left(\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\right)_\varphi &= \left(\boldsymbol{\lambda}_1 \cos\alpha + \boldsymbol{\lambda}_2 \sin\alpha\right)_\varphi \\
&= \left(\boldsymbol{\lambda}_1 \cos\alpha + \boldsymbol{\lambda}_2 \sin\alpha\right) \cdot \left(-\sin\varphi\hat{x} + \cos\varphi\hat{y}\right) \\
&= \left(\boldsymbol{\lambda}_1 \cos\alpha + \boldsymbol{\lambda}_2 \sin\alpha\right)_x \left(-\sin\varphi\right) + \left(\boldsymbol{\lambda}_1 \cos\alpha + \boldsymbol{\lambda}_2 \sin\alpha\right)_y \cos\varphi \\
&= \left(\cos\theta\cos\varphi\cos\alpha + \sin\varphi\sin\alpha\right)\left(-\sin\varphi\right) + \left(\cos\theta\sin\varphi\cos\alpha - \cos\varphi\sin\alpha\right)\cos\varphi \\
&= -\sin\varphi\cos\theta\cos\varphi\cos\alpha - \sin^2\varphi\sin\alpha + \cos\varphi\cos\theta\sin\varphi\cos\alpha - \cos^2\varphi\sin\alpha \\
&= -\sin\alpha
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\left|\langle m_f| \boldsymbol{\lambda}_{\boldsymbol{k},\alpha} \boldsymbol{j}_{-\boldsymbol{k}} |m_i\rangle\right|^2 &= \left| \langle m_f| \left(\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\right)_\varphi \cdot \frac{q}{2MR} \left[L_z \left(e^{ikR\cos\varphi_1} \mp e^{-ikR\cos\varphi_1}\right) + \left(e^{ikR\cos\varphi_1} \mp e^{-ikR\cos\varphi_1}\right) L_z \right] |m_i\rangle \right|^2 \\
&= \frac{q^2}{4M^2R^2} \sin^2\alpha \left| \langle m_f| L_z \left(e^{ikR\cos\varphi_1} \mp e^{-ikR\cos\varphi_1}\right) + \left(e^{ikR\cos\varphi_1} \mp e^{-ikR\cos\varphi_1}\right) L_z |m_i\rangle \right|^2 \\
&= \frac{q^2}{4M^2R^2} \sin^2\alpha \left| \hbar m_f \langle m_f| \left(e^{ikR\cos\varphi_1} \mp e^{-ikR\cos\varphi_1}\right) |m_i\rangle + \langle m_f| \left(e^{ikR\cos\varphi_1} \mp e^{-ikR\cos\varphi_1}\right) |m_i\rangle \hbar m_i \right|^2 \\
&= \frac{\hbar^2 q^2}{4M^2R^2} \sin^2\alpha \left(m_f + m_i\right)^2 \left| \langle m_f| \left(e^{ikR\cos\varphi_1} \mp e^{-ikR\cos\varphi_1}\right) |m_i\rangle \right|^2
\end{aligned}
$$

Let us calculate the term in the braket. Denoting $\Delta m = m_f - m_i$, and by using long wave approximation (up to E1/B2, $e^{i\boldsymbol{k}\boldsymbol{r}} \approx 1 + i\boldsymbol{k}\boldsymbol{r}$), we get

$$
\begin{aligned}
\langle m_f| \left(e^{ikR\cos\varphi_1} \mp e^{-ikR\cos\varphi_1}\right) |m_i\rangle &= \frac{1}{2\pi} \int d\varphi\, e^{im_f\varphi_1} \left(e^{ikR\cos\varphi_1} \mp e^{-ikR\cos\varphi_1}\right) e^{-im_i\varphi_1} \\
&= \frac{1}{2\pi} \int d\varphi\, e^{i(m_f - m_i)\varphi_1} \left(e^{ikR\cos\varphi_1} \mp e^{-ikR\cos\varphi_1}\right) \\
&\approx \frac{1}{2\pi} \int d\varphi\, e^{i(\Delta m)\varphi_1} \left[\left(1 + ikR\cos\varphi_1\right) \mp \left(1 - ikR\cos\varphi_1\right)\right] \\
&= \frac{1}{2\pi} \int d\varphi\, e^{i(\Delta m)\varphi_1} \left[\left(1 \mp 1\right) + \left(ikR\cos\varphi_1 \pm ikR\cos\varphi_1\right)\right] \qquad (5.23)
\end{aligned}
$$

For $q_1 = q_2$

$$
\begin{aligned}
\langle m_f | \left(e^{ikR\cos\varphi_1} - e^{-ikR\cos\varphi_1}\right) | m_i \rangle &\approx \frac{1}{2\pi}\int d\varphi \, e^{i(\Delta m)\varphi_1} \cdot 2ikR\cos\varphi_1 \\
&= \frac{ikR}{\pi}\int d\varphi \, e^{i(\Delta m)\varphi_1} \cdot \frac{1}{2}\left(e^{i\varphi} + e^{-i\varphi}\right) \\
&= \frac{ikR}{\pi}\left(\int d\varphi \, e^{i(\Delta m+1)\varphi_1} + \int d\varphi \, e^{i(\Delta m-1)\varphi_1}\right) \\
&= \frac{ikR}{\pi}\left(\delta\left(\Delta m + 1\right) + \delta\left(\Delta m - 1\right)\right) \qquad (5.24)
\end{aligned}
$$

and therefore we get the selection rule $\Delta m = \pm 1$. The transition rate in such a case will be

$$
\begin{aligned}
\Gamma_{\boldsymbol{k},\alpha} &= \frac{2\pi}{\hbar} \left|\langle f | H_{\text{int}} | i \rangle\right|^2 \delta\left(E_{n_i} - E_{n_f}\right) \\
&= \frac{2\pi}{\hbar}\frac{\hbar N_{\boldsymbol{k},\alpha}}{\omega\Omega}\left|\langle m_f | \boldsymbol{\lambda}_{\boldsymbol{k},\alpha} \boldsymbol{j}_{-\boldsymbol{k}} | m_i \rangle\right|^2 \delta\left(\frac{\hbar^2 m_f^2}{ML^2} + \hbar\omega - \frac{\hbar^2 m_i^2}{ML^2}\right) \\
&= \frac{2\pi}{\hbar}\frac{\hbar N_{\boldsymbol{k},\alpha}}{\omega\Omega}\frac{\hbar^2 q^2}{4M^2R^2}\sin^2\alpha\left(m_f + m_i\right)^2 \left|\langle m_f | \left(e^{ikR\cos\varphi_1} - e^{-ikR\cos\varphi_1}\right) | m_i \rangle\right|^2 \delta\left(\frac{\hbar}{ML^2}\left(m_f^2 - m_i^2\right) + \omega\right) \\
&= \frac{2\pi}{\hbar}\frac{\hbar N_{\boldsymbol{k},\alpha}}{\omega\Omega}\frac{\hbar^2 q^2}{4M^2R^2}\sin^2\alpha\left(m_f + m_i\right)^2 \left|\frac{ikR}{\pi}\right|^2 \delta\left(\frac{\hbar}{ML^2}\left(m_f^2 - m_i^2\right) + \omega\right) \\
&= \frac{N_{\boldsymbol{k},\alpha}\hbar^2 q^2}{2\pi M^2\omega\Omega}\sin^2\alpha\left(m_f + m_i\right)^2 k^2 \delta\left(\frac{\hbar}{ML^2}\left(m_f^2 - m_i^2\right) + \omega\right) \\
&= \frac{N_{\boldsymbol{k},\alpha}\hbar^2 \omega q^2}{2\pi M^2 c^2\Omega}\sin^2\alpha\left(m_f + m_i\right)^2 \delta\left(\frac{\hbar}{ML^2}\left(m_f^2 - m_i^2\right) + \omega\right) \qquad (5.25)
\end{aligned}
$$

The power per unit solid angle in a given direction and for a given polarization is

$$
\begin{aligned}
\frac{dP_\alpha}{d\gamma} &= \int \frac{\Omega\omega^2 d\omega}{\left(2\pi c\right)^3}\hbar\omega\Gamma_{\boldsymbol{k},\alpha} \\
&= \int \frac{\Omega\omega^2 d\omega}{\left(2\pi c\right)^3}\hbar\omega\frac{N_{\boldsymbol{k},\alpha}\hbar^2\omega q^2}{2\pi M^2c^2\Omega}\sin^2\alpha\left(m_f + m_i\right)^2\delta\left(\frac{\hbar}{ML^2}\left(m_f^2 - m_i^2\right) + \omega\right) \\
&= \int d\omega \, \frac{N_{\boldsymbol{k},\alpha}\hbar^3\omega^4 q^2}{16\pi^4 M^2 c^5}\sin^2\alpha\left(m_f + m_i\right)^2\delta\left(\frac{\hbar}{ML^2}\left(m_f^2 - m_i^2\right) + \omega\right) \\
&= \frac{N_{\boldsymbol{k},\alpha}\hbar^3\left(\frac{\hbar}{ML^2}\left(m_i^2 - m_f^2\right)\right)^4 q^2}{16\pi^4 M^2 c^5}\sin^2\alpha\left(m_f + m_i\right)^2 \\
&= \frac{N_{\boldsymbol{k},\alpha}\hbar^7 q^2}{16\pi^4 M^6 c^5 L^8}\sin^2\alpha\left(m_f + m_i\right)^2\left(m_i^2 - m_f^2\right)^4 \\
&= \frac{N_{\boldsymbol{k},\alpha}\hbar^7 q^2}{16\pi^4 M^6 c^5 L^8}\sin^2\alpha\left(m_f + m_i\right)^2\left(m_i + m_f\right)^4\left(m_i - m_f\right)^4 \\
&= \frac{N_{\boldsymbol{k},\alpha}\hbar^7 q^2}{16\pi^4 M^6 c^5 L^8}\sin^2\alpha\left(\Delta m + 2m_i\right)^6\left(\Delta m\right)^4 \\
&= \frac{N_{\boldsymbol{k},\alpha}\hbar^7 q^2}{16\pi^4 M^6 c^5 L^8}\sin^2\alpha\left(\Delta m + 2m_i\right)^6 \qquad (5.26)
\end{aligned}
$$

For $q_1 = -q_2$

$$\langle m_f | \left(e^{ikR\cos\varphi_1} + e^{-ikR\cos\varphi_1} \right) | m_i \rangle \approx \frac{1}{2\pi} \int d\varphi \, e^{i(\Delta m)\varphi_1} \cdot 2 = 2\delta_{\Delta m,0} \tag{5.27}$$

In this case the system is essentially a dipole. Indeed we got an electric dipole (where $e^{ikR\cos\varphi_1} \approx 1$), for which there is no change in m.

6

Question

A charged particle with spin 1/2 (electron) is in a tightly bound level of an atom. It is subjected to a uniform constant magnetic field $\boldsymbol{B}_0$. Neglect the influence of $\boldsymbol{B}_0$ on the orbital part and consider only the spin splitting of the level. Discuss the interaction of this system with radiation.

Full Question (2014, 5)

a. First write the Hamiltonian of this problem and then consider how it is modified in the (forever) presence of the radiation EM field.

b. Assume that the spin is in the (energetically) up state. Discuss its de-excitation by a photon emission.

c. What is the angular distribution of the emitted radiation? Does it depend on the polarization? What would you tell experimentalist to expect if his photon detector does not distinguish between polarizations?

d. What about the reverse process i.e. the photon absorption? How is it probability related to the emission? How does it depend on polarization?

Solution Outline

1. The matter Hamiltonian: $H_{\text{matter}} = -\mu B_0 S_z$. The interaction Hamiltonian: $H_{\text{int}} = -\mu \boldsymbol{B} \cdot \boldsymbol{S}$.
2. Write the magnetic operator $\boldsymbol{B}(\boldsymbol{r})$ and get to $H_{\text{int}} \sim (\boldsymbol{k} \times \boldsymbol{\lambda}) \cdot \boldsymbol{S}$.
3. The Fermi golden rule: $\Gamma_{\boldsymbol{k},\boldsymbol{\lambda}} \sim \omega \left|\langle\downarrow| (\boldsymbol{k} \times \boldsymbol{\lambda}) \cdot \boldsymbol{S} |\uparrow\rangle\right|^2$

Solution

The Hamiltonian without radiation is

$$H = \frac{\boldsymbol{p}^2}{2M} - \frac{e^2}{r} - \mu \boldsymbol{B}_0 \cdot \boldsymbol{S} \tag{6.1}$$

Adding the radiation will give

$$H = \frac{\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2}{2M} - \frac{e^2}{r} - \mu \left(\boldsymbol{B}_0 + \underbrace{\nabla \times \boldsymbol{A}}_{\boldsymbol{B}}\right) \cdot \boldsymbol{S} \tag{6.2}$$

We can write this Hamiltonian as

$$H = H_{\text{atom}} + H_{\text{atom-rad}} \overbrace{-\mu \boldsymbol{B}_0 \cdot \boldsymbol{S}}^{\text{spin (Zeeman)}} \underbrace{\overbrace{-\mu \boldsymbol{B} \cdot \boldsymbol{S}}^{spin-rad}}_{H_{\text{int}}} + H_{\text{rad}} \tag{6.3}$$

Spin It is simple to align the coordinate system with the direction of B_0 , or equivalently assume $\boldsymbol{B}_0 = B_0 \hat{z}$. Hence, the Hamiltonian for the spin in this problem is

$$H_{\text{spin}} = -\mu B_0 S_z \tag{6.4}$$

The eigenstates are the ordinary $|\uparrow\rangle$ $(m = 1/2)$ and $|\downarrow\rangle$ $(m = -1/2)$ with the energies $E_m = \mu B_0 \hbar m$.

Interaction

The interaction of the spin with the EM field is given by

$$H_{\text{int}} = -\mu \boldsymbol{B} \cdot \boldsymbol{S} \tag{6.5}$$

The spin operator is

$$\boldsymbol{S} = \begin{pmatrix} S_x \\ S_y \\ S_z \end{pmatrix} = \begin{pmatrix} \frac{1}{2}\left(S_+ + S_-\right) \\ \frac{1}{2i}\left(S_+ - S_-\right) \\ S_z \end{pmatrix} \tag{6.6}$$

The electric field operator is

$$\boldsymbol{E}\left(\boldsymbol{r}\right) = i \sum_{\boldsymbol{k},\boldsymbol{\lambda}} \sqrt{\frac{2\pi\omega}{\Omega}} \boldsymbol{\lambda} \left(a_{\boldsymbol{k},\boldsymbol{\lambda}} e^{i\boldsymbol{kr}} - a^{\dagger}_{\boldsymbol{k},\boldsymbol{\lambda}} e^{-i\boldsymbol{kr}}\right) \tag{6.7}$$

The magnetic field operator is

$$\boldsymbol{B}\left(\boldsymbol{r}\right) = i \sum_{\boldsymbol{k},\boldsymbol{\lambda}} \sqrt{\frac{2\pi\omega}{\Omega c}} \left(\boldsymbol{k} \times \boldsymbol{\lambda}\right) \left(a_{\boldsymbol{k},\boldsymbol{\lambda}} e^{i\boldsymbol{kr}} - a^{\dagger}_{\boldsymbol{k},\boldsymbol{\lambda}} e^{-i\boldsymbol{kr}}\right) \tag{6.8}$$

The interaction Hamiltonian is

$$H_{\text{int}} = -\mu \boldsymbol{B} \cdot \boldsymbol{S} = -i\mu \sum_{\boldsymbol{k},\boldsymbol{\lambda}} \sqrt{\frac{2\pi\omega}{\Omega c}} \left(\boldsymbol{k} \times \boldsymbol{\lambda}\right) \cdot \boldsymbol{S} \left(a_{\boldsymbol{k},\boldsymbol{\lambda}} e^{i\boldsymbol{kr}} - a^{\dagger}_{\boldsymbol{k},\boldsymbol{\lambda}} e^{-i\boldsymbol{kr}}\right) \tag{6.9}$$

The rate for emission/absorption using Fermi golden rule, is

$$\begin{aligned}
\Gamma &= \frac{2\pi}{\hbar} \left|\left\langle f\right| H_{\text{int}} \left|i\right\rangle\right|^2 \delta\left(E_f - E_i\right) \\
&= \frac{2\pi}{\hbar} \left| \left\langle N'_{\boldsymbol{k},\alpha}, m'_z\right| \mu \sum_{\boldsymbol{k},\boldsymbol{\lambda}} \sqrt{\frac{2\pi\omega}{\Omega c}} \left(\boldsymbol{k} \times \boldsymbol{\lambda}\right) \cdot \boldsymbol{S} e^{i\boldsymbol{kr}} \left(a_{\boldsymbol{k},\boldsymbol{\lambda}} - a^{\dagger}_{\boldsymbol{k},\boldsymbol{\lambda}}\right) \left|N_{\boldsymbol{k},\alpha}, m_z\right\rangle \right|^2 \delta\left(E_f - E_i\right) \\
&= \frac{4\pi^2\mu^2}{\Omega\hbar c} \sum_{\boldsymbol{k},\boldsymbol{\lambda}} \omega \left|\left\langle m'_z\right| \left(\boldsymbol{k} \times \boldsymbol{\lambda}\right) \cdot \boldsymbol{S} \left|m_z\right\rangle\right|^2 \left|\left\langle N'_{\boldsymbol{k},\alpha}\right| \left(a_{\boldsymbol{k},\boldsymbol{\lambda}} - a^{\dagger}_{\boldsymbol{k},\boldsymbol{\lambda}}\right) \left|N_{\boldsymbol{k},\alpha}\right\rangle\right|^2 \delta\left(E_f - E_i\right)
\end{aligned} \tag{6.10}$$

The initial and final states are

$$\left|i\right\rangle = \left|N_{\boldsymbol{k},\alpha}, m_z\right\rangle \tag{6.11}$$

$$\left|f\right\rangle = \left|N'_{\boldsymbol{k},\alpha}, m'_z\right\rangle \tag{6.12}$$

Emission

In this case:

$$\left|N'_{\boldsymbol{k},\alpha}\right\rangle = \left|N_{\boldsymbol{k},\alpha} + 1\right\rangle \tag{6.13}$$

Denoting $\Delta m = m'_z - m_z$ (for now let us make this part general for both emission and absorption), the energy difference is

$$E_f - E_i = \hbar\omega - \mu B_0 \hbar m'_z - \left(-\mu B_0 \hbar m_z\right) = \hbar\omega - \mu B_0 \hbar \left(m'_z - m_z\right) = \hbar\omega - \mu B_0 \hbar \Delta m \tag{6.14}$$

Hence,

$$\Gamma = \frac{4\pi^2\mu^2}{\Omega\hbar c}\sum_{\boldsymbol{k},\boldsymbol{\lambda}}\omega\left|\langle m_z'|\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)\cdot\boldsymbol{S}\left|m_z\right\rangle\right|^2\left|\langle N_{\boldsymbol{k},\alpha}+1|\left(a_{\boldsymbol{k},\boldsymbol{\lambda}}-a_{\boldsymbol{k},\boldsymbol{\lambda}}^{\dagger}\right)|N_{\boldsymbol{k},\alpha}\rangle\right|^2\delta\left(\hbar\omega-\mu B_0\hbar\Delta m\right) \tag{6.15}$$

The "radiation" part (for emission):

$$\left|\langle N_{\boldsymbol{k},\alpha}+1|\left(a_{\boldsymbol{k},\boldsymbol{\lambda}}-a_{\boldsymbol{k},\boldsymbol{\lambda}}^{\dagger}\right)|N_{\boldsymbol{k},\alpha}\rangle\right|^2 = N_{\boldsymbol{k},\alpha}+1 \tag{6.16}$$

The "interaction" part:

$$\boldsymbol{k} = k\left(\sin\theta\cos\varphi,\sin\theta\sin\varphi,\cos\theta\right) \tag{6.17}$$
$$\boldsymbol{\lambda}_1 = \left(\sin\varphi,-\cos\varphi,0\right) \tag{6.18}$$
$$\boldsymbol{\lambda}_2 = \left(\cos\theta\cos\varphi,\cos\theta\sin\varphi,-\sin\theta\right) \tag{6.19}$$

Let us assume that the polarization will be a linear combination of $\boldsymbol{\lambda}_1$ and $\boldsymbol{\lambda}_2$ (linear polarization), as follows,

$$\boldsymbol{\lambda} = \boldsymbol{\lambda}_1\cos\alpha+\boldsymbol{\lambda}_2\sin\alpha = \begin{pmatrix}\sin\varphi\cos\alpha+\cos\theta\cos\varphi\sin\alpha\\ -\cos\varphi\cos\alpha+\cos\theta\sin\varphi\sin\alpha\\ -\sin\theta\sin\alpha\end{pmatrix} \tag{6.20}$$

Therefore,

$$\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_x = k_y\lambda_z-k_z\lambda_y = k\left(\cos\theta\cos\varphi\cos\alpha-\sin\varphi\sin\alpha\right) \tag{6.21}$$
$$\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_y = -k_x\lambda_z+k_z\lambda_x = k\left(\cos\theta\sin\varphi\cos\alpha+\cos\varphi\sin\alpha\right) \tag{6.22}$$
$$\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_z = k_x\lambda_y-k_y\lambda_x = -k\sin\theta\cos\alpha \tag{6.23}$$

So (valid for both emission and absorption),

$$\begin{aligned}
\langle m_z'|\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)\cdot\boldsymbol{S}\left|m_z\right\rangle &= \langle m_z'|\left[\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_x\cdot S_x+\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_y\cdot S_y+\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_z\cdot S_z\right]|m_z\rangle\\
&= \langle m_z'|\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_x\cdot S_x\left|m_z\right\rangle+\langle m_z'|\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_y\cdot S_y\left|m_z\right\rangle+\langle m_z'|\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_z\cdot S_z\left|m_z\right\rangle\\
&= \langle m_z'|\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_x\cdot\frac{1}{2}\left(S_++S_-\right)|m_z\rangle+\langle m_z'|\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_y\cdot\frac{1}{2i}\left(S_+-S_-\right)|m_z\rangle+\cancelto{0}{\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_z\cdot\hbar m_z\langle m_z'|m_z\rangle}\\
&= \left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_x\frac{\hbar}{2}\left[\langle m_z'|m_z+1\rangle+\langle m_z'|m_z-1\rangle\right]+\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_y\frac{\hbar}{2i}\left[\langle m_z'|m_z+1\rangle-\langle m_z'|m_z-1\rangle\right]\\
&= \left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_x\frac{\hbar}{2}\left[\delta_{m_z',m_z+1}+\delta_{m_z',m_z-1}\right]+\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_y\frac{\hbar}{2i}\left[\delta_{m_z',m_z+1}-\delta_{m_z',m_z-1}\right]\\
&= \left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_x\frac{\hbar}{2}\left[\delta_{\Delta m,1}+\delta_{\Delta m,-1}\right]+\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_y\frac{\hbar}{2i}\left[\delta_{\Delta m,1}-\delta_{\Delta m,-1}\right]
\end{aligned} \tag{6.24}$$

Hence, the selection rule is $\Delta m=\pm 1$. The case of emission where $\Delta m=-1$ ($m_z'=-1/2$, $m_z=1/2$) will give

$$\langle\downarrow|\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)\cdot\boldsymbol{S}\left|\uparrow\right\rangle = \left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_x\frac{\hbar}{2}-\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_y\frac{\hbar}{2i} = \frac{\hbar}{2}\left[\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_x+i\left(\boldsymbol{k}\times\boldsymbol{\lambda}\right)_y\right] \tag{6.25}$$

and therefore,

$$\begin{aligned}
|\langle\downarrow|(\boldsymbol{k}\times\boldsymbol{\lambda})\cdot\boldsymbol{S}|\uparrow\rangle|^2 &= \left|\frac{\hbar}{2}\left[(\boldsymbol{k}\times\boldsymbol{\lambda})_x + i(\boldsymbol{k}\times\boldsymbol{\lambda})_y\right]\right|^2 \\
&= \frac{\hbar^2}{4}\left[(\boldsymbol{k}\times\boldsymbol{\lambda})_x^2 + (\boldsymbol{k}\times\boldsymbol{\lambda})_y^2\right] \\
&= \frac{\hbar^2}{4}k^2\left[(\cos\theta\cos\varphi\cos\alpha - \sin\varphi\sin\alpha)^2 + (\cos\theta\sin\varphi\cos\alpha + \cos\varphi\sin\alpha)^2\right] \\
&= \frac{\hbar^2}{4}k^2\left[\cos^2\theta\cos^2\varphi\cos^2\alpha - 2\cos\theta\cos\varphi\cos\alpha\sin\varphi\sin\alpha + \sin^2\varphi\sin^2\alpha\right. \\
&\qquad \left. + \cos^2\theta\sin^2\varphi\cos^2\alpha + 2\cos\theta\sin\varphi\cos\alpha\cos\varphi\sin\alpha + \cos^2\varphi\sin^2\alpha\right] \\
&= \frac{\hbar^2}{4}k^2\left[\cos^2\theta\cos^2\alpha + \sin^2\alpha\right] \qquad (6.26)
\end{aligned}$$

Finally, the emission rate will be

$$\begin{aligned}
\Gamma_{\boldsymbol{k},\alpha} &= \frac{4\pi^2\mu^2}{\Omega\hbar c}\omega\cdot\frac{\hbar^2}{4}k^2\left[\cos^2\theta\cos^2\alpha + \sin^2\alpha\right]\cdot N_{\boldsymbol{k},\alpha}\delta(\hbar\omega - \mu B_0\hbar) \\
&= \frac{\pi^2\mu^2}{\Omega c}\hbar\omega k^2\left(N_{\boldsymbol{k},\alpha}+1\right)\left[\cos^2\theta\cos^2\alpha + \sin^2\alpha\right]\delta(\hbar\omega - \mu B_0\hbar) \qquad (6.27)
\end{aligned}$$

Assuming $N_{\boldsymbol{k},\alpha} = 0$ for all $\boldsymbol{k}$ (vacuum),

$$\Gamma_{\boldsymbol{k},\alpha} = \frac{\pi^2\mu^2}{\Omega c}\hbar\omega k^2\left[\cos^2\theta\cos^2\alpha + \sin^2\alpha\right]\delta(\hbar\omega - \mu B_0\hbar)$$

The power dP of light of polarization $\boldsymbol{\lambda}$ (angle α), radiated into a small solid angle $d\gamma$ in the direction $\boldsymbol{k}$, due to spontaneous emission, is

$$\begin{aligned}
dP_\alpha &= \sum_{\boldsymbol{k}\text{ in }d\gamma}\Gamma_{\boldsymbol{k},\alpha} \\
&= d\gamma\int\frac{\Omega\omega^2 d\omega}{(2\pi c)^3}\cdot\Gamma_{\boldsymbol{k},\alpha} \\
&= d\gamma\int\frac{\Omega\omega^2 d\omega}{(2\pi c)^3}\cdot\frac{\pi^2\mu^2}{\Omega c}\hbar\omega k^2\left[\cos^2\theta\cos^2\alpha + \sin^2\alpha\right]\delta(\hbar\omega - \mu B_0\hbar) \\
&= d\gamma\int d\omega\,\frac{\hbar\omega^3\mu^2}{8\pi c^4}\left(\frac{\omega}{c}\right)^2\left[\cos^2\theta\cos^2\alpha + \sin^2\alpha\right]\delta(\hbar\omega - \mu B_0\hbar) \\
&= d\gamma\int d\omega\,\frac{\hbar\omega^5\mu^2}{8\pi c^6}\left[\cos^2\theta\cos^2\alpha + \sin^2\alpha\right]\delta(\hbar\omega - \mu B_0\hbar) \\
&= d\gamma\frac{\hbar(\mu B_0)^5\mu^2}{8\pi c^6}\left[\cos^2\theta\cos^2\alpha + \sin^2\alpha\right] \\
&= d\gamma\frac{\hbar\mu^7 B_0^5}{8\pi c^6}\left[\cos^2\theta\cos^2\alpha + \sin^2\alpha\right] \qquad (6.28)
\end{aligned}$$

Therefore,

$$\frac{dP_\alpha}{d\gamma} = \frac{\hbar\mu^7 B_0^5}{8\pi c^6}\left[\cos^2\theta\cos^2\alpha + \sin^2\alpha\right] \qquad (6.29)$$

7

Question

Consider spontaneous emission of a photon by an excited atom. Consider E1 transition. Suppose the magnetic number of the atom decreases by one unit. Discuss how would you find the angular distribution of the emitted photon?

Solution Outline

1. For E1 (electric dipole) transition, use $\frac{dP_{\boldsymbol{\lambda}}}{d\gamma} = \frac{\omega^4 e^2}{2\pi c^3} \left|\boldsymbol{d}_{f,i} \cdot \boldsymbol{\lambda}^*\right|^2$.
2. Initial: $|i\rangle = |2l_i m_i\rangle |0_k\rangle$. Final: $|f\rangle = |100\rangle |1_k\rangle$.
3. Write the position operator (atom) as $\boldsymbol{R} = r' \left(\sin\theta' \cos\varphi', \sin\theta' \sin\varphi', \cos\theta'\right) = r' \left(\sqrt{\frac{2\pi}{3}} \left(Y_{1,-1} - Y_{1,1}\right), i\sqrt{\frac{2\pi}{3}} \left(Y_{1,-1} + Y_1\right.\right.$
4. Calculate $\boldsymbol{d}_{f,i} = \langle 100| \boldsymbol{R} |2l_i m_i\rangle$ by explicitly write the $Y_{l,m}$ and integrating over θ', φ'. Denote the integration over r' as some constant (which doesn't affect the angular distribution).

Solution

The interaction Hamiltonian is

$$\begin{aligned}
H_{\text{int}} &= -\frac{1}{c} \int d^3r \, \boldsymbol{j}\left(\boldsymbol{r}\right) \boldsymbol{A}\left(\boldsymbol{r}\right) \\
&= -\frac{1}{c} \int d^3r \, \boldsymbol{j}\left(\boldsymbol{r}\right) \sum_{\boldsymbol{k},\alpha} \sqrt{\frac{\hbar c^2}{\omega \Omega}} \left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha} a_{\boldsymbol{k},\alpha} e^{i\boldsymbol{k}\boldsymbol{r}} + \boldsymbol{\lambda}^*_{\boldsymbol{k},\alpha} a^\dagger_{\boldsymbol{k},\alpha} e^{-i\boldsymbol{k}\boldsymbol{r}}\right] \\
&= -\sum_{\boldsymbol{k},\alpha} \sqrt{\frac{\hbar}{\omega \Omega}} \left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha} a_{\boldsymbol{k},\alpha} \int d^3r \, \boldsymbol{j}\left(\boldsymbol{r}\right) e^{i\boldsymbol{k}\boldsymbol{r}} + \boldsymbol{\lambda}^*_{\boldsymbol{k},\alpha} a^\dagger_{\boldsymbol{k},\alpha} \int d^3r \, \boldsymbol{j}\left(\boldsymbol{r}\right) e^{-i\boldsymbol{k}\boldsymbol{r}}\right] \\
&= -\sum_{\boldsymbol{k},\alpha} \sqrt{\frac{\hbar}{\omega \Omega}} \left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha} \boldsymbol{j}_{-\boldsymbol{k}} a_{\boldsymbol{k},\alpha} + a^\dagger_{\boldsymbol{k},\alpha} \boldsymbol{\lambda}^*_{\boldsymbol{k},\alpha} \boldsymbol{j}_{\boldsymbol{k}}\right] \qquad (7.1)
\end{aligned}$$

Initial and final states:

$$|i\rangle = |n_i l_i m_i\rangle \qquad (7.2)$$

$$|f\rangle = |n_f l_f m_f\rangle \qquad (7.3)$$

Let us calculate the emission rate using Fermi's golden rule,

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar} \left|\langle f| H_{\text{int}} |i\rangle\right|^2 \delta\left(E_i - E_f\right) \qquad (7.4)$$

Calculating,

$$
\begin{aligned}
\left|\langle f| H_{\text{int}} |i\rangle\right|^2 &= \left|\langle f| \left[-\sum_{\boldsymbol{k},\alpha}\sqrt{\frac{\hbar}{\omega\Omega}}\left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-\boldsymbol{k}}a_{\boldsymbol{k},\alpha}+a^{\dagger}_{\boldsymbol{k},\alpha}\boldsymbol{\lambda}^{*}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{\boldsymbol{k}}\right]\right]|i\rangle\right|^2 \\
&= \left|\sum_{\boldsymbol{k},\alpha}\sqrt{\frac{\hbar}{\omega\Omega}}\langle n_f l_f m_f|\left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-\boldsymbol{k}}a_{\boldsymbol{k},\alpha}+a^{\dagger}_{\boldsymbol{k},\alpha}\boldsymbol{\lambda}^{*}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{\boldsymbol{k}}\right]|n_i l_i m_i\rangle\right|^2 \\
&= \left|\sum_{\boldsymbol{k},\alpha}\sqrt{\frac{\hbar}{\omega\Omega}}\langle l_f m_f|\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-\boldsymbol{k}}|l_i m_i\rangle\langle n_f|a_{\boldsymbol{k},\alpha}|n_i\rangle+\underbrace{\cancel{\langle n_f|a^{\dagger}_{\boldsymbol{k},\alpha}|n_i\rangle\langle l_f m_f|\boldsymbol{\lambda}^{*}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{\boldsymbol{k}}|l_i m_i\rangle}}_{\text{absorption}}\right|^2
\end{aligned} \tag{7.5}
$$

and therefore,

$$
\Gamma_{\boldsymbol{k},\boldsymbol{\lambda}}=\frac{\hbar}{\omega\Omega}\left|\langle l_f m_f|\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-\boldsymbol{k}}|l_i m_i\rangle\right|^2\left|\langle n_f|a_{\boldsymbol{k},\alpha}|n_i\rangle\right|^2\delta\left(E_i-E_f\right) \tag{7.6}
$$

assuming $n_i = 2$ and $n_f = 1$, and taking $\boldsymbol{k}$ s.t $\hbar\omega = \hbar ck$ is equal to the energy level spacing ($\Delta E = E_1 - E_0$),

$$
\Gamma_{\boldsymbol{k},\boldsymbol{\lambda}}=\frac{\hbar}{\omega\Omega}\left|\langle l_f m_f|\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-\boldsymbol{k}}|l_i m_i\rangle\right|^2 \tag{7.7}
$$

Parametrization

$$
\boldsymbol{k}=k\left(\sin\theta\cos\varphi,\sin\theta\sin\varphi,\cos\theta\right)=k\left(\sqrt{\frac{2\pi}{3}}\left(Y_{1,-1}-Y_{1,1}\right),i\sqrt{\frac{2\pi}{3}}\left(Y_{1,-1}+Y_{1,1}\right)\sqrt{\frac{4\pi}{3}}Y_{1,0}\right) \tag{7.8}
$$

$$
\boldsymbol{\lambda}_1=\left(\cos\theta\cos\varphi,\cos\theta\sin\varphi,-\sin\theta\right) \tag{7.9}
$$

$$
\boldsymbol{\lambda}_2=\left(\sin\varphi,-\cos\varphi,0\right) \tag{7.10}
$$

$$
\boldsymbol{\lambda}=\boldsymbol{\lambda}_1\cos\alpha+\boldsymbol{\lambda}_2\sin\alpha=\begin{pmatrix}\cos\theta\cos\varphi\cos\alpha+\sin\varphi\sin\alpha\\ \cos\theta\sin\varphi\cos\alpha-\cos\varphi\sin\alpha\\ -\sin\theta\cos\alpha\end{pmatrix}
$$

The dipole approximation:

$$
e^{-i\boldsymbol{k}\boldsymbol{r}}\approx 1 \tag{7.11}
$$

$$
\begin{aligned}
\langle f|\boldsymbol{j}_k|i\rangle &= \int d^3r\, e^{-i\boldsymbol{k}\boldsymbol{r}}\langle f|\boldsymbol{j}\left(\boldsymbol{r}\right)|i\rangle \\
&= \int d^3r\,\left(1-i\boldsymbol{k}\boldsymbol{r}+\ldots\right)\langle f|\boldsymbol{j}\left(\boldsymbol{r}\right)|i\rangle \\
&= \langle f|\boldsymbol{j}_0|i\rangle - i\langle f|\int d^3r\,\boldsymbol{k}\boldsymbol{r}\boldsymbol{j}\left(\boldsymbol{r}\right)|i\rangle+\ldots
\end{aligned} \tag{7.12}
$$

$$
\begin{aligned}
\langle f|\boldsymbol{j}_0|i\rangle &= \langle f|\frac{\boldsymbol{P}}{m}|i\rangle \\
&= \langle f|\frac{i}{\hbar}\left[H_0,\boldsymbol{R}\right]|i\rangle \\
&= \frac{i}{\hbar}\langle f|\left(H_0\boldsymbol{R}-\boldsymbol{R}H_0\right)|i\rangle \\
&= \frac{i}{\hbar}\left(E_f-E_i\right)\langle f|\boldsymbol{R}|i\rangle
\end{aligned} \tag{7.13}
$$

Therefore, to the lowest order, where $e^{-i\boldsymbol{kr}} \approx 1$ (electric dipole transition),

$$\langle 0|\, \boldsymbol{j}_k \,|n\rangle \approx \frac{i}{\hbar}\left(0 - \hbar\omega\right)\langle n|\, \boldsymbol{R}\,|0\rangle = -i\omega \underbrace{\langle f|\, \boldsymbol{R}\,|i\rangle}_{\boldsymbol{d}_{f,i}} \tag{7.14}$$

Hence,

$$\frac{dP_{\boldsymbol{\lambda}}}{d\gamma} = \frac{\omega^4 e^2}{2\pi c^3}\left|\boldsymbol{d}_{f,i}\cdot\boldsymbol{\lambda}^*\right|^2 \tag{7.15}$$

Let us assume the final state is the ground state, denoted by $|f\rangle = |100\rangle$. Now,

$$\boldsymbol{R} = r'\left(\sin\theta'\cos\varphi', \sin\theta'\sin\varphi', \cos\theta'\right) = r'\begin{pmatrix} \sqrt{\frac{2\pi}{3}}\left(Y_{1,-1} - Y_{1,1}\right) \\ i\sqrt{\frac{2\pi}{3}}\left(Y_{1,-1} + Y_{1,1}\right) \\ \sqrt{\frac{4\pi}{3}}Y_{1,0} \end{pmatrix}$$

Let us write $\langle r,\theta,\varphi|nlm\rangle$ as $\psi_{n,l,m}\left(r,\theta,\varphi\right) = R_{n,l}\left(r\right)Y_{l,m}\left(\theta,\varphi\right)$. Using $Y^*_{l,m} = \left(-1\right)^m Y_{l,-m}$,

$$\begin{aligned}
\boldsymbol{d}_{f,i}\cdot\boldsymbol{\lambda}^* &= \langle 100|\, \boldsymbol{R}\cdot\boldsymbol{\lambda}^*\,|2l_im_i\rangle \\
&= \langle 100|\, r'\sqrt{\frac{2\pi}{3}}\left[\lambda^*_x\left(Y_{1,-1} - Y_{1,1}\right) + i\lambda^*_y\left(Y_{1,-1} + Y_{1,1}\right) + \sqrt{2}\lambda^*_z Y_{1,0}\right]|2l_im_i\rangle \\
&= \langle 100|\, r'\sqrt{\frac{2\pi}{3}}\left[\left(\lambda^*_x + i\lambda^*_y\right)Y_{1,-1} + \sqrt{2}\lambda^*_z Y_{1,0} - \left(\lambda^*_x - i\lambda^*_y\right)Y_{1,1}\right]|2l_im_i\rangle \\
&= \int dr'\, r'^2 \underbrace{\int d\theta'\,\sin\theta \int d\varphi'}_{\int d\Omega}\left\{\psi^*_{1,0,0}r'\sqrt{\frac{2\pi}{3}}\left[\left(\lambda^*_x + i\lambda^*_y\right)Y_{1,-1} + \sqrt{2}\lambda^*_z Y_{1,0} - \left(\lambda^*_x - i\lambda^*_y\right)Y_{1,1}\right]\psi_{2,l_i,m_i}\right\} \\
&= \int dr'\, r'^2 \int d\Omega\left\{R^*_{1,0}Y^*_{0,0}r'\sqrt{\frac{2\pi}{3}}\left[\left(\lambda^*_x + i\lambda^*_y\right)Y_{1,-1} + \sqrt{2}\lambda^*_z Y_{1,0} - \left(\lambda^*_x - i\lambda^*_y\right)Y_{1,1}\right]\psi_{2,l_i,m_i}R_{2,l_i}Y_{l_i,m_i}\right\} \\
&= \underbrace{\left(\int_0^\infty dr'\, r'^2 R^*_{1,0}r' R_{2,l_i}\right)}_{C_{l_i}}\sqrt{\frac{2\pi}{3}}\int d\Omega Y^*_{0,0}\left[\left(\lambda^*_x + i\lambda^*_y\right)Y_{1,-1} + \sqrt{2}\lambda^*_z Y_{1,0} - \left(\lambda^*_x - i\lambda^*_y\right)Y_{1,1}\right]Y_{l_i,m_i} \\
&= C_{l_i}\sqrt{\frac{2\pi}{3}}Y^*_{0,0}\int d\Omega\,\left[\left(\lambda^*_x + i\lambda^*_y\right)Y_{1,-1} + \sqrt{2}\lambda^*_z Y_{1,0} - \left(\lambda^*_x - i\lambda^*_y\right)Y_{1,1}\right]Y^*_{l_i,-m_i}\left(-1\right)^{m_i} \\
&= -C_{l_i}\sqrt{\frac{2\pi}{3}}Y^*_{0,0}\left[\left(\lambda^*_x + i\lambda^*_y\right)\delta_{l_i,1}\delta_{m_i,1}\left(-1\right)^{m_i} + \sqrt{2}\lambda^*_z\delta_{l_i,1}\delta_{m_i,0}\left(-1\right)^{m_i} - \left(\lambda^*_x - i\lambda^*_y\right)\delta_{l_i,1}\delta_{m_i,-1}\left(-1\right)^{m_i}\right] \\
&= -C_{l_i}\sqrt{\frac{2\pi}{3}}\frac{1}{\sqrt{4\pi}}\delta_{l_i,1}\left[-\left(\lambda^*_x + i\lambda^*_y\right)\delta_{m_i,1} + \sqrt{2}\lambda^*_z\delta_{m_i,0} + \left(\lambda^*_x - i\lambda^*_y\right)\delta_{m_i,-1}\right] \\
&= C_{l_i}\frac{1}{\sqrt{6}}\delta_{l_i,1}\left[\left(\lambda^*_x + i\lambda^*_y\right)\delta_{m_i,1} - \sqrt{2}\lambda^*_z\delta_{m_i,0} - \left(\lambda^*_x - i\lambda^*_y\right)\delta_{m_i,-1}\right] \qquad (7.16)
\end{aligned}$$

From this we get the selection rules (where $l_f = 0$) $\Delta l = l_f - l_i = -1$. In addition, in our problem we were given $\Delta m = -1$, namely $m_i = 1$. Therefore,

$$
\begin{aligned}
\frac{dP_{\boldsymbol{\lambda}}}{d\gamma} &= \frac{\omega^4 e^2}{2\pi c^3} \left| \boldsymbol{d}_{f,i} \cdot \boldsymbol{\lambda}^* \right|^2 \\
&= \frac{\omega^4 e^2}{2\pi c^3} \left| C_{l_i} \frac{1}{\sqrt{6}} \left(\lambda_x^* + i\lambda_y^* \right) \right|^2 \\
&= \frac{\omega^4 e^2 C_{l_i}^2}{12\pi c^3} \left| \lambda_x^* + i\lambda_y^* \right|^2 \\
&= \frac{\omega^4 e^2 C_{l_i}^2}{12\pi c^3} \left(\lambda_x^* + i\lambda_y^* \right) \left(\lambda_x - i\lambda_y \right) \\
&= \frac{\omega^4 e^2 C_{l_i}^2}{12\pi c^3} \left(|\lambda_x|^2 + |\lambda_y|^2 \right) \\
&= \frac{\omega^4 e^2 C_{l_i}^2}{12\pi c^3} \left[\left(\cos\theta \cos\varphi \cos\alpha + \sin\varphi \sin\alpha \right)^2 + \left(\cos\theta \sin\varphi \cos\alpha - \cos\varphi \sin\alpha \right)^2 \right] \\
&= \frac{\omega^4 e^2 C_{l_i}^2}{12\pi c^3} \left[\cos^2\theta \cos^2\varphi \cos^2\alpha + 2\cos\theta \cos\varphi \cos\alpha \sin\varphi \sin\alpha + \sin^2\varphi \sin^2\alpha \right. \\
&\qquad \left. + \cos^2\varphi \sin^2\alpha - 2\cos\theta \sin\varphi \cos\alpha \cos\varphi \sin\alpha + \cos^2\theta \sin^2\varphi \cos^2\alpha \right] \\
&= \frac{\omega^4 e^2 C_{l_i}^2}{12\pi c^3} \left[\cos^2\theta \cos^2\alpha + \sin^2\alpha \right]
\end{aligned}
\tag{7.17}
$$

8

Question

Consider the interaction of a charged pendulum with radiation. (Charged pendulum is a point like massive charged particle hanging on a weightless string.)

Solution Outline

1. The matter Hamiltonian: $H_{\text{matter}} = \frac{\boldsymbol{p}^2}{2M} + MgR\left(1 - \cos\theta\right)$
2. Expand in small angles: $\cos\theta = \sqrt{1 - \sin^2\theta} = \sqrt{1 - \left(\frac{r}{R}\right)^2} \approx 1 - \frac{1}{2}\frac{x^2+y^2}{R}$. Get a 2D H.O. (ignore $z = r\cos\theta$, it is constant)
3. $\left|i\right\rangle = \left|n_x n_y\right\rangle \left|0_k\right\rangle$, $\left|f\right\rangle = \left|n_x' n_y'\right\rangle \left|0_k\right\rangle$
4. Use E1 transition to get $\boldsymbol{j}_{-\boldsymbol{k}} = \frac{q}{m}\boldsymbol{p} = \frac{q}{m}\begin{pmatrix} p_x \\ p_y \end{pmatrix} = i\frac{q}{m}\sqrt{\frac{\hbar m\omega_0}{2}}\begin{pmatrix} a_x^\dagger - a_x \\ a_y^\dagger - a_y \end{pmatrix}$.
5. Calculate $\Gamma \sim \left|\boldsymbol{\lambda}\left\langle n_x' n_y'\right| \boldsymbol{j}_{-\boldsymbol{k}} \left|n_x n_y\right\rangle\right|^2$.

Solution

The Hamiltonian is

$$
\begin{aligned}
H &= \frac{\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}\right)^2}{2M} + MgR\left(1 - \cos\theta\right) + H_{\text{rad}} \\
&= \underbrace{\frac{\boldsymbol{p}^2}{2M} + MgR\left(1 - \cos\theta\right)}_{H_{\text{matter}}} \underbrace{- \frac{e}{2Mc}\left(\boldsymbol{p}\boldsymbol{A} + \boldsymbol{A}\boldsymbol{p}\right)}_{H_{\text{int}}} + \cancelto{\text{quadratic}}{\frac{e^2}{2Mc^2}\boldsymbol{A}^2} + H_{\text{rad}}
\end{aligned}
\tag{8.1}
$$

The non-interacting Hamiltonian

We will use small θ angles, thus getting

$$
\begin{aligned}
H_{\text{matter}} &= \frac{\boldsymbol{p}^2}{2M} + MgR\left(1 - \cos\theta\right) \\
&\approx \frac{\boldsymbol{p}^2}{2M} + MgR\left(1 - \sqrt{1 - \left(\frac{r}{R}\right)^2}\right) \\
&\approx \frac{\boldsymbol{p}^2}{2M} + MgR\left(1 - \left(1 - \frac{1}{2}\left(\frac{r}{R}\right)^2\right)\right) \\
&= \frac{p_x^2}{2M} + \frac{p_y^2}{2M} + \frac{p_z^2}{2M} + \frac{1}{2}M\frac{g}{R}r^2 \\
&= \frac{p_x^2}{2M} + \frac{p_y^2}{2M} + \frac{p_z^2}{2M} + \frac{1}{2}M\frac{g}{R}x^2 + \frac{1}{2}M\frac{g}{R}y^2
\end{aligned}
\tag{8.2}
$$

Denoting $\omega_0 = \sqrt{g/R}$, and ignoring the non interesting z dimension, we get 2 dimensional harmonic oscillator in x-y plane, as follows,

$$
H_{\text{matter}} = \frac{p_x^2}{2M} + \frac{1}{2}M\omega_0^2 x^2 + \frac{p_y^2}{2M} + \frac{1}{2}M\omega_0^2 y^2 \tag{8.3}
$$

so we will denote the eigenstates as $\left\{\left|n_x n_y\right\rangle\right\}_{n_x,n_y=0}^{\infty}$, with the energies

$$
E_{n_x n_y} = \hbar\omega_0\left(n_x + n_y + 1\right) \tag{8.4}
$$

The interaction Hamiltonian

$$A\left(\boldsymbol{r}\right)=\sum_{\boldsymbol{k},\alpha}\sqrt{\frac{\hbar c^{2}}{\omega\Omega}}\left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}a_{\boldsymbol{k},\alpha}e^{i\boldsymbol{k}\boldsymbol{r}}+\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}^{*}a_{\boldsymbol{k},\alpha}^{\dagger}e^{-i\boldsymbol{k}\boldsymbol{r}}\right] \tag{8.5}$$

$$\begin{aligned}
H_{\text{int}} &= -\frac{1}{c}\int d^{3}r\,\boldsymbol{j}\left(\boldsymbol{r}\right)\boldsymbol{A}\left(\boldsymbol{r}\right)\\
&= -\frac{1}{c}\int d^{3}r\,\boldsymbol{j}\left(\boldsymbol{r}\right)\sum_{\boldsymbol{k},\alpha}\sqrt{\frac{\hbar c^{2}}{\omega\Omega}}\left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}a_{\boldsymbol{k},\alpha}e^{i\boldsymbol{k}\boldsymbol{r}}+\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}^{*}a_{\boldsymbol{k},\alpha}^{\dagger}e^{-i\boldsymbol{k}\boldsymbol{r}}\right]\\
&= -\sum_{\boldsymbol{k},\alpha}\sqrt{\frac{\hbar}{\omega\Omega}}\left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}a_{\boldsymbol{k},\alpha}\int d^{3}r\,\boldsymbol{j}\left(\boldsymbol{r}\right)e^{i\boldsymbol{k}\boldsymbol{r}}+\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}^{*}a_{\boldsymbol{k},\alpha}^{\dagger}\int d^{3}r\,\boldsymbol{j}\left(\boldsymbol{r}\right)e^{-i\boldsymbol{k}\boldsymbol{r}}\right]\\
&= -\sum_{\boldsymbol{k},\alpha}\sqrt{\frac{\hbar}{\omega\Omega}}\left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-\boldsymbol{k}}a_{\boldsymbol{k},\alpha}+a_{\boldsymbol{k},\alpha}^{\dagger}\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}^{*}\boldsymbol{j}_{\boldsymbol{k}}\right]
\end{aligned} \tag{8.6}$$

The initial and final states:

$$\left|i\right\rangle=\left|n_{x}n_{y},N_{\boldsymbol{k},\alpha}\right\rangle \tag{8.7}$$

$$\left|f\right\rangle=\left|n_{x}'n_{y}',N_{\boldsymbol{k},\alpha}'\right\rangle \tag{8.8}$$

Emission

We will discuss emission of one photon, so

$$N_{\boldsymbol{k},\alpha}'=N_{\boldsymbol{k},\alpha}+1 \tag{8.9}$$

and the energies:

$$E_{i}=\hbar\omega_{0}\left(n_{x}+n_{y}+1\right) \tag{8.10}$$

$$E_{f}=\hbar\omega_{0}\left(n_{x}'+n_{y}'+1\right)+\hbar\omega \tag{8.11}$$

The Fermi golden rule is

$$\Gamma=\frac{2\pi}{\hbar}\left|\left\langle f\right|H_{\text{int}}\left|i\right\rangle\right|^{2}\delta\left(E_{f}-E_{i}\right) \tag{8.12}$$

and

$$\begin{aligned}
\left|\left\langle f\right|H_{\text{int}}\left|i\right\rangle\right|^{2} &= \left|\left\langle n_{x}'n_{y}',N_{\boldsymbol{k},\alpha}+1\right|\left\{-\sum_{\boldsymbol{k}',\alpha'}\sqrt{\frac{\hbar}{\omega'\Omega}}\left[\boldsymbol{\lambda}_{\boldsymbol{k}',\alpha'}\boldsymbol{j}_{-\boldsymbol{k}'}a_{\boldsymbol{k}',\alpha}+a_{\boldsymbol{k}',\alpha}^{\dagger}\boldsymbol{\lambda}_{\boldsymbol{k}',\alpha}^{*}\boldsymbol{j}_{\boldsymbol{k}'}\right]\right\}\left|n_{x}n_{y},N_{\boldsymbol{k},\alpha}\right\rangle\right|^{2}\\
&= \frac{\hbar}{\omega\Omega}\left|\left\langle n_{x}'n_{y}',N_{\boldsymbol{k},\alpha}+1\right|\left[\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-k}a_{\boldsymbol{k},\alpha}+a_{\boldsymbol{k},\alpha}^{\dagger}\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}^{*}\boldsymbol{j}_{k}\right]\left|n_{x}n_{y},N_{\boldsymbol{k},\alpha}\right\rangle\right|^{2}\\
&= \frac{\hbar}{\omega\Omega}\left|\left\langle n_{x}'n_{y}'\right|\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-k}\left|n_{x}n_{y}\right\rangle\cancelto{0}{\left\langle N_{\boldsymbol{k},\alpha}+1\right|a_{\boldsymbol{k},\alpha}\left|N_{\boldsymbol{k},\alpha}\right\rangle}+\left\langle N_{\boldsymbol{k},\alpha}+1\right|a_{\boldsymbol{k},\alpha}^{\dagger}\left|N_{\boldsymbol{k},\alpha}\right\rangle\left\langle n_{x}'n_{y}'\right|\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}^{*}\boldsymbol{j}_{k}\left|n_{x}n_{y}\right\rangle\right|^{2}\\
&= \frac{\hbar}{\omega\Omega}\left|\sqrt{N_{\boldsymbol{k},\alpha}+1}\left\langle N_{\boldsymbol{k},\alpha}+1|N_{\boldsymbol{k},\alpha}+1\right\rangle\left\langle n_{x}'n_{y}'\right|\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}^{*}\boldsymbol{j}_{k}\left|n_{x}n_{y}\right\rangle\right|^{2}\\
&= \frac{\hbar\left(N_{\boldsymbol{k},\alpha}+1\right)}{\omega\Omega}\left|\left\langle n_{x}'n_{y}'\right|\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-k}\left|n_{x}n_{y}\right\rangle\right|^{2}
\end{aligned} \tag{8.13}$$

The current density is

$$
\begin{aligned}
\boldsymbol{j}_{-k} &= \int d^3r\, \boldsymbol{j}\left(\boldsymbol{r}\right) e^{i\boldsymbol{k}\boldsymbol{r}} \\
&= \int d^3r\, \frac{1}{2}\left[\frac{\boldsymbol{p}}{M} q\delta\left(\boldsymbol{r}-\boldsymbol{r}_a\right) + q_a\delta\left(\boldsymbol{r}-\boldsymbol{r}_a\right)\frac{\boldsymbol{p}}{M}\right] e^{i\boldsymbol{k}\boldsymbol{r}} \\
&= \frac{q}{2}\left[\frac{\boldsymbol{p}}{M} e^{i\boldsymbol{k}\boldsymbol{r}_a} + e^{i\boldsymbol{k}\boldsymbol{r}_a}\frac{\boldsymbol{p}}{M}\right]
\end{aligned}
\tag{8.14}
$$

Electric dipole approximation:

$$
\boldsymbol{j}_{-k} \approx \frac{q\boldsymbol{p}}{M} \tag{8.15}
$$

Assuming $n'_x \leq n_x$ and $n'_y \leq n_y$,

$$
\begin{aligned}
\left|\left\langle n'_x n'_y\right| \boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-k}\left|n_x n_y\right\rangle\right|^2 &= \left|\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\frac{q}{M}\left\langle n'_x n'_y\right| \boldsymbol{p}\left|n_x n_y\right\rangle\right|^2 \\
&= \frac{q^2}{M^2}\left|\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\left\langle n'_x n'_y\right| \begin{pmatrix} p_x \\ p_y \end{pmatrix}\left|n_x n_y\right\rangle\right|^2 \\
&= \frac{q^2}{M^2}\left|\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\left\langle n'_x n'_y\right| \begin{pmatrix} i\sqrt{\frac{\hbar\omega_0}{2}}\left(a_x^\dagger - a_x\right) \\ i\sqrt{\frac{\hbar\omega_0}{2}}\left(a_y^\dagger - a_y\right) \end{pmatrix}\left|n_x n_y\right\rangle\right|^2 \\
&= \frac{\hbar\omega_0 q^2}{2M^2}\left|\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\begin{pmatrix} \cancelto{0}{\left\langle n'_x n'_y\right| a_x^\dagger\left|n_x n_y\right\rangle} - \left\langle n'_x n'_y\right| a_x\left|n_x n_y\right\rangle \\ \cancelto{0}{\left\langle n'_x n'_y\right| a_y^\dagger\left|n_x n_y\right\rangle} - \left\langle n'_x n'_y\right| a_y\left|n_x n_y\right\rangle \end{pmatrix}\right|^2 \\
&= \frac{\hbar\omega_0 q^2}{2M^2}\left|\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\begin{pmatrix} -\sqrt{n_x}\left\langle n'_x, n'_y\middle| n_x - 1, n_y\right\rangle \\ -\sqrt{n_y}\left\langle n'_x, n'_y\middle| n_x, n_y - 1\right\rangle \end{pmatrix}\right|^2 \\
&= \frac{\hbar\omega_0 q^2}{2M^2}\left|\lambda_x\sqrt{n_x}\delta_{n'_x,n_x-1}\delta_{n'_y,n_y} + \lambda_y\sqrt{n_y}\delta_{n'_x,n_x}\delta_{n'_y,n_y-1}\right|^2
\end{aligned}
\tag{8.16}
$$

Denoting $\Delta n_x = n'_x - n_x$ and $\Delta n_y = n'_y - n_y$,

$$
\begin{aligned}
\left|\left\langle n'_x n'_y\right| \boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-k}\left|n_x n_y\right\rangle\right|^2 &= \frac{\hbar\omega_0 q^2}{2M^2}\left|\lambda_x\sqrt{n_x}\delta_{\Delta n_x,1}\delta_{\Delta n_y,0} + \lambda_y\sqrt{n_y}\delta_{\Delta n_x,0}\delta_{\Delta n_y,1}\right|^2 \\
&= \frac{\hbar\omega_0 q^2}{2M^2}\Big[\lambda_x^2 n_x\delta_{\Delta n_x,1}^2\delta_{\Delta n_y,0}^2 \\
&\quad + 2\lambda_x\lambda_y\sqrt{n_x n_y}\delta_{\Delta n_x,1}\delta_{\Delta n_y,0}\delta_{\Delta n_x,0}\delta_{\Delta n_y,1} \\
&\quad + \lambda_y^2 n_y\delta_{\Delta n_x,0}^2\delta_{\Delta n_y,1}^2\Big]
\end{aligned}
\tag{8.17}
$$

The second term will be vanish due to the delta functions, so the selection rules for non-vanishing emission rate will be

$$
\Delta n_x = -1,\, \Delta n_y = 0 \quad \text{OR} \quad \Delta n_x = 0,\, \Delta n_y = -1 \tag{8.18}
$$

which also imply that $\Delta n = \Delta n_x + \Delta n_y = -1$. Denoting $n = n_x + n_y$ and $\left|n\right\rangle = \left|n_x n_y\right\rangle$,

$$
\begin{aligned}
\left|\left\langle n'_x n'_y\right| \boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-k}\left|n_x n_y\right\rangle\right|^2 &= \left|\left\langle n-1\right| \boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-k}\left|n\right\rangle\right|^2 \\
&= \frac{\hbar\omega_0 q^2}{2M^2}\left[\lambda_x^2 n_x\delta_{\Delta n_x,1}\delta_{\Delta n_y,0} + \lambda_y^2 n_y\delta_{\Delta n_x,0}\delta_{\Delta n_y,1}\right]
\end{aligned}
\tag{8.19}
$$

and by energy conservation

$$\begin{aligned}\hbar\omega_0\left(n'_x+n'_y+1\right)+\hbar\omega&=\hbar\omega_0\left(n_x+n_y+1\right)\\ \omega_0\left(\Delta n_x+\Delta n_y\right)+\omega&=0\\ \omega_0\Delta n+\omega&=0\end{aligned}\tag{8.20}$$

Wrapping it all together we get

$$\begin{aligned}\Gamma_{\boldsymbol{k},\alpha}&=\frac{2\pi}{\hbar}\frac{\hbar\left(N_{\boldsymbol{k},\alpha}+1\right)}{\omega\Omega}\left|\langle n-1|\,\boldsymbol{\lambda}_{\boldsymbol{k},\alpha}\boldsymbol{j}_{-k}\,|n\rangle\right|^2\delta\left(\omega+\omega_0\Delta n\right)\\ &=\frac{2\pi}{\hbar}\frac{\hbar\left(N_{\boldsymbol{k},\alpha}+1\right)}{\omega\Omega}\frac{\hbar\omega_0q^2}{2M^2}\left[\lambda_x^2n_x\delta_{\Delta n_x,1}\delta_{\Delta n_y,0}+\lambda_y^2n_y\delta_{\Delta n_x,0}\delta_{\Delta n_y,1}\right]\delta\left(\omega+\omega_0\Delta n\right)\\ &=\frac{\pi\hbar\omega_0q^2}{M^2\omega\Omega}\left(N_{\boldsymbol{k},\alpha}+1\right)\left[\lambda_x^2n_x\delta_{\Delta n_x,1}\delta_{\Delta n_y,0}+\lambda_y^2n_y\delta_{\Delta n_x,0}\delta_{\Delta n_y,1}\right]\delta\left(\omega+\omega_0\Delta n\right)\end{aligned}\tag{8.21}$$

$$\boldsymbol{k}=k\left(\sin\theta\cos\varphi,\sin\theta\sin\varphi,\cos\theta\right)\tag{8.22}$$

$$\boldsymbol{\lambda}_1=\left(\sin\varphi,-\cos\varphi,0\right)\tag{8.23}$$

$$\boldsymbol{\lambda}_2=\left(\cos\theta\cos\varphi,\cos\theta\sin\varphi,-\sin\theta\right)\tag{8.24}$$

We can further choose w.l.o.g. $\Delta n_x=-1$ and $\Delta n_y=0$, so by using

$$\lambda_x=\left(\boldsymbol{\lambda}_1\cos\alpha+\boldsymbol{\lambda}_2\sin\alpha\right)_x=\sin\varphi\cos\alpha+\cos\theta\cos\varphi\sin\alpha\tag{8.25}$$

we get

$$\Gamma_{\boldsymbol{k},\alpha}=\frac{\pi\hbar\omega_0q^2}{M^2\omega\Omega}\left(N_{\boldsymbol{k},\alpha}+1\right)n_x\left(\sin\varphi\cos\alpha+\cos\theta\cos\varphi\sin\alpha\right)^2\delta\left(\omega+\omega_0\Delta n\right)\tag{8.26}$$

Assuming $N_{\boldsymbol{k},\alpha}=0$ for all $\boldsymbol{k},\alpha$, the power of light of polarization $\boldsymbol{\lambda}$ (with angle α), radiated in to a small solid angle $d\gamma$ in the direction $\boldsymbol{k}$, is

$$\begin{aligned}dP_\alpha&=\sum_{\boldsymbol{k}\text{ in }d\gamma}\hbar\omega\Gamma_{\boldsymbol{k},\alpha}\delta\left(\omega+\omega_0\Delta n\right)\\ &=d\gamma\int\frac{\Omega\omega^2d\omega}{\left(2\pi c\right)^3}\hbar\omega\cdot\frac{\pi\hbar\omega_0q^2}{M^2\omega\Omega}n_x\left(\sin\varphi\cos\alpha+\cos\theta\cos\varphi\sin\alpha\right)^2\cdot\delta\left(\omega+\omega_0\Delta n\right)\\ &=d\gamma\cdot\frac{\hbar^2q^2n_x\omega_0}{8\pi^2M^2c^3}\left(-\omega_0\Delta n\right)^2\left(\sin\varphi\cos\alpha+\cos\theta\cos\varphi\sin\alpha\right)^2\end{aligned}\tag{8.27}$$

Thus the power per unit solid angle in a given direction and for a given polarization is

$$\frac{dP_\alpha}{d\gamma}=\frac{\hbar^2q^2\omega_0^3\left(\Delta n\right)^2}{8\pi^2M^2c^3}\left(\sin\varphi\cos\alpha+\cos\theta\cos\varphi\sin\alpha\right)^2\tag{8.28}$$

9

Full Question

A two level system is interacting with a bosonic system

$$H = \sigma_x \sum_\alpha \lambda_\alpha \left(a_\alpha + a_\alpha^\dagger\right) + \sum_\alpha \epsilon_\alpha a_\alpha^\dagger a_\alpha$$

where σ_x is the Pauli matrix, a_α, $a_\alpha^\dagger$ are boson operators and λ_α, ϵ_α are positive constants. Find the eigenvalues and eigenfunctions of this Hamiltonian.

Solution Outline

1. Define a new operator $b_\alpha = a_\alpha + \frac{\lambda_\alpha}{\epsilon_\alpha}\sigma_x$, by completing the square. Diagonalize σ_x (spin space) and get $b_{\alpha,\pm} = a_\alpha \pm \frac{\lambda_\alpha}{\epsilon_\alpha}$.
2. Verify that the new operator $b_\alpha, b_\alpha^\dagger$ obey the bosonic commutation relations.
3. Define $|\beta_{\alpha,\pm}\rangle$ as a coherent state of a_α, and get the condition for which $|\beta_{\alpha,\pm}\rangle$ will be the vacuum state of b_α ($b_\alpha |\beta_{\alpha,\pm}\rangle = 0$). Get $\beta_{a,\pm} = \mp\frac{\lambda_\alpha}{\epsilon_\alpha}$.
4. Write the eigenstates and eigenvalues for bosons.

Solution

The Hamiltonian is

$$\begin{aligned}
H &= \sigma_x \sum_\alpha \lambda_\alpha \left(a_\alpha + a_\alpha^\dagger\right) + \mathbb{I} \cdot \sum_\alpha \epsilon_\alpha a_\alpha^\dagger a_\alpha \\
&= \sum_\alpha \epsilon_\alpha \left[a_\alpha^\dagger a_\alpha + \frac{\lambda_\alpha}{\epsilon_\alpha}\sigma_x \left(a_\alpha + a_\alpha^\dagger\right)\right] \\
&= \sum_\alpha \epsilon_\alpha \left[\left(a_\alpha^\dagger + \frac{\lambda_\alpha}{\epsilon_\alpha}\sigma_x\right)\left(a_\alpha + \frac{\lambda_\alpha}{\epsilon_\alpha}\sigma_x\right) - \left(\frac{\lambda_\alpha}{\epsilon_\alpha}\sigma_x\right)^2\right] \\
&= \sum_\alpha \epsilon_\alpha \left(a_\alpha^\dagger + \frac{\lambda_\alpha}{\epsilon_\alpha}\sigma_x\right)\left(a_\alpha + \frac{\lambda_\alpha}{\epsilon_\alpha}\sigma_x\right) - \sum_\alpha \frac{\lambda_\alpha^2}{\epsilon_\alpha}
\end{aligned} \tag{9.1}$$

Let us define $b_\alpha = a_\alpha + \frac{\lambda_\alpha}{\epsilon_\alpha}\sigma_x$ and $b_\alpha^\dagger = a_\alpha^\dagger + \frac{\lambda_\alpha}{\epsilon_\alpha}\sigma_x$. It is easy to see that

$$\left[b_\alpha, b_{\alpha'}^\dagger\right] = \left[a_\alpha + \frac{\lambda_\alpha}{\epsilon_\alpha}\sigma_x, a_{\alpha'}^\dagger + \frac{\lambda_{\alpha'}}{\epsilon_{\alpha'}}\sigma_x\right] = \left[a_\alpha, a_{\alpha'}^\dagger\right] = \delta_{\alpha\alpha'} \tag{9.2}$$

So

$$H = \sum_\alpha \epsilon_\alpha b_\alpha^\dagger b_\alpha - \sum_\alpha \frac{\lambda_\alpha^2}{\epsilon_\alpha} \tag{9.3}$$

Let us denote the eigenstates of σ_x as

$$|\pm\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle \pm |\downarrow\rangle\right) \tag{9.4}$$

with ± 1 as the corresponding eigenvalues. Therefore we can diagonalize the spin part in b_α and get

$$b_{\alpha,\pm} = a_\alpha \pm \frac{\lambda_\alpha}{\epsilon_\alpha} \tag{9.5}$$

Moreover, we will denote $|n_\alpha\rangle$ as the number state of a_α.

$$|n_{\alpha,\pm}\rangle = |n_\alpha\rangle \otimes |\pm\rangle \tag{9.6}$$

We will define $|\beta_{\alpha,\pm}\rangle$ as the coherent state of a_α, and therefore

$$a_\alpha |\beta_{\alpha,\pm}\rangle = \beta_{\alpha,\pm} |\beta_{\alpha,\pm}\rangle \tag{9.7}$$

Using (9.7) and the eigenvalues of σ_x,

$$b_{\alpha,\pm} |\beta_{\alpha,\pm}\rangle = \left(a_\alpha + \frac{\lambda_\alpha}{\epsilon_\alpha}\sigma_x\right) |\beta_{\alpha,\pm}\rangle = \left(\beta_{\alpha,\pm} \pm \frac{\lambda_\alpha}{\epsilon_\alpha}\right) |\beta_{\alpha,\pm}\rangle \tag{9.8}$$

The state $|\beta_{\alpha,\pm}\rangle$ will be the ground state (vacuum) of $b_{\alpha,\pm}$, namely $b_{\alpha,\pm} |\beta_{\alpha,\pm}\rangle = 0$, if we use the constraint

$$\beta_{\alpha,\pm} = \mp\frac{\lambda_\alpha}{\epsilon_\alpha} \tag{9.9}$$

In this case,

$$\begin{aligned}
|\beta_{\alpha,\pm}\rangle &= e^{-\frac{|\beta_\alpha|^2}{2}} \sum_{n_\alpha} \frac{(\beta_{\alpha,\pm})^{n_\alpha}}{\sqrt{n_\alpha!}} |n_{\alpha,\pm}\rangle \\
&= e^{-\frac{\left|-\frac{\lambda_\alpha}{\epsilon_\alpha}\right|^2}{2}} \sum_{n_\alpha} \frac{\left(\mp\frac{\lambda_\alpha}{\epsilon_\alpha}\right)^{n_\alpha}}{\sqrt{n_\alpha!}} |n_{\alpha,\pm}\rangle \\
&= e^{-\frac{1}{2}\left(\frac{\lambda_\alpha}{\epsilon_\alpha}\right)^2} \sum_{n_\alpha} \frac{(\mp 1)^{n_\alpha}\left(\frac{\lambda_\alpha}{\epsilon_\alpha}\right)^{n_\alpha}}{\sqrt{n_\alpha!}} |n_{\alpha,\pm}\rangle
\end{aligned} \tag{9.10}$$

and the eigenstates of a system with N bosons will be

$$\left|\{n_\alpha\}_\pm\right\rangle = \prod_\alpha \frac{\left(b^\dagger_{\alpha,\pm}\right)^{n_\alpha}}{\sqrt{n_\alpha!}} |\beta_{\alpha,\pm}\rangle, \quad \sum_\alpha n_\alpha = N \tag{9.11}$$

with the corresponding energies

$$E_{\{n_\alpha\}} = \sum_\alpha \left(\epsilon_\alpha n_\alpha - \frac{\lambda_\alpha^2}{\epsilon_\alpha}\right) \tag{9.12}$$

10

Question

Consider the following simplified model of spinless fermions placed in a potential well and interacting via a very long range interaction

$$H = \sum_{i,j=1}^{\infty} h_{ij} a_i^\dagger a_j + \frac{V_0}{2}\left(\hat{N} - N_0\right)^2$$

Here h_{ij} is a single particle hamiltonian of the well. It is a hermitian matrix with known eigenvalues ϵ_n and eigenfunctions $\psi_n(i)$. The operator $\hat{N}$ is $\hat{N} = \sum_{j=1}^{\infty} a_j^\dagger a_j$ and N_0 is a fixed integer.

Full Question (2014, 9)

a. Find the ground state of the model for a fixed number M of electrons.

b. Derive and solve the Heisenberg equations of motion for the operators a_i and $a_i^\dagger$. Use the solutions to find the excitation energies and the wave functions of excitations with respectively $M+1$ and $M-1$ particles relative to energy of the M particle system.

c. Repeat for particle-hole operators $a_k^\dagger a_i$ and find the excitations of the M particle system.

Solution Outline

1. Preform the following expansion: $a_i = \sum_i \psi_n(i) b_n = \sum_i \langle i|n\rangle b_n$.
2. Verify that $b_n, b_n^\dagger$ obey the fermionic anti-commutation relations.
3. Get to $H = \sum_n \epsilon_n b_n^\dagger b_n + \frac{1}{2}V_0\left(\sum_n b_n^\dagger b_n - N_0\right)^2 = \sum_n \epsilon_n \hat{N}_n + \frac{1}{2}V_0\left(\hat{N} - N_0\right)^2$, and now we can denote the vacuum as $|0\rangle$ and the ground state will be $|M\rangle = \prod_{i=1}^{M} b_{n_i}^\dagger |0\rangle$.
4. Use the Heisenberg equation to find $da_k(t)/dt$ and $da_k^\dagger(t)/dt$, and then get to $db_k(t)/dt$ and $db_k^\dagger(t)/dt$. The solutions are exponents.
5. Find excitation energy ΔE by: $H|M+1\rangle = Hb_n^\dagger|M\rangle = \left(\left[H, b_n^\dagger\right] + b_n^\dagger H\right)|M\rangle = \left(-i\hbar\frac{db_n^\dagger}{dt} + b_n^\dagger E_M\right)|M\rangle$, and by using (4) get to $\underbrace{(\Delta E + E_M)}_{E_{M+1}}|M+1\rangle$. To a similar calculation for $|M-1\rangle$.
6. For particle-hole, calculate $\frac{d\left(a_k^\dagger a_l\right)}{dt} = \frac{i}{\hbar}\left[H, a_k^\dagger a_l\right]$ and perform a similar calculation with $b_m^\dagger b_n|M\rangle$.

Solution

a

The Hamiltonian can be written as

$$H = \sum_{i,j} h_{ij} a_i^\dagger a_j + \frac{1}{2}V_0\left(\sum_j a_j^\dagger a_j - N_0\right)^2 \tag{10.1}$$

Let us perform the following change of basis:

$$a_i = \sum_n \phi_n(i) b_n = \sum_n \langle i|n\rangle b_n \tag{10.2}$$

$$a_i^\dagger = \sum_n \phi_n^*(i) b_n^\dagger = \sum_n \langle i|n\rangle^* b_n^\dagger \tag{10.3}$$

where $\phi_n(i) \equiv \psi_n(i)$ the given eigenfunctions. Let us calculate the expressions in the Hamiltonian. The first is

$$\begin{aligned}
\sum_{i,j} h_{ij} a_i^\dagger a_j &= \sum_{i,j} \langle i| h |j\rangle a_i^\dagger a_j \\
&= \sum_{i,j} \langle i| h |j\rangle \left(\sum_n \langle i|n\rangle^* b_n^\dagger \right) \left(\sum_m \langle j|m\rangle b_m \right) \\
&= \sum_{i,j} \sum_{n,m} \langle n|i\rangle \langle i| h |j\rangle \langle j|m\rangle b_n^\dagger b_m \\
&= \sum_{n,m} \langle n| h |m\rangle b_n^\dagger b_m \\
&= \sum_{n,m} h_{nm} \delta_{nm} b_n^\dagger b_m \\
&= \sum_n \epsilon_n b_n^\dagger b_n
\end{aligned} \tag{10.4}$$

and the second is

$$\begin{aligned}
\sum_j a_j^\dagger a_j &= \sum_j \left(\sum_n \langle j|n\rangle^* b_n^\dagger \right) \left(\sum_m \langle j|m\rangle b_m \right) \\
&= \sum_j \sum_{n,m} \langle n|j\rangle \langle j|m\rangle b_n^\dagger b_m \\
&= \sum_{n,m} \langle n|m\rangle b_n^\dagger b_m \\
&= \sum_{n,m} \delta_{nm} b_n^\dagger b_m \\
&= \sum_n b_n^\dagger b_n
\end{aligned} \tag{10.5}$$

Moreover, we will show that $b_n, b_n^\dagger$ obey the anti-commutation relations, as follows,

$$\begin{aligned}
\left\{ b_n, b_m^\dagger \right\} &= b_n b_m^\dagger + b_m^\dagger b_n \\
&= \left(\sum_i \langle i|n\rangle^* a_i \right) \left(\sum_j \langle j|m\rangle a_j^\dagger \right) + \left(\sum_j \langle j|m\rangle a_j^\dagger \right) \left(\sum_i \langle i|n\rangle^* a_i \right) \\
&= \sum_i \sum_j \langle n|i\rangle \langle j|m\rangle a_i a_j^\dagger + \sum_i \sum_j \langle j|m\rangle \langle n|i\rangle a_j^\dagger a_i \\
&= \sum_i \sum_j \langle n|i\rangle \langle j|m\rangle \left(\left\{ a_i, a_j^\dagger \right\} - a_j^\dagger a_i \right) + \sum_i \sum_j \langle j|m\rangle \langle n|i\rangle a_j^\dagger a_i \\
&= \sum_i \sum_j \langle n|i\rangle \langle j|m\rangle \delta_{ij} \\
&= \sum_i \langle n|i\rangle \langle i|m\rangle \\
&= \langle n|m\rangle \\
&= \delta_{mn}
\end{aligned} \tag{10.6}$$

Using (10.4) and (10.5), we will get

$$H = \sum_n \epsilon_n b_n^\dagger b_n + \frac{1}{2} V_0 \left(\sum_n b_n^\dagger b_n - N_0 \right)^2 = \sum_n \epsilon_n \hat{N}_n + \frac{1}{2} V_0 \left(\hat{N} - N_0 \right)^2 \tag{10.7}$$

Consider the following state of M electrons:

$$|M\rangle = \prod_{i=1}^{M} b_{n_i}^\dagger |0\rangle \tag{10.8}$$

So

$$H|\psi\rangle = \left[\sum_n \epsilon_n \hat{N}_n + \frac{1}{2} V_0 \left(\hat{N} - N_0 \right)^2 \right] |M\rangle = \left[\sum_{n_i} \epsilon_{n_i} + \frac{1}{2} V_0 \left(M - N_0 \right)^2 \right] |M\rangle \tag{10.9}$$

The energies are

$$E_{\{n_i\}} = \sum_{n_i} \epsilon_{n_i} + \frac{1}{2} V_0 \left(M - N_0 \right)^2 \tag{10.10}$$

GS: $\{n_i\}$ s.t. $\sum_{n_i} \epsilon_{n_i}$ minimal, i.e. occupie lowest ϵ but follow pauli principle

b

Derivation of the Heisenberg equation:

$$\begin{aligned}
\frac{dA(t)}{dt} &= \frac{d}{dt}\left(e^{iHt/\hbar} A e^{-iHt/\hbar} \right) \\
&= \frac{i}{\hbar} H e^{iHt/\hbar} A e^{-iHt/\hbar} + e^{iHt/\hbar} \left(\frac{\partial A}{\partial t} \right) e^{-iHt/\hbar} + e^{iHt/\hbar} A \left(-\frac{i}{\hbar} H \right) e^{-iHt/\hbar} \\
&= \frac{i}{\hbar} H A(t) + e^{iHt/\hbar} \left(\frac{\partial A}{\partial t} \right) e^{-iHt/\hbar} - \frac{i}{\hbar} A(t) H \\
&= \frac{i}{\hbar} (HA - AH) + e^{iHt/\hbar} \left(\frac{\partial A}{\partial t} \right) e^{-iHt/\hbar} \\
&= \frac{i}{\hbar} [H, A] + e^{iHt/\hbar} \left(\frac{\partial A}{\partial t} \right) e^{-iHt/\hbar}
\end{aligned} \tag{10.11}$$

Let us calculate the following useful expressions:

$$\left[a_i^\dagger a_j, a_k \right] = a_i^\dagger \cancel{\{a_j, a_k\}} - \left\{ a_i^\dagger, a_k \right\} a_j = -\delta_{ik} a_j \tag{10.12}$$

$$\left[\hat{N}, a_k \right] = \left[\sum_i a_i^\dagger a_i, a_k \right] = \sum_i \left[a_i^\dagger a_i, a_k \right] = -\sum_i \delta_{ik} a_i = -a_k \tag{10.13}$$

The Heisenberg equation of motion for the operator a_k is

$$
\begin{aligned}
\frac{da_k(t)}{dt} &= \frac{i}{\hbar}\left[H, a_k\right] \\
&= \frac{i}{\hbar}\left(\sum_{i,j} h_{ij}\left[a_i^\dagger a_j, a_k\right] + \frac{1}{2}V_0\left[\left(\hat{N}-N_0\right)^2, a_k\right]\right) \\
&= \frac{i}{\hbar}\left(\sum_{i,j} h_{ij}\left(-\delta_{ik}a_j\right) + \frac{1}{2}V_0\left[\hat{N}^2 - 2N_0\hat{N} + N_0^2, a_k\right]\right) \\
&= \frac{i}{\hbar}\left(-\sum_{i,j} h_{ij}\delta_{ik}a_j + \frac{1}{2}V_0\left(\hat{N}\left[\hat{N}, a_k\right] + \left[\hat{N}, a_k\right]\hat{N} - 2N_0\left[\hat{N}, a_k\right]\right)\right) \\
&= \frac{i}{\hbar}\left(-\sum_{j} h_{kj}a_j + \frac{1}{2}V_0\left(-\hat{N}a_k - a_k\hat{N} + 2N_0 a_k\right)\right) \\
&= \frac{i}{\hbar}\left(-\sum_{j} h_{kj}a_j + \frac{1}{2}V_0\left(-\hat{N}a_k + \left[\hat{N}, a_k\right] - \hat{N}a_k + 2N_0 a_k\right)\right) \\
&= \frac{i}{\hbar}\left(-\sum_{j} h_{kj}a_j + \frac{1}{2}V_0\left(-2\hat{N}a_k - a_k + 2N_0 a_k\right)\right) \\
&= \frac{i}{\hbar}\left(-\sum_{j} h_{kj}a_j - V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)a_k\right) \\
&= -\frac{i}{\hbar}\left(\sum_{j} h_{kj}a_j + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)a_k\right) \qquad (10.14)
\end{aligned}
$$

The Heisenberg equation of motion for the operator $a_k^\dagger$ is

$$
\frac{da_k^\dagger(t)}{dt} = \left(\frac{i}{\hbar}\left[H, a_k\right]\right)^\dagger = -\frac{i}{\hbar}\left[H, a_k\right]^\dagger = \frac{i}{\hbar}\left(\sum_j h_{jk}a_j^\dagger + V_0 a_k^\dagger\left(\hat{N} - N_0 + \frac{1}{2}\right)\right) \qquad (10.15)
$$

The two equations for a_k and $a_k^\dagger$ are essentially coupled, since on the R.H.S there is a dependency in a_i ($a_i^\dagger$) where $i \neq k$. In order to decouple them we want to transform these equations to b_n and $b_n^\dagger$.

$$
\begin{aligned}
\frac{d}{dt}\left(\sum_n \psi_n(k)\, b_n(t)\right) &= -\frac{i}{\hbar}\left(\sum_j h_{kj}\left(\sum_n \psi_n(j)\, b_n\right) + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)\left(\sum_n \psi_n(k)\, b_n\right)\right) \\
\sum_n \psi_n(k)\, \frac{db_n(t)}{dt} &= -\frac{i}{\hbar}\left(\sum_n \sum_j h_{kj}\psi_n(j)\, b_n + V_0\left(\hat{N} - N_0 + \frac{1}{2}\right)\sum_n \psi_n(k)\, b_n\right) \qquad (10.16)
\end{aligned}
$$

Multiplying 10.14 by $\sum_k \psi_l^* (k)$, and get

$$\begin{aligned}
\sum_k \psi_l^* (k) \sum_n \psi_n (k) \frac{db_n (t)}{dt} &= -\frac{i}{\hbar} \left(\sum_n \sum_j \sum_k \psi_l^* (k) h_{kj} \psi_n (j) b_n + V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) \sum_n \sum_k \psi_l^* (k) \psi_n (k) b_n \right) \\
\sum_n \delta_{nl} \frac{db_n (t)}{dt} &= -\frac{i}{\hbar} \left(\sum_n \sum_j \sum_k \psi_l^* (k) h_{kj} \psi_n (j) b_n + V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) \sum_n \delta_{nl} b_n \right) \\
\frac{db_l (t)}{dt} &= -\frac{i}{\hbar} \left(\sum_n \sum_j \sum_k \langle l|k\rangle \langle k| h |j\rangle \langle j|n\rangle b_n + V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) b_l \right) \\
\frac{db_l (t)}{dt} &= -\frac{i}{\hbar} \left(\sum_n \langle l| h |n\rangle b_n + V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) b_l \right) \\
\frac{db_l (t)}{dt} &= -\frac{i}{\hbar} \left(\sum_n \epsilon_n \delta_{nl} b_n + V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) b_l \right) \\
\frac{db_l (t)}{dt} &= -\frac{i}{\hbar} \left(\epsilon_l b_l + V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) b_l \right) \\
\frac{db_l (t)}{dt} &= -\frac{i}{\hbar} \left(\epsilon_l + V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) \right) b_l
\end{aligned} \tag{10.17}$$

and the second equation will be

$$\frac{db_l^\dagger (t)}{dt} = \frac{i}{\hbar} b_l^\dagger \left(\epsilon_l + V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) \right) \tag{10.18}$$

Now the two equations are decoupled and therefore we can simply solve them and get

$$b_l (t) = b_l (0) e^{-\frac{i}{\hbar} \left(\epsilon_l + V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) \right) t} \qquad b_l^\dagger (t) = b_l^\dagger (0) e^{\frac{i}{\hbar} \left(\epsilon_l + V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) \right) t} \tag{10.19}$$

and so the solutions for $a_i, a_i^\dagger$ will be

$$a_i (t) = \sum_n \psi_n (i) b_n (t) \qquad a_i^\dagger (t) = \sum_n \psi_n^* (i) b_n^\dagger (t) \tag{10.20}$$

Let us now consider the state of M electrons as $|M\rangle$. Acting the Hamiltonian on the excited state $|M+1\rangle = b_n^\dagger |M\rangle$ will give

$$\begin{aligned}
H |M+1\rangle &= H b_n^\dagger |M\rangle \\
&= \left(\left[H, b_n^\dagger \right] + b_n^\dagger H \right) |M\rangle \\
&= \left(-i\hbar \frac{db_n^\dagger}{dt} + b_n^\dagger E_M \right) |M\rangle \\
&= \left(-i\hbar \frac{i}{\hbar} b_n^\dagger \left(\epsilon_n + V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) \right) + b_n^\dagger E_M \right) |M\rangle \\
&= \left(b_n^\dagger \left(\epsilon_n + V_0 \left(M - N_0 + \frac{1}{2} \right) \right) + b_n^\dagger E_M \right) |M\rangle \\
&= \left(\epsilon_n + V_0 \left(M - N_0 + \frac{1}{2} \right) + E_M \right) b_n^\dagger |M\rangle \\
&= \underbrace{\left(\epsilon_n + V_0 \left(M - N_0 + \frac{1}{2} \right) + E_M \right)}_{E_{M+1}} |M+1\rangle
\end{aligned} \tag{10.21}$$

Therefore, the excitation energy is

$$\Delta E = E_{M+1} - E_M = \epsilon_n + V_0 \left(M - N_0 + \frac{1}{2} \right) \tag{10.22}$$

Similar calculation for the state $|M-1\rangle$ will give

$$\begin{aligned}
H |M-1\rangle &= H b_n |M\rangle \\
&= ([H, b_n] + b_n H) |M\rangle \\
&= \left(-i\hbar \frac{db_n}{dt} + b_n E_M \right) |M\rangle \\
&= \left(-i\hbar \left(-\frac{i}{\hbar} \left(\epsilon_n + V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) \right) b_n \right) + b_n E_M \right) |M\rangle \\
&= \left(- \left(\epsilon_l + V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) \right) b_n + b_n E_M \right) |M\rangle \\
&= \left(-\epsilon_l - V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) + E_M \right) b_n |M\rangle \\
&= \left(-\epsilon_l - V_0 \left(\hat{N} - N_0 + \frac{1}{2} \right) + E_M \right) |M-1\rangle \\
&= \left(-\epsilon_l - V_0 \left((M-1) - N_0 + \frac{1}{2} \right) + E_M \right) |M-1\rangle \\
&= \underbrace{\left(-\epsilon_l - V_0 \left(M - N_0 - \frac{1}{2} \right) + E_M \right)}_{E_{M-1}} |M-1\rangle
\end{aligned} \tag{10.23}$$

Therefore, the excitation energy is

$$\Delta E = E_{M-1} - E_M = -\epsilon_l - V_0 \left(M - N_0 - \frac{1}{2} \right) \tag{10.24}$$

c

We will do the calculations similar to the previous section (b). First of all we will calculate the following expressions:

$$\begin{aligned}
\left[a_i^\dagger a_j, a_k^\dagger a_l \right] &= a_i^\dagger \left[a_j, a_k^\dagger a_l \right] + \left[a_i^\dagger, a_k^\dagger a_l \right] a_j \\
&= a_i^\dagger \left(\cancel{a_k^\dagger \{a_j, a_l\}} - \left\{ a_j, a_k^\dagger \right\} a_l \right) + \left(a_k^\dagger \left\{ a_i^\dagger, a_l \right\} - \cancel{\left\{ a_i^\dagger, a_k^\dagger \right\}} a_l \right) a_j \\
&= -\delta_{jk} a_i^\dagger a_l + \delta_{il} a_k^\dagger a_j
\end{aligned} \tag{10.25}$$

$$\left[\hat{N}, a_k^\dagger a_l \right] = \left[\sum_i a_i^\dagger a_i, a_k^\dagger a_l \right] = \sum_i \left[a_i^\dagger a_i, a_k^\dagger a_l \right] = \sum_i \left(-a_i^\dagger \delta_{ik} a_l + a_k^\dagger \delta_{il} a_i \right) = -a_k^\dagger a_l + a_k^\dagger a_l = 0 \tag{10.26}$$

Calculating

$$
\begin{aligned}
\frac{d\left(a_k^\dagger a_l\right)}{dt} &= \frac{i}{\hbar}\left[H, a_k^\dagger a_l\right] \\
&= \frac{i}{\hbar}\left(\sum_{i,j} h_{ij}\left[a_i^\dagger a_j, a_k^\dagger a_l\right] + \frac{1}{2}V_0\left[\left(\hat{N}-N_0\right)^2, a_k^\dagger a_l\right]\right) \\
&= \frac{i}{\hbar}\left(\sum_{i,j} h_{ij}\left(-\delta_{jk}a_i^\dagger a_l + \delta_{il}a_k^\dagger a_j\right) + \frac{1}{2}V_0\left[\hat{N}^2 - 2N_0\hat{N} + N_0^2, a_k^\dagger a_l\right]\right) \\
&= \frac{i}{\hbar}\left(-\sum_{i,j} h_{ij}\delta_{jk}a_i^\dagger a_l + \sum_{i,j} h_{ij}\delta_{il}a_k^\dagger a_j + \frac{1}{2}V_0\left(\hat{N}\cancelto{0}{\left[\hat{N}, a_k^\dagger a_l\right]} + \cancelto{0}{\left[\hat{N}, a_k^\dagger a_l\right]}\hat{N} - 2N_0\cancelto{0}{\left[\hat{N}, a_k^\dagger a_l\right]}\right)\right) \\
&= \frac{i}{\hbar}\left(-\sum_{i} h_{ik}a_i^\dagger a_l + \sum_{j} h_{lj}a_k^\dagger a_j\right) \\
&= \frac{i}{\hbar}\left(-\sum_{i} \epsilon_k\delta_{ik}a_i^\dagger a_l + \sum_{j} \epsilon_l\delta_{jl}a_k^\dagger a_j\right) \\
&= \frac{i}{\hbar}\left(-\epsilon_k a_k^\dagger a_l + \epsilon_l a_k^\dagger a_l\right) \\
&= \frac{i}{\hbar}\left(\epsilon_l - \epsilon_k\right)a_k^\dagger a_l
\end{aligned} \tag{10.27}
$$

Therefore,

$$
\frac{d\left(b_n^\dagger b_m\right)}{dt} = \frac{i}{\hbar}\left(\epsilon_m - \epsilon_n\right)b_n^\dagger b_m \tag{10.28}
$$

Acting the Hamiltonian on the particle-hole state $b_n^\dagger b_m \left|M\right\rangle$ will give

$$
\begin{aligned}
Hb_n^\dagger b_m\left|M\right\rangle &= \left(\left[H, b_n^\dagger b_m\right] + b_n^\dagger b_m H\right)\left|M\right\rangle \\
&= \left(-i\hbar\frac{d\left(b_n^\dagger b_m\right)}{dt} + b_n^\dagger b_m E_M\right)\left|M\right\rangle \\
&= \left(\left(\epsilon_m - \epsilon_n\right)b_n^\dagger b_m + E_M b_n^\dagger b_m\right)\left|M\right\rangle \\
&= \left(E_M + \epsilon_m - \epsilon_n\right)b_n^\dagger b_m\left|M\right\rangle
\end{aligned} \tag{10.29}
$$

Therefore, the excitation energy for particle-hole is

$$
\Delta E = \left(E_M + \epsilon_m - \epsilon_n\right) - E_M = \epsilon_m - \epsilon_n \tag{10.30}
$$

11

Question

Consider the following Hamiltonian

$$H=\int\psi^{\dagger}(x)\left(-\frac{\hbar^{2}}{2m}\frac{\partial^{2}}{\partial x^{2}}\right)\psi(x)\,dx+\int\left(\psi^{\dagger}(x)+\psi(x)\right)V(x-y)\,\mu(y)\,dxdy$$

where $\psi(x)$ and $\psi^{\dagger}(x)$ are boson operators.,

$$\mu(y)=\frac{1}{2}\sum_{\alpha,\beta=1}^{2}\xi_{\alpha}^{\dagger}(y)\,\sigma_{\alpha\beta}^{z}\xi_{\beta}(y)$$

$\xi_{\alpha}(y)$ and $\xi_{\beta}^{\dagger}(y)$ are fermion operators, $\alpha,\beta=1,2$, $\sigma_{\alpha\beta}^{z}$ - is the Pauli matrix.

Full Question (2014, 11)

a. Find eigenstates and eigenvalues of H with one fermion and arbitrary number of bosons. (Hint: you may find it a bit easier to do some of the calculations in momentum representation) What is the meaning of the infinite energy term which you obtain in your solution?

b. Repeat (a) for several fermions.

Solution Outline

1. $\mu(y)=\frac{1}{2}(n_1(y)-n_2(y))$. The wave function: $|\psi\rangle=|N_B\rangle\otimes|1_{y_F,\sigma}\rangle=|N_B\rangle\otimes\left(\xi_{\sigma}^{\dagger}(y_F)\,|0_F\rangle\right)$.
2. Use the expansion $\psi(x)=\frac{1}{\sqrt{2\pi}}\int a_k e^{ikx}dk$ to rewrite H. Should Fourier transform V, use: $\frac{1}{\sqrt{2\pi}}\int dx\, e^{ikx}V(x-y)=\frac{1}{\sqrt{2\pi}}V_k e^{iky}$.
3. Define a new operator $A_{y_F,\sigma}(k)=a_k+\frac{m}{\hbar^2k^2}(-1)^{\sigma+1}V_{-k}e^{iky_F}$, by completing the square, and reach decoupling.
4. Verify that $A_{y_F,\sigma}(k)\,,A_{y_F,\sigma}^{\dagger}(k)$ obey the bosonic commutation relations.
5. After the decoupling we can write the solution: $|\{n_i\}\rangle=\prod_{i=0}^{N_B}\frac{\left(A_{y_F,\sigma}^{\dagger}(k_i)\right)^{n_i}}{\sqrt{n_i!}}\,|0_B\rangle$.
6. The infinite energy term originate in the delta function of the potential $\rightarrow$ inferring the particles as point-like (not physical).

Solution

Let us define the state of one fermion and arbitrary number N of bosons,

$$|\psi\rangle=|N_B\rangle\otimes|1_{y_F,\sigma}\rangle=|N_B\rangle\otimes\left(\xi_{\sigma}^{\dagger}(y_F)\,|0_F\rangle\right)\tag{11.1}$$

where y_F is the position of the fermion. The expression $\mu(y)$ can be also written as

$$\begin{aligned}\mu(y)&=\frac{1}{2}\sum_{\alpha,\beta=1}^{2}\xi_{\alpha}^{\dagger}(y)\,\sigma_{\alpha\beta}^{z}\xi_{\beta}(y)\\&=\frac{1}{2}\left(\xi_{1}^{\dagger}(y)\,\xi_1(y)-\xi_{2}^{\dagger}(y)\,\xi_2(y)\right)\\&=\frac{1}{2}(n_1(y)-n_2(y))\end{aligned}\tag{11.2}$$

The Hamiltonian composed of H_0 which is the non-interaction part and H_{int} which describes the boson-fermion interaction, as follows,

$$H = \underbrace{\int \psi^\dagger(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi(x)\,dx}_{H_0} + \underbrace{\iint \left(\psi^\dagger(x)+\psi(x)\right)V(x-y)\,\mu(y)\,dxdy}_{H_{\text{int}}} \tag{11.3}$$

Using the expansion,

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\int a_k e^{ikx}dk \tag{11.4}$$

$$\psi^\dagger(x) = \frac{1}{\sqrt{2\pi}}\int a_k^\dagger e^{-ikx}dk \tag{11.5}$$

we will rewrite H_0 and H_{int}. The non-interaction Hamiltonian will be

$$\begin{aligned}
H_0 &= \int \psi^\dagger(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi(x)\,dx \\
&= \int \left(\frac{1}{\sqrt{2\pi}}\int a_k^\dagger e^{-ikx}dk\right)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\left(\frac{1}{\sqrt{2\pi}}\int a_{k'}e^{ik'x}dk'\right)dx \\
&= \frac{1}{2\pi}\left(-\frac{\hbar^2}{2m}\right)\int dx\int dk\int dk'\,a_k^\dagger e^{-ikx}\left(-k'^2\right)a_{k'}e^{ik'x} \\
&= \frac{1}{2\pi}\frac{\hbar^2}{2m}\int dx\int dk\int dk'\,a_k^\dagger a_{k'}e^{-i(k-k')x}k'^2 \\
&= \frac{1}{2\pi}\frac{\hbar^2}{2m}\int dk\int dk'\,a_k^\dagger a_{k'}\delta(k-k')\,k'^2 \\
&= \int dk\,\frac{\hbar^2k^2}{2m}a_k^\dagger a_k
\end{aligned} \tag{11.6}$$

The interaction part will be

$$\begin{aligned}
H_{\text{int}} &= \iint \left(\psi^\dagger(x)+\psi(x)\right)V(x-y)\,\mu(y)\,dxdy \\
&= \int dx\int dy\left(\frac{1}{\sqrt{2\pi}}\int a_k^\dagger e^{-ikx}dk + \frac{1}{\sqrt{2\pi}}\int a_k e^{ikx}dk\right)V(x-y)\,\mu(y) \\
&= \int dk\int dy\left(a_k^\dagger\int\frac{dx}{\sqrt{2\pi}}e^{-ikx}V(x-y) + a_k\int\frac{dx}{\sqrt{2\pi}}e^{ikx}V(x-y)\right)\mu(y)
\end{aligned} \tag{11.7}$$

Since $V(x-y)$ is hermitian, $V(x-y) = V^*(x-y)$, and therefore

$$\begin{aligned}
H_{\text{int}} &= \int dk\int dy\left(a_k^\dagger\int\frac{dx}{\sqrt{2\pi}}e^{-ikx}V^*(x-y) + a_k\int\frac{dx}{\sqrt{2\pi}}e^{ikx}V(x-y)\right)\mu(y) \\
&= \int dk\int dy\left(a_k^\dagger V_{-k}(y)\,e^{-iky} + a_kV_k(y)\,e^{iky}\right)\mu(y)
\end{aligned} \tag{11.8}$$

Acting the Hamiltonian on $|\psi\rangle$ will give

$$
\begin{aligned}
H|\psi\rangle &= \int dk\,\left[\frac{\hbar^2k^2}{2m}a_k^\dagger a_k+\int dy\,\left(a_k^\dagger V_{-k}(y)\,e^{-iky}+a_kV_k(y)\,e^{iky}\right)\mu(y)\right]|N_B\rangle\otimes|1_{y_F,\sigma}\rangle\\
&= \int dk\,\left[\frac{\hbar^2k^2}{2m}a_k^\dagger a_k+\int dy\,\left(a_k^\dagger V_{-k}(y)\,e^{-iky}+a_kV_k(y)\,e^{iky}\right)\frac{1}{2}(-1)^{\sigma+1}\delta(y-y_F)\right]|N_B\rangle\otimes|1_{y_F,\sigma}\rangle\\
&= \int dk\,\left[\frac{\hbar^2k^2}{2m}a_k^\dagger a_k+\frac{1}{2}(-1)^{\sigma+1}\left(a_k^\dagger V_{-k}(y_F)\,e^{-iky_F}+a_kV_k(y_F)\,e^{iky_F}\right)\right]|N_B\rangle\otimes|1_{y_F,\sigma}\rangle\\
&= \int dk\,\Bigg[\frac{\hbar^2k^2}{2m}\underbrace{\left(a_k^\dagger+\frac{m}{\hbar^2k^2}(-1)^{\sigma+1}V_k(y_F)\,e^{-iky_F}\right)}_{A^\dagger_{y_F,\sigma}(k)}\underbrace{\left(a_k+\frac{m}{\hbar^2k^2}(-1)^{\sigma+1}V_{-k}(y_F)\,e^{-iky_F}\right)}_{A_{y_F,\sigma}(k)}\\
&\qquad -\frac{1}{2}\frac{m}{\hbar^2k^2}|V_k(y_F)|^2\Bigg]|N_B\rangle\otimes|1_{y_F,\sigma}\rangle
\end{aligned}
\tag{11.9}
$$

We define the following operators

$$A_{y_F,\sigma}(k)=a_k+\frac{1}{\sqrt{2\pi}}\frac{m}{\hbar^2k^2}\lambda(-1)^{\sigma+1}V_{-k}e^{iky_F}\tag{11.10}$$

$$A^\dagger_{y_F,\sigma}(k)=a_k^\dagger+\frac{1}{\sqrt{2\pi}}\frac{m}{\hbar^2k^2}\lambda(-1)^{\sigma+1}V_ke^{-iky_F}\tag{11.11}$$

with the following boson commutation relations

$$\left[A_{y_F,\sigma}(k),A^\dagger_{y_F,\sigma}(k)\right]=\left[a_k,a^\dagger_{k'}\right]=\delta(k-k')\tag{11.12}$$

Therefore, the total Hamiltonian, after reducing the fermion degree of freedom of position, is

$$H=\int dk\,\left[\frac{\hbar^2k^2}{2m}A^\dagger_{y,\alpha}(k)\,A_{y,\alpha}(k)-\frac{1}{2}\frac{m}{\hbar^2k^2}|V_k(y_F)|^2\right]\tag{11.13}$$

Now we can address the interaction potential. Assuming $V(x-y)=\lambda\delta(x-y)$,

$$V_k=\frac{1}{\sqrt{2\pi}}\int dx\,e^{ikx}V(x-y)=\frac{1}{\sqrt{2\pi}}\int dx\,e^{ikx}\lambda\delta(x-y)=\frac{1}{\sqrt{2\pi}}\lambda e^{iky}\tag{11.14}$$

So the Hamiltonian will have the following form,

$$H=\int dk\,\left[\frac{\hbar^2k^2}{2m}A^\dagger_{y_F,\sigma}(k)\,A_{y_F,\sigma}(k)-\frac{1}{4\pi}\frac{m}{\hbar^2k^2}\lambda^2\right]\tag{11.15}$$

The Hamiltonian is now diagonalized with the following eighenstates:

$$|\{n_i\}\rangle=\prod_{i=0}^{N_B}\frac{\left(A^\dagger_{y_F,\sigma}(k_i)\right)^{n_i}}{\sqrt{n_i!}}|0_B\rangle\tag{11.16}$$

while given y_F and σ of the fermion, where N_B is the number of bosons and $\sum_i n_i=N_B$. The energies

$$E_{\{n_i\}}=\sum_i\frac{\hbar^2k_i^2}{2m}n_i-\underbrace{\frac{m\lambda^2}{4\pi\hbar^2}\int\frac{dk}{k^2}}_{\text{diverges}}\tag{11.17}$$

The last divergent term originates in the delta function in the potential energy describing the interaction between the bosons and the fermion. This potential is not physical since we infer the bosons and the fermion as point-like particles. A more physical approach is perhaps defining a typical length scale of a particle, and as a result, setting a lower cut-off for k which will give a finite energy.

12

Question

Find eigenfunctions and eigenvalues of the boson operator $\psi_{op}(\boldsymbol{r})$.

Full Question (2015, 9)

a. Find eigenfunctions and eigenvalues of the boson operator $\psi_{op}(\boldsymbol{r})$. Can you do the same for $\psi^{\dagger}_{op}(\boldsymbol{r})$. For the fermionic field operator?

b. Return back to the case of the eigenstate of the bosonic $\psi_{op}(\boldsymbol{r})$ and calculate the average of H_{op} (with the two body interaction $V(r - r_0)$) in this state. What is the average of N_{op}?

Help: to facilitate the understanding of how to deal with the first question write momentarily $\psi_{op}(\boldsymbol{r})$ in terms of an expansion in some complete set. But then reformulate your answer for the "unexpanded" $\psi_{op}(\boldsymbol{r})$ i.e. give it with no relation to the set into which you have expanded. (it was anyways arbitrary, wasn't it?).

Solution Outline

1. For $\psi(\boldsymbol{r})$: *(exist)*
   (a) Use $\psi(\boldsymbol{r}) = \sum_i \phi_i(\boldsymbol{r})\, a_i$ where a_i is a bosonic annihilation operator.
   (b) Define $|\alpha_i\rangle$ as the coherent state of a_i. Define $|\Phi\rangle = \bigotimes_i |\alpha_i\rangle = \prod_i e^{-\frac{|\alpha_i|^2}{2}} e^{\alpha a_i^{\dagger}} |0\rangle$.
   (c) The eigenstates are $|\Phi\rangle$, with the eigenvalues $\Phi(\boldsymbol{r}) = \sum_i \phi_i(\boldsymbol{r})\, \alpha_i$.
2. For $\psi^{\dagger}(\boldsymbol{r})$: *(does not exist)*
   (a) Assume eigenstate $|\Phi\rangle$. Expand it as $|\Phi\rangle = \sum_{n=0}^{\infty} \alpha_n |\Phi_n\rangle$ where $|\Phi_n\rangle$ is a projection of $|\Phi\rangle$ on the subspace of the Fock state with n particles.
   (b) Since $\psi^{\dagger}(\boldsymbol{r})$ adds a particle, the new state does not consist of $|\Phi_0\rangle$, and therefore cannot be an eigenstate.
3. For the fermionic field operator: *(does not exist)*
   (a) $\psi(\boldsymbol{r})$: via anti-commutation, $\Phi^2 |\Phi\rangle = \psi(\boldsymbol{r})\psi(\boldsymbol{r})|\Phi\rangle = -\psi(\boldsymbol{r})\psi(\boldsymbol{r})|\Phi\rangle = -\Phi^2|\Phi\rangle \implies \Phi^2 = 0$.
   (b) $\psi^{\dagger}(\boldsymbol{r})$: the same as the bosonic case.
4. For averages calculate $\langle\Phi| H_{op} |\Phi\rangle$ and $\langle\Phi| N_{op} |\Phi\rangle$.

Solution

a

Let us expand the operator $\psi(\boldsymbol{r})$, as follows,

$$\psi(\boldsymbol{r}) = \sum_i \phi_i(\boldsymbol{r})\, a_i \tag{12.1}$$

where a_i is a bosonic annihilation operator. Let us now define $|\alpha_i\rangle$ as the coherent state of a_i as follow,

$$|\alpha_i\rangle = e^{-\frac{|\alpha_i|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha_i^n}{\sqrt{n!}} |n\rangle = e^{-\frac{|\alpha_i|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha_i^n}{\sqrt{n!}} \left(a_i^{\dagger}\right)^n |0\rangle = e^{-\frac{|\alpha_i|^2}{2}} e^{\alpha a_i^{\dagger}} |0\rangle \tag{12.2}$$

and therefore

$$a_i |\alpha_i\rangle = \alpha_i |\alpha_i\rangle \tag{12.3}$$

Let us define the general state $|\Phi\rangle$ as a tensor product of $|\alpha_i\rangle$,

$$|\Phi\rangle = \bigotimes_i |\alpha_i\rangle = \prod_i e^{-\frac{|\alpha_i|^2}{2}} e^{\alpha a_i^\dagger} |0\rangle \tag{12.4}$$

and therefore

$$a_j |\Phi\rangle = a_j \bigotimes_i |\alpha_i\rangle = (\alpha_j |\alpha_j\rangle) \otimes \left(\bigotimes_{i\neq j} |\alpha_i\rangle\right) = \alpha_j \left(|\alpha_j\rangle \otimes \bigotimes_{i\neq j} |\alpha_i\rangle\right) = \alpha_j |\Phi\rangle \tag{12.5}$$

Since we got that $|\Phi\rangle$ is an eigenfunction of a_i and $\psi(\boldsymbol{r})$ is a linear combination of a_i, $|\Phi\rangle$ is also an eigenfunction of $\psi(\boldsymbol{r})$,

$$\psi(\boldsymbol{r}) |\Phi\rangle = \left(\sum_i \phi_i(\boldsymbol{r}) a_i\right) |\Phi\rangle = \sum_i \phi_i(\boldsymbol{r}) \alpha_i |\Phi\rangle \equiv \Phi(\boldsymbol{r}) |\Phi\rangle \tag{12.6}$$

where $\Phi(\boldsymbol{r})$ is the corresponding eigenvalue of $\psi(\boldsymbol{r})$.

Can you do the same for $\psi^\dagger_{op}(\boldsymbol{r})$? Assume $|\Phi\rangle$ (different from the defined above) is an eigenstate of $\psi^\dagger(\boldsymbol{r})$ and write it in the following way

$$|\Phi\rangle = \sum_{n=0}^{\infty} \alpha_n |\Phi_n\rangle \tag{12.7}$$

where $|\Phi_n\rangle$ is a projection of $|\Phi\rangle$ on the subspace of the Fock state with n particles. Since $\psi^\dagger(\boldsymbol{r})$ adds a particle,

$$\psi^\dagger |\Phi_n\rangle \sim |\Phi_{n+1}\rangle \tag{12.8}$$

therefore,

$$\psi^\dagger |\Phi\rangle = \psi^\dagger \sum_{n=0}^{\infty} \alpha_n |\Phi_n\rangle \sim \sum_{n=0}^{\infty} \alpha_n |\Phi_{n+1}\rangle \tag{12.9}$$

This new state does not consist of $|\Phi_0\rangle$. But we assume $|\Phi\rangle$ is an eigenstate so it must hold $\alpha_0 = 0$. By induction we get$\alpha_n = 0$ for all n, which imply that $|\Phi\rangle = 0$. Hence, $\psi^\dagger(\boldsymbol{r})$ does not have an eigenstate.

For the fermionic field operator? Let us assume $\psi(\boldsymbol{r})$ is a fermion operator with an eigenstate $|\Phi\rangle$ and a corresponding eigenvalue Φ. Therefore,

$$\psi(\boldsymbol{r}) \psi(\boldsymbol{r}) |\Phi\rangle = \Phi^2 |\Phi\rangle \tag{12.10}$$

However, we can use the anti-commutation relation $\{\psi(\boldsymbol{r}), \psi(\boldsymbol{r})\} = 0$, and get

$$\psi(\boldsymbol{r}) \psi(\boldsymbol{r}) |\Phi\rangle = (\{\psi(\boldsymbol{r}), \psi(\boldsymbol{r})\} - \psi(\boldsymbol{r}) \psi(\boldsymbol{r})) |\Phi\rangle = -\psi(\boldsymbol{r}) \psi(\boldsymbol{r}) |\Phi\rangle = -\Phi^2 |\Phi\rangle \tag{12.11}$$

which says that $\Phi = 0$, and therefore there is no eigenstate for a fermion operator $\psi(\boldsymbol{r})$. The same goes for the fermion operator $\psi^\dagger(\boldsymbol{r})$.

b

The Hamiltonian with two body interaction $V\left(r-r'\right)$, is

$$H=\int d^3r\,\psi^{\dagger}\left(\boldsymbol{r}\right)\underbrace{\left(-\frac{\hbar^2}{2m}\nabla^2+U\left(\boldsymbol{r}\right)\right)}_{h}\psi\left(\boldsymbol{r}\right)+\int d^3r\int d^3r'\,\psi^{\dagger}\left(\boldsymbol{r}\right)\psi^{\dagger}\left(\boldsymbol{r}'\right)V\left(r-r'\right)\psi\left(\boldsymbol{r}'\right)\psi\left(\boldsymbol{r}\right) \tag{12.12}$$

and the average of H_{op} is

$$\begin{aligned}\left\langle\Phi\right|H\left|\Phi\right\rangle &=\int d^3r\,\left\langle\Phi\right|\psi^{\dagger}\left(\boldsymbol{r}\right)h\psi\left(\boldsymbol{r}\right)\left|\Phi\right\rangle+\int d^3r\int d^3r'\,\left\langle\Phi\right|\psi^{\dagger}\left(\boldsymbol{r}\right)\psi^{\dagger}\left(\boldsymbol{r}'\right)V\left(r-r'\right)\psi\left(\boldsymbol{r}'\right)\psi\left(\boldsymbol{r}\right)\left|\Phi\right\rangle\\ &=\int d^3r\,\left\langle\Phi\right|\Phi^{*}\left(\boldsymbol{r}\right)h\Phi\left(\boldsymbol{r}\right)\left|\Phi\right\rangle+\int d^3r\int d^3r'\,\left\langle\Phi\right|\Phi^{*}\left(\boldsymbol{r}\right)\Phi^{*}\left(\boldsymbol{r}'\right)V\left(r-r'\right)\Phi\left(\boldsymbol{r}'\right)\Phi\left(\boldsymbol{r}\right)\left|\Phi\right\rangle\\ &=\int d^3r\,\left|\Phi\left(\boldsymbol{r}\right)\right|^2h+\int d^3r\int d^3r'\,\left|\Phi\left(\boldsymbol{r}\right)\right|^2\left|\Phi\left(\boldsymbol{r}'\right)\right|^2V\left(r-r'\right)\end{aligned} \tag{12.13}$$

The average of N_{op} is

$$\left\langle\Phi\right|N_{op}\left|\Phi\right\rangle=\left\langle\Phi\right|\int d^3r\,\psi^{\dagger}\left(\boldsymbol{r}\right)\psi\left(\boldsymbol{r}\right)\left|\Phi\right\rangle=\int d^3r\,\left\langle\Phi\right|\Phi^{*}\left(\boldsymbol{r}\right)\Phi\left(\boldsymbol{r}\right)\left|\Phi\right\rangle=\int d^3r\,\left|\Phi\left(\boldsymbol{r}\right)\right|^2 \tag{12.14}$$

13

Question

Describe differences and similarities between second quantization of the harmonic oscillator and its description in terms of a and $a^\dagger$ operators, i.e. $a = p/\sqrt{2m\hbar\omega} - i\sqrt{m\omega/(2\hbar)}x$, etc.

Solution

	Second Quantization	**First Quantization**
Hamiltonian	$H = \int \psi^\dagger(x) h\psi(x) = \sum_k \epsilon_k a_k^\dagger a_k$	$h = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$
	Convenient to describe many body systems	Convenient to describe a single wave function (one “particle”). Not convenient to describe many body systems (need Slater determinant).
	Number of particles is <u>not</u> pre-determined	Describes constant number of “particles”
	Grand canonical ensemble	Canonical ensemble
	$a_k^\dagger$ raises the number of particles in mode k	$a_i^\dagger$ raises the energy of the i^{th} particle
	Using creation operator: Particle reservoir	Using creation (ladder) operator: Energy reservoir
Eigenenergies	$E = \overbrace{\sum_k}^{\text{modes}} \epsilon_k = \sum_k \hbar\omega_k\left(n_k + \frac{1}{2}\right)$	$E = \overbrace{\sum_i}^{\text{particles}} \epsilon_i = \sum_i \hbar\omega\left(n_i + \frac{1}{2}\right)$
Eigenstates	$\lvert\{n_k\}\rangle = \prod_k \lvert n_k\rangle = \prod_k \frac{\left(a_k^\dagger\right)^{n_k}}{\sqrt{n_k!}}\lvert 0\rangle$	$\left\lvert\{n_i\}_{i=0}^N\right\rangle = \lvert n_1\rangle \otimes \lvert n_2\rangle \otimes \cdots \otimes \lvert n_1\rangle$
s.p. eigenstate	$\lvert\ldots 0_{k-1}1_k0_{k+1}\ldots\rangle = a_k^\dagger\lvert\ldots 0_{k-1}0_k0_{k+1}\ldots\rangle$	$\lvert n_i\rangle = \frac{\left(a^\dagger\right)^{n_i}}{\sqrt{n_i!}}\lvert 0_i\rangle$
	$a_k\lvert 0_k\rangle = 0$	$a\lvert 0\rangle = 0$

Description of the annihilation operator

Suppose a is a first quantization annihilation operator of an harmonic oscillator with eigenfunctions $\phi_n(x)$, and b is a bosonic annihilation operator. Let us see how the annihilation operator a looks like in the second quantization. We will denote it as $\tilde{a}$, and get

$$
\begin{aligned}
\tilde{a} &= \int dx\, \psi^\dagger(x)\, a\psi(x) \\
&= \int dx \left(\sum_m \phi_m^*(x)\, b_m^\dagger\right) a \left(\sum_n \phi_n(x)\, b_n\right) \\
&= \sum_{n,m} b_m^\dagger b_n \int dx\, \phi_m^*(x)\, a\phi_n(x) \\
&= \sum_{n,m} b_m^\dagger b_n \langle m| a |n\rangle \\
&= \sum_{n,m} b_m^\dagger b_n \sqrt{n}\langle m|n-1\rangle \\
&= \sum_{n,m} b_m^\dagger b_n \sqrt{n}\delta_{m,n-1} \\
&= \sum_n b_{n-1}^\dagger b_n \sqrt{n} \qquad (13.1)
\end{aligned}
$$

We can see that decreasing an harmonic oscillator quantum number using a, in first quantization “language”, is equivalent to annihilate one boson in every mode n and create instead of it a boson in mode $n-1$, in the second quantization “language”.

14

Question

Find a variational solution for the "spin-phonon" Hamiltonian

$$H = \omega b^\dagger b + \lambda\left(b + b^\dagger\right)\sigma_x + \mu\sigma_z$$

where λ and μ are constants, b and $b^\dagger$ are boson (phonon) operators and σ_x, σ_z - the Pauli matrices. Use a product trial wave function $\psi = \phi\,(\text{phonons})\,\xi\,(\text{spin})$ with general ϕ and ξ.

Solution Outline

1. We want to solve $\delta\left(\langle\psi|H|\psi\rangle - \epsilon\langle\psi|\psi\rangle\right) \equiv \delta f = 0$. Use a product trial wave function $|\psi\rangle = |\phi\rangle|\xi\rangle$.
2. Calculate $\langle\psi|H|\psi\rangle$ by reducing the Hamiltonian to only the phonons degree of freedom, using partial trace with $|\xi\rangle = \begin{pmatrix}\cos\theta \\ \sin\theta e^{i\varphi}\end{pmatrix}$. Get $\langle\psi|H|\psi\rangle = \langle\phi|\langle H\rangle_\xi|\phi\rangle$.
3. Solve $\langle H\rangle_\xi$ by completing the square and define a new operator $A = b + \frac{\lambda}{\omega}\sin(2\theta)\cos\varphi$. Now $\langle H\rangle_\xi$ depends on θ, φ.
4. Verify that $A, A^\dagger$ obey the boson (phonon) commutation relations.
5. In order to perform the variation, since f depends on $\theta, \varphi, |\phi\rangle$ we will take the derivatives of f with respect to these variables, and equate them to zero.
6. Find the condition for θ and φ where f is minimal, and write the solution $|\psi\rangle = |n\rangle|\xi(\theta_m, \varphi_m)\rangle$ and the corresponding energy.

Solution

Let us find the variational solution by solving

$$\delta\left(\langle\psi|H|\psi\rangle - \epsilon\langle\psi|\psi\rangle\right) \equiv \delta f = 0 \tag{14.1}$$

where $|\psi\rangle = |\phi\rangle|\xi\rangle$ is the trial wave function, and

$$|\xi\rangle = \begin{pmatrix}\cos\theta \\ \sin\theta e^{i\varphi}\end{pmatrix} \tag{14.2}$$

Calculating $\langle\psi|H|\psi\rangle$ will give

$$\langle\psi|H|\psi\rangle = \langle\xi|\langle\phi|H|\phi\rangle|\xi\rangle = \omega\langle\phi|b^\dagger b|\phi\rangle + \lambda\langle\phi|\left(b + b^\dagger\right)|\phi\rangle\langle\xi|\sigma_x|\xi\rangle + \mu\langle\phi|\phi\rangle\langle\xi|\sigma_z|\xi\rangle \tag{14.3}$$

where $\langle\xi|\sigma_x|\xi\rangle$ and $\langle\xi|\sigma_z|\xi\rangle$ can be calculated as follows,

$$\begin{aligned}
\langle\xi|\sigma_x|\xi\rangle &= \begin{pmatrix}\cos\theta & \sin\theta e^{-i\varphi}\end{pmatrix}\begin{pmatrix}0 & 1 \\ 1 & 0\end{pmatrix}\begin{pmatrix}\cos\theta \\ \sin\theta e^{i\varphi}\end{pmatrix} \\
&= \begin{pmatrix}\cos\theta & \sin\theta e^{-i\varphi}\end{pmatrix}\begin{pmatrix}\sin\theta e^{i\varphi} \\ \cos\theta\end{pmatrix} \\
&= \sin\theta\cos\theta e^{i\varphi} + \cos\theta\sin\theta e^{-i\varphi} \\
&= 2\sin\theta\cos\theta\cos\varphi \\
&= \sin(2\theta)\cos\varphi
\end{aligned} \tag{14.4}$$

$$\begin{aligned}
\langle\xi|\,\sigma_z\,|\xi\rangle &= \begin{pmatrix}\cos\theta & \sin\theta e^{-i\varphi}\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\cos\theta\\ \sin\theta e^{i\varphi}\end{pmatrix}\\
&= \begin{pmatrix}\cos\theta & \sin\theta e^{-i\varphi}\end{pmatrix}\begin{pmatrix}\cos\theta\\ -\sin\theta e^{i\varphi}\end{pmatrix}\\
&= \cos^2\theta - \sin^2\theta\\
&= \cos(2\theta)
\end{aligned} \tag{14.5}$$

Therefore,

$$\begin{aligned}
\langle\psi|H|\psi\rangle &= \omega\,\langle\phi|\,b^\dagger b\,|\phi\rangle + \lambda\,\langle\phi|\left(b+b^\dagger\right)|\phi\rangle\sin(2\theta)\cos\varphi + \mu\cos(2\theta)\,\langle\phi|\phi\rangle\\
&= \langle\phi|\left[\omega b^\dagger b + \lambda\left(b+b^\dagger\right)\sin(2\theta)\cos\varphi\right]|\phi\rangle + \mu\cos(2\theta)\,\langle\phi|\phi\rangle\\
&= \langle\phi|\left[\omega\underbrace{\left(b^\dagger + \frac{\lambda}{\omega}\sin(2\theta)\cos\varphi\right)}_{\equiv A^\dagger}\underbrace{\left(b + \frac{\lambda}{\omega}\sin(2\theta)\cos\varphi\right)}_{\equiv A} - \frac{\lambda^2}{\omega}\sin^2(2\theta)\cos^2\varphi\right]|\phi\rangle + \mu\cos(2\theta)\,\langle\phi|\phi\rangle\\
&= \langle\phi|\left[\omega A^\dagger A - \frac{\lambda^2}{\omega}\sin^2(2\theta)\cos^2\varphi\right]|\phi\rangle + \mu\cos(2\theta)\,\langle\phi|\phi\rangle\\
&= \langle\phi|\underbrace{\left[\omega A^\dagger A - \frac{\lambda^2}{\omega}\sin^2(2\theta)\cos^2\varphi + \mu\cos(2\theta)\right]}_{\langle H\rangle_\xi}|\phi\rangle
\end{aligned} \tag{14.6}$$

The newly defined operators A and $A^\dagger$ will obey the bosonic commutation relations,

$$\left[A, A^\dagger\right] = \left[b, b^\dagger\right] = 1 \tag{14.7}$$

We got that $\langle H\rangle_\xi$ is a shifted harmonic oscillator, with the following energies:

$$\epsilon_n = \omega n - \frac{\lambda^2}{\omega}\sin^2(2\theta)\cos^2\varphi + \mu\cos(2\theta) \tag{14.8}$$

Since $|\xi\rangle$ is normalized (we chose it so), $\langle\psi|\psi\rangle = \langle\phi|\phi\rangle$, and we can write

$$\delta f = \delta\left(\langle\psi|H|\psi\rangle - \epsilon\,\langle\psi|\psi\rangle\right) = \delta\,\langle\phi|\left[\omega A^\dagger A - \frac{\lambda^2}{\omega}\sin^2(2\theta)\cos^2\varphi + \mu\cos(2\theta) - \epsilon\right]|\phi\rangle \tag{14.9}$$

Since f depends on $\theta, \varphi, |\phi\rangle$ we will take the derivatives of f with respect to these variables, and equate them to zero. The derivatives are:

$$\frac{\partial f}{\partial\theta} = \left(-4\frac{\lambda^2}{\omega}\sin(2\theta)\cos(2\theta)\cos^2\varphi - 2\mu\sin(2\theta)\right)\langle\phi|\phi\rangle = -2\mu\sin(2\theta)\left(\frac{2\lambda^2}{\mu\omega}\cos(2\theta)\cos^2\varphi + 1\right) \tag{14.10}$$

$$\frac{\partial f}{\partial\varphi} = 2\frac{\lambda^2}{\omega}\sin^2(2\theta)\cos\varphi\sin\varphi\,\langle\phi|\phi\rangle = \frac{\lambda^2}{\omega}\sin^2(2\theta)\sin(2\varphi) \tag{14.11}$$

$$\frac{\partial f}{\partial\,\langle\phi|} = \underbrace{\left(\langle H\rangle_\xi - \epsilon\right)|\phi\rangle}_{\text{Sch. eq. for } \langle H\rangle_\xi} = \left[\omega n - \frac{\lambda^2}{\omega}\sin^2(2\theta)\cos^2\varphi + \mu\cos(2\theta)\right]|\phi\rangle \tag{14.12}$$

From $\partial_{\langle\phi|} f = 0$ we get

$$\langle H \rangle_{\xi} |\phi\rangle = \epsilon |\phi\rangle \tag{14.13}$$

and we already solved $\langle H \rangle_{\xi}$, so $\epsilon = \epsilon_n$. From $\partial_{\varphi} f = 0$ we get

$$\sin^2(2\theta)\sin(2\varphi) = 0 \qquad \Longrightarrow \qquad \varphi = 0, \frac{\pi}{2}, \pi, \frac{3\pi}{2} \quad \text{OR} \quad \theta = 0, \frac{\pi}{2}, \pi \tag{14.14}$$

Using that, and from $\partial_{\theta} f = 0$ we get one of the following

$$\varphi = 0, \pi \qquad \Longrightarrow \qquad \cos(2\theta) = -\frac{\mu\omega}{2\lambda^2} \tag{14.15}$$

$$\varphi = \frac{\pi}{2}, \frac{3\pi}{2} \qquad \Longrightarrow \qquad \cos(2\theta) = \frac{\mu\omega}{2\lambda^2} \tag{14.16}$$

$$\theta = 0, \frac{\pi}{2}, \pi \tag{14.17}$$

Since we want to find the gourd state we want to minimize the energy ϵ. First of all we immediately can set $n = 0$, and get

$$\epsilon = -\frac{\lambda^2}{\omega}\sin^2(2\theta)\cos^2\varphi + \mu\cos(2\theta) \tag{14.18}$$

Now, we need to examine all the different cases, we from the variation (can also check for minima points). After doing that we finally get

$$\cos(2\theta_m) = -\frac{\mu\omega}{2\lambda^2} \tag{14.19}$$

$$\varphi_m = 0, \pi \tag{14.20}$$

with the minimal energy

$$\epsilon = -\frac{\lambda^2}{\omega}\left(1 - \left(-\frac{\mu\omega}{2\lambda^2}\right)^2\right) - \frac{\mu^2\omega}{2\lambda^2} = -\frac{\lambda^2}{\omega} + \frac{\mu^2\omega}{4\lambda^2} - \frac{\mu^2\omega}{2\lambda^2} = -\frac{\lambda^2}{\omega} - \frac{\mu^2\omega}{4\lambda^2} \tag{14.21}$$

Hence, the ground state $|\psi\rangle$ is

$$|\psi\rangle = |n = 0\rangle\,|\xi(\theta = \theta_m, \varphi = \varphi_m)\rangle = |0\rangle \otimes \begin{pmatrix} \cos\theta_m \\ \sin\theta_m e^{i\varphi_m} \end{pmatrix} \tag{14.22}$$

where $|n\rangle$ is the known solution of the harmonic oscillator.

15

Question

In the lectures we have derived the Bogoliubov spectrum using the zero range approximation for the two body potential $V(|\boldsymbol{r}-\boldsymbol{r}_0|) = V_0\delta(\boldsymbol{r}-\boldsymbol{r}_0)$. How will this spectrum change if one does not use this simplification?

Solution Outline

1. Write the (time-dependent) Gross-Pitaevski equation.
2. Consider a solution of small deviation $\psi(\boldsymbol{r},t) = \left(\sqrt{\rho_0}+\delta\psi(\boldsymbol{r},t)\right)e^{-i\mu t/\hbar}$, insert it into GP equation and simplify.
3. Use the guess: $\delta\psi(\boldsymbol{r},t) = A_{\boldsymbol{k}}e^{i(\boldsymbol{kr}-\omega t)} + A^*_{-\boldsymbol{k}}e^{-i(\boldsymbol{kr}-\omega t)}$.
4. Extract two equations, for $e^{i(\boldsymbol{kr}-\omega t)}$ and $e^{-i(\boldsymbol{kr}-\omega t)}$. Write the system of equations in matrix notation $M\begin{pmatrix}A_{\boldsymbol{k}}\\ A_{-\boldsymbol{k}}\end{pmatrix}=0$ and get the Bogoliubov spectrum by solving det[M]=0.

Solution

The Gross-Pitaevski equation is

$$i\hbar\frac{\partial\psi(\boldsymbol{r},t)}{\partial t} = h\psi(\boldsymbol{r},t) + \int d^3r'\,V(\boldsymbol{r}-\boldsymbol{r}')\left|\psi(\boldsymbol{r}',t)\right|^2\psi(\boldsymbol{r},t) \tag{15.1}$$

where

$$h = -\frac{\hbar^2}{2m}\nabla^2 \tag{15.2}$$

The simple solution, which is constant in space, is

$$\psi_0 = \sqrt{\rho_0}e^{-i\mu t/\hbar} \tag{15.3}$$

where $\mu = V_0\rho_0$ and $V_0 = \int d^3r'\,V(\boldsymbol{r}')$. We want to consider solutions for the GP equation which are small deviations from ψ_0. Namely,

$$\psi(\boldsymbol{r},t) = \left(\sqrt{\rho_0}+\delta\psi(\boldsymbol{r},t)\right)e^{-i\mu t/\hbar} \tag{15.4}$$

Inserting $\psi(\boldsymbol{r},t)$ into the GP equation will give

$$\begin{aligned}
i\hbar\frac{\partial\psi(\boldsymbol{r},t)}{\partial t} &= h\psi(\boldsymbol{r},t) + \int d^3r'\,V(\boldsymbol{r}-\boldsymbol{r}')\left|\psi(\boldsymbol{r}',t)\right|^2\psi(\boldsymbol{r},t)\\
i\hbar\left[-i\frac{\mu}{\hbar}\left(\sqrt{\rho_0}+\delta\psi(\boldsymbol{r},t)\right)+\frac{\partial\delta\psi(\boldsymbol{r},t)}{\partial t}\right]e^{-i\mu t/\hbar} &= h\delta\psi(\boldsymbol{r},t)e^{-i\mu t/\hbar} + \int d^3r'\,V(\boldsymbol{r}-\boldsymbol{r}')\left|\sqrt{\rho_0}+\delta\psi(\boldsymbol{r}',t)\right|^2\left(\sqrt{\rho_0}+\delta\psi(\boldsymbol{r},t)\right)e^{-i\mu t/\hbar}\\
\mu\left(\sqrt{\rho_0}+\delta\psi(\boldsymbol{r},t)\right)+i\hbar\frac{\partial\delta\psi(\boldsymbol{r},t)}{\partial t} &= h\delta\psi(\boldsymbol{r},t) + \int d^3r'\,V\left[\rho_0+\sqrt{\rho_0}\left(\delta\psi(\boldsymbol{r}',t)+\delta\psi^*(\boldsymbol{r}',t)\right)\right]\left(\sqrt{\rho_0}+\delta\psi(\boldsymbol{r},t)\right)\\
\mu\left(\sqrt{\rho_0}+\delta\psi(\boldsymbol{r},t)\right)+i\hbar\frac{\partial\delta\psi(\boldsymbol{r},t)}{\partial t} &= h\delta\psi(\boldsymbol{r},t) + \left[\underbrace{\rho_0V_0}_{\mu} + \int d^3r'\,V(\boldsymbol{r}-\boldsymbol{r}')\sqrt{\rho_0}\left(\delta\psi(\boldsymbol{r}',t)+\delta\psi^*(\boldsymbol{r}',t)\right)\right]\left(\sqrt{\rho_0}+\delta\psi(\boldsymbol{r},t)\right)\\
i\hbar\frac{\partial\delta\psi(\boldsymbol{r},t)}{\partial t} &= h\delta\psi(\boldsymbol{r},t) + \int d^3r'\,V(\boldsymbol{r}-\boldsymbol{r}')\sqrt{\rho_0}\left(\delta\psi(\boldsymbol{r}',t)+\delta\psi^*(\boldsymbol{r}',t)\right)\left(\sqrt{\rho_0}+\delta\psi(\boldsymbol{r},t)\right)\\
i\hbar\frac{\partial\delta\psi(\boldsymbol{r},t)}{\partial t} &= h\delta\psi(\boldsymbol{r},t) + \rho_0\int d^3r'\,V(\boldsymbol{r}-\boldsymbol{r}')\left(\delta\psi(\boldsymbol{r}',t)+\delta\psi^*(\boldsymbol{r}',t)\right)
\end{aligned} \tag{15.5}$$

Using the following guess,

$$\delta\psi(\boldsymbol{r},t) = A_{\boldsymbol{k}} e^{i(\boldsymbol{kr}-\omega t)} + A^*_{-\boldsymbol{k}} e^{-i(\boldsymbol{kr}-\omega t)} \tag{15.6}$$

will give the following expressions:

$$i\hbar \frac{\partial \delta\psi(\boldsymbol{r},t)}{\partial t} = i\hbar \left[-i\omega A_{\boldsymbol{k}} e^{i(\boldsymbol{kr}-\omega t)} + i\omega A^*_{-\boldsymbol{k}} e^{-i(\boldsymbol{kr}-\omega t)}\right] = \hbar\omega \left[A_{\boldsymbol{k}} e^{i(\boldsymbol{kr}-\omega t)} - A^*_{-\boldsymbol{k}} e^{-i(\boldsymbol{kr}-\omega t)}\right] \tag{15.7}$$

$$h\delta\psi(\boldsymbol{r},t) = -\frac{\hbar^2}{2m}\nabla^2 \left[A_{\boldsymbol{k}} e^{i(\boldsymbol{kr}-\omega t)} + A^*_{-\boldsymbol{k}} e^{-i(\boldsymbol{kr}-\omega t)}\right] = \frac{\hbar^2 k^2}{2m}\delta\psi(\boldsymbol{r},t) \tag{15.8}$$

$$\begin{aligned} \delta\psi(\boldsymbol{r}',t) + \delta\psi^*(\boldsymbol{r}',t) &= A_{\boldsymbol{k}} e^{i\left(\boldsymbol{kr}'-\omega t\right)} + A^*_{-\boldsymbol{k}} e^{-i\left(\boldsymbol{kr}'-\omega t\right)} + A^*_{\boldsymbol{k}} e^{-i\left(\boldsymbol{kr}'-\omega t\right)} + A_{-\boldsymbol{k}} e^{i\left(\boldsymbol{kr}'-\omega t\right)} \\ &= \left(A_{\boldsymbol{k}} + A_{-\boldsymbol{k}}\right) e^{i\left(\boldsymbol{kr}'-\omega t\right)} + \left(A^*_{\boldsymbol{k}} + A^*_{-\boldsymbol{k}}\right) e^{-i\left(\boldsymbol{kr}'-\omega t\right)} \end{aligned} \tag{15.9}$$

and therefore, keeping in mind that V is symmetric and real,

$$\begin{aligned} \hbar\omega \left[A_{\boldsymbol{k}} e^{i(\boldsymbol{kr}-\omega t)} - A^*_{-\boldsymbol{k}} e^{-i(\boldsymbol{kr}-\omega t)}\right] &= \frac{\hbar^2 k^2}{2m}\delta\psi(\boldsymbol{r},t) + \rho_0 \int d^3r'\, V\left(\boldsymbol{r}-\boldsymbol{r}'\right) \left[\left(A_{\boldsymbol{k}} + A_{-\boldsymbol{k}}\right) e^{i\left(\boldsymbol{kr}'-\omega t\right)} + \left(A^*_{\boldsymbol{k}} + A^*_{-\boldsymbol{k}}\right) e^{-i\left(\boldsymbol{kr}'-\omega t\right)}\right] \\ &= \frac{\hbar^2 k^2}{2m}\delta\psi(\boldsymbol{r},t) + \rho_0 \int d^3r'\, V\left(\boldsymbol{r}'-\boldsymbol{r}\right) \left[\left(A_{\boldsymbol{k}} + A_{-\boldsymbol{k}}\right) e^{i\left(\boldsymbol{kr}'-\omega t\right)} + \left(A^*_{\boldsymbol{k}} + A^*_{-\boldsymbol{k}}\right) e^{-i\left(\boldsymbol{kr}'-\omega t\right)}\right] \\ &= \frac{\hbar^2 k^2}{2m}\delta\psi(\boldsymbol{r},t) + \rho_0 \int d^3r'\, V\left(\boldsymbol{r}'\right) \left[\left(A_{\boldsymbol{k}} + A_{-\boldsymbol{k}}\right) e^{i\left(\boldsymbol{kr}'-\omega t\right)} e^{i\boldsymbol{kr}} + \left(A^*_{\boldsymbol{k}} + A^*_{-\boldsymbol{k}}\right) e^{-i\left(\boldsymbol{kr}'-\omega t\right)} e^{-i\boldsymbol{kr}}\right] \\ &= \frac{\hbar^2 k^2}{2m}\delta\psi(\boldsymbol{r},t) + \rho_0 \left[\left(A_{\boldsymbol{k}} + A_{-\boldsymbol{k}}\right) V_{\boldsymbol{k}} e^{i(\boldsymbol{kr}-\omega t)} + \left(A^*_{\boldsymbol{k}} + A^*_{-\boldsymbol{k}}\right) V_{-\boldsymbol{k}} e^{-i(\boldsymbol{kr}-\omega t)}\right] \\ &= \frac{\hbar^2 k^2}{2m}\delta\psi(\boldsymbol{r},t) + \rho_0 \left[\left(A_{\boldsymbol{k}} + A_{-\boldsymbol{k}}\right) V_{\boldsymbol{k}} e^{i(\boldsymbol{kr}-\omega t)} + \left(A^*_{\boldsymbol{k}} + A^*_{-\boldsymbol{k}}\right) V^*_{\boldsymbol{k}} e^{-i(\boldsymbol{kr}-\omega t)}\right] \end{aligned} \tag{15.10}$$

We can extract two equations, for $e^{i(\boldsymbol{kr}-\omega t)}$ and $e^{-i(\boldsymbol{kr}-\omega t)}$, and get

$$\hbar\omega A_{\boldsymbol{k}} = \frac{\hbar^2 k^2}{2m} A_{\boldsymbol{k}} + \rho_0 \left(A_{\boldsymbol{k}} + A_{-\boldsymbol{k}}\right) V_{\boldsymbol{k}} \tag{15.11}$$

$$-\hbar\omega A_{-\boldsymbol{k}} = \frac{\hbar^2 k^2}{2m} A_{-\boldsymbol{k}} + \rho_0 \left(A_{\boldsymbol{k}} + A_{-\boldsymbol{k}}\right) V_{\boldsymbol{k}} \tag{15.12}$$

In matrix notations:

$$\begin{pmatrix} \hbar\omega - \frac{\hbar^2 k^2}{2m} - \rho_0 V_{\boldsymbol{k}} & \rho_0 V_{\boldsymbol{k}} \\ \rho_0 V_{\boldsymbol{k}} & -\hbar\omega - \frac{\hbar^2 k^2}{2m} - \rho_0 V_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} A_{\boldsymbol{k}} \\ A_{-\boldsymbol{k}} \end{pmatrix} = 0 \tag{15.13}$$

For a solution the determinant must be zero,

$$\begin{aligned} 0 &= \left| \begin{pmatrix} \hbar\omega - \frac{\hbar^2 k^2}{2m} - \rho_0 V_{\boldsymbol{k}} & \rho_0 V_{\boldsymbol{k}} \\ \rho_0 V_{\boldsymbol{k}} & -\hbar\omega - \frac{\hbar^2 k^2}{2m} - \rho_0 V_{\boldsymbol{k}} \end{pmatrix} \right| \\ &= \left(\hbar\omega - \frac{\hbar^2 k^2}{2m} - \rho_0 V_{\boldsymbol{k}}\right)\left(-\hbar\omega - \frac{\hbar^2 k^2}{2m} - \rho_0 V_{\boldsymbol{k}}\right) - \rho_0^2 V_{\boldsymbol{k}}^2 \\ &= \left(\frac{\hbar^2 k^2}{2m} + \rho_0 V_{\boldsymbol{k}}\right)^2 - (\hbar\omega)^2 - \rho_0^2 V_{\boldsymbol{k}}^2 \\ &= \left(\frac{\hbar^2 k^2}{2m}\right)^2 + 2\left(\frac{\hbar^2 k^2}{2m}\right)\rho_0 V_{\boldsymbol{k}} + \rho_0^2 V_{\boldsymbol{k}}^2 - (\hbar\omega)^2 - \rho_0^2 V_{\boldsymbol{k}}^2 \\ &= \left(\frac{\hbar^2 k^2}{2m}\right)^2 + 2\left(\frac{\hbar^2 k^2}{2m}\right)\rho_0 V_{\boldsymbol{k}} - (\hbar\omega)^2 \end{aligned} \tag{15.14}$$

and we get Bogoliubov spectrum

$$(\hbar\omega)^2 = \frac{\hbar^2 k^2}{2m}\left(\frac{\hbar^2 k^2}{2m} + 2\rho_0 V_{\boldsymbol{k}}\right) \tag{15.15}$$

This form of the spectrum is for a general potential V. Using the zero range approximation for the two body potential $V\left(|\boldsymbol{r}-\boldsymbol{r'}|\right) = V_0\delta\left(\boldsymbol{r}-\boldsymbol{r'}\right)$, we get

$$V_{\boldsymbol{k}} = \int d^3r\, e^{-i\boldsymbol{k}\left(\boldsymbol{r}-\boldsymbol{r}'\right)} V\left(|\boldsymbol{r}-\boldsymbol{r'}|\right) = \int d^3r\, e^{-i\boldsymbol{k}\boldsymbol{r}} V\left(\boldsymbol{r}\right) = V_0 \int d^3r\, e^{-i\boldsymbol{k}\boldsymbol{r}} \delta\left(\boldsymbol{r}-\boldsymbol{r'}\right) = V_0 \tag{15.16}$$

and therefore,

$$\hbar\omega\left(k\right) = \sqrt{\frac{\hbar^2 k^2}{2m}\left(\frac{\hbar^2 k^2}{2m} + 2\rho_0 V_0\right)} \tag{15.17}$$

16

Question

Consider a Hamiltonian

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2M} + \frac{k\left(x^2+y^2\right)}{2} + \alpha xy, \quad |\alpha| < k$$

and assume that $M \gg m$. Discuss solutions of this problem using the Born-Oppenheimer approximation.

Solution Outline

1. Write the Hamiltonian as $H = H_{\text{slow}}\left(p_y, y\right) + H_{\text{fast}}\left(p_x, x; y\right)$.
2. Solve the "fast" Hamiltonian, while keeping y as a parameter.
3. Show that the Berry potential (connection) $A_{n_x}(y)$ is zero.
4. Write $H_{\text{BO}}\left(p_y, y\right) = H_{\text{slow}} + \left\langle H_{\text{fast}}\right\rangle_x$ and solve it.
5. Check the validity of the BH approximation: $\frac{\Delta E_{\text{fast}}}{\Delta E_{\text{slow}}} \gg 1$.

Solution

The Hamiltonian can be divided into "fast" part (x) and "slow" part (y).

$$H = \underbrace{\frac{p_x^2}{2m} + \frac{1}{2}kx^2 + \alpha xy}_{H_{\text{fast}}} + \frac{p_y^2}{2M} + \frac{1}{2}ky^2 \tag{16.1}$$

The "fast" part

The Hamiltonian of the fast part is

$$H_{\text{fast}}\left(p_x, x; y\right) = \frac{p_x^2}{2m} + \frac{1}{2}kx^2 + \alpha xy = \frac{p_x^2}{2m} + \frac{1}{2}m\underbrace{\frac{k}{m}}_{\omega_x^2}\left(x - \underbrace{\left(-\frac{\alpha y}{k}\right)}_{x_0}\right)^2 - \frac{\alpha^2}{2k}y^2 \tag{16.2}$$

It is a shifted harmonic oscillator with the known solutions denoted as $\phi_{n_x}\left(x - x_0; y\right)$ with the corresponding energies

$$E_{n_x}(y) = \hbar\omega_x\left(n_x + \frac{1}{2}\right) - \frac{\alpha^2}{2k}y^2 \tag{16.3}$$

where $\omega_x = \sqrt{k/m}$.

Berry potential (connection)

The Berry potential is

$$A_{n_x}(y) = i\left\langle\phi_{n_x}\right|\partial_y\left|\phi_{n_x}\right\rangle \tag{16.4}$$

however,

$$\left\langle\phi_{n_x}\right|\partial_y\left|\phi_{n_x}\right\rangle = \left\langle\phi_{n_x}\middle|\partial_y\phi_{n_x}\right\rangle = \cancel{\partial_y\underbrace{\left\langle\phi_{n_x}\middle|\phi_{n_x}\right\rangle}_{\text{const}}} - \left\langle\partial_y\phi_{n_x}\middle|\phi_{n_x}\right\rangle = -\left\langle\phi_{n_x}\middle|\partial_y\phi_{n_x}\right\rangle^* \tag{16.5}$$

and since ϕ_{n_x} is real, $\left\langle\phi_{n_x}\middle|\partial_y\phi_{n_x}\right\rangle$ must be zero and therefore

$$A_{n_x}(y) = 0 \tag{16.6}$$

Solving the Born-Oppenheimer Hamiltonian

We will now try to find a solution of the form

$$\psi(x,y) = \sum_{n_y} \xi_{n_x}(y)\,\phi_{n_x}\left(x + \frac{\alpha y}{k}; y\right) \tag{16.7}$$

where $\xi_{n_x}(y)$ are the eigenfunction of the Born-Oppenheimer Hamiltonian:

$$\begin{aligned}
H_{\mathrm{BO}}(p_y, y) &= \frac{p_y^2}{2M} + \frac{1}{2}ky^2 + \langle H_{\mathrm{fast}}\rangle_x \\
&= \frac{p_y^2}{2M} + \frac{1}{2}ky^2 + \hbar\omega_x\left(n_x + \frac{1}{2}\right) - \frac{\alpha^2}{2k}y^2 \\
&= \frac{p_y^2}{2M} + \frac{1}{2}k\left(1 - \frac{\alpha^2}{k^2}\right)y^2 + \hbar\omega_x\left(n_x + \frac{1}{2}\right)
\end{aligned} \tag{16.8}$$

Solving the Sch. equation for H_{BO},

$$H_{\mathrm{BO}}\xi_{n_x}(y) = E_{n_x n_y}\xi_{n_x}(y) \tag{16.9}$$

will give the solution for a shifted harmonic oscillator, with the energies

$$E_{n_x n_y} = \hbar\omega_y\left(n_y + \frac{1}{2}\right) + \hbar\omega_x\left(n_x + \frac{1}{2}\right) \tag{16.10}$$

where

$$\omega_y = \sqrt{\frac{k}{M}\left(1 - \frac{\alpha^2}{k^2}\right)} \tag{16.11}$$

Born-Oppenheimer approximation validity

The criterion is

$$\frac{\Delta E_{\mathrm{fast}}}{\Delta E_{\mathrm{slow}}} \gg 1 \tag{16.12}$$

where

$$\Delta E_{\mathrm{fast}} = E_{n_x+1}(y) - E_{n_x}(y) = \hbar\omega_x \tag{16.13}$$

$$\Delta E_{\mathrm{slow}} = E_{n_x(n_y+1)} - E_{n_x n_y} = \hbar\omega_y \tag{16.14}$$

Hence,

$$\frac{\Delta E_{\mathrm{fast}}}{\Delta E_{\mathrm{slow}}} = \frac{\omega_x}{\omega_y} = \frac{\sqrt{\frac{k}{m}}}{\sqrt{\frac{k}{M}\left(1 - \frac{\alpha^2}{k^2}\right)}} = \sqrt{\frac{M}{m}\left(1 - \frac{\alpha^2}{k^2}\right)} \tag{16.15}$$

Since given $M \gg m$, (16.12) is satisfied.

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Question

A localized spin-1/2 (quantum two-level system) is subjected to the time-dependent magnetic field,

$$b(t) = (b\cos(\omega t), b\sin(\omega t), b_0)$$

where b_0 is a constant component of the field, b is the amplitude of the rotating component. Assume that the perturbation is sufficiently slow and calculate the dynamic phase and Berry phase within the adiabatic approximation.

Solution Outline

1. Write the Hamiltonian $H = \boldsymbol{\Omega} \cdot \boldsymbol{S}$.
2. Find the direction angles θ, φ of $\boldsymbol{\Omega}$.
3. Find the eigenstates $|\phi_+\rangle$ and $|\phi_-\rangle$ of the spin in the θ, φ direction (rotate the up and down states to these angles). $E_\pm = \pm\frac{\hbar}{2}|\boldsymbol{\Omega}|$.
4. Calculate the dynamic phase: $\varphi(t) = -\frac{1}{\hbar}\int_0^t dt'\, E_\pm(t')$.
5. Calculate the Berry connection: $A_\pm = i\langle\phi_\pm|\nabla_{\boldsymbol{R}}|\phi_\pm\rangle$.
6. Calculate the Berry phase: $\gamma_\pm = \int d\boldsymbol{R}\, A_\pm$.

Solution

The Hamiltonian is

$$\begin{aligned}
H &= -\mu \boldsymbol{S} \cdot \boldsymbol{b}(t) \\
&= -\mu\frac{\hbar}{2}\left[\sigma_x b\cos(\omega t) + \sigma_y b\sin(\omega t) + \sigma_z b_0\right] \\
&= -\mu\frac{\hbar}{2}\left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} b\cos(\omega t) + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} b\sin(\omega t) + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} b_0\right] \\
&= -\mu\frac{\hbar}{2}\begin{pmatrix} b_0 & b\cos(\omega t) - ib\sin(\omega t) \\ b\cos(\omega t) + ib\sin(\omega t) & -b_0 \end{pmatrix} \\
&= -\mu\frac{\hbar}{2}\begin{pmatrix} b_0 & be^{-i\omega t} \\ be^{i\omega t} & -b_0 \end{pmatrix}
\end{aligned} \tag{17.1}$$

The Hamiltonian can also be written as

$$H = \boldsymbol{\Omega} \cdot \boldsymbol{S} \tag{17.2}$$

where

$$\boldsymbol{\Omega} = -\mu(b\cos(\omega t), b\sin(\omega t), b_0) \tag{17.3}$$

Therefore, the precession frequency is

$$\Omega = |\boldsymbol{\Omega}| = \mu\sqrt{b^2 + b_0^2} \tag{17.4}$$

and the precession axis is tilted relative to the z axis with an angle

$$\theta = \arctan\left(\frac{\sqrt{\Omega_x^2 + \Omega_y^2}}{\Omega_z}\right) = \arctan\left(\frac{\sqrt{b^2\cos^2(\omega t) + b^2\sin^2(\omega t)}}{b_0}\right) = \arctan\left(\frac{b}{b_0}\right) \tag{17.5}$$

and the angle φ in the $x-y$ plane, is

$$\varphi = \arctan\left(\frac{\Omega_y}{\Omega_x}\right) = \arctan\left(\frac{b\sin(\omega t)}{b\cos(\omega t)}\right) = \arctan(\tan(\omega t)) = \omega t \tag{17.6}$$

Accordingly the eigenstates can be obtained from the $|\uparrow\rangle$ and from the $|\downarrow\rangle$ states, and by rotating them to θ and φ, we get

$$|\phi_+\rangle = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) e^{i\varphi} \end{pmatrix} \tag{17.7}$$

$$|\phi_-\rangle = \begin{pmatrix} \sin\left(\frac{\theta}{2}\right) \\ -\cos\left(\frac{\theta}{2}\right) e^{i\varphi} \end{pmatrix} \tag{17.8}$$

where θ and φ are the angles found in (17.5) and (17.6). The energies are

$$E_\pm = \pm\frac{\hbar}{2}\Omega = \pm\mu\frac{\hbar}{2}\sqrt{b^2+b_0^2} \tag{17.9}$$

Dynamic phase

The dynamic phase is

$$\begin{aligned} \varphi(t) &= -\frac{1}{\hbar}\int_0^t dt'\, E_\pm(t') \\ &= -\frac{E_\pm}{\hbar}t \\ &= \mp\frac{\mu}{2}\sqrt{b_0^2+b^2}t \end{aligned} \tag{17.10}$$

Berry phase

The Berry potential (connection) is

$$A_\pm = i\langle\phi_\pm|\nabla_{\boldsymbol{R}}|\phi_\pm\rangle \tag{17.11}$$

Conducting the calculations for A_+ and A_- will give

$$\begin{aligned} A_+ &= i\langle\phi_+|\nabla_{\boldsymbol{R}}|\phi_+\rangle \\ &= i\begin{pmatrix}\cos\left(\frac{\theta}{2}\right) & \sin\left(\frac{\theta}{2}\right)e^{-i\varphi}\end{pmatrix}\left[\hat{R}\frac{\partial}{\partial R} + \hat{\theta}\frac{1}{R}\frac{\partial}{\partial\theta} + \hat{\varphi}\frac{1}{R\sin\theta}\frac{\partial}{\partial\varphi}\right]\begin{pmatrix} \cos\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) e^{i\varphi} \end{pmatrix} \\ &= i\begin{pmatrix}\cos\left(\frac{\theta}{2}\right) & \sin\left(\frac{\theta}{2}\right)e^{-i\varphi}\end{pmatrix}\begin{pmatrix} -\hat{\theta}\frac{1}{2R}\sin\left(\frac{\theta}{2}\right) \\ \hat{\theta}\frac{1}{2R}\cos\left(\frac{\theta}{2}\right)e^{i\varphi} + \hat{\varphi}\frac{i}{R\sin\theta}\sin\left(\frac{\theta}{2}\right)e^{i\varphi} \end{pmatrix} \\ &= i\left[-\hat{\theta}\cos\left(\frac{\theta}{2}\right)\frac{1}{2R}\sin\left(\frac{\theta}{2}\right) + \sin\left(\frac{\theta}{2}\right)e^{-i\varphi}\left(\hat{\theta}\frac{1}{2R}\cos\left(\frac{\theta}{2}\right)e^{i\varphi} + \hat{\varphi}\frac{i}{R\sin\theta}\sin\left(\frac{\theta}{2}\right)e^{i\varphi}\right)\right] \\ &= i\left[\hat{\theta}\frac{1}{2R}\left(\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right) - \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\right) + \hat{\varphi}\frac{i}{R\sin\theta}\sin^2\left(\frac{\theta}{2}\right)\right] \\ &= i\hat{\varphi}\frac{i}{2R\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right)}\sin^2\left(\frac{\theta}{2}\right) \\ &= -\hat{\varphi}\frac{1}{2R}\tan\left(\frac{\theta}{2}\right) \end{aligned} \tag{17.12}$$

$$
\begin{aligned}
A_- &= i \langle \phi_- | \nabla_{\boldsymbol{R}} | \phi_- \rangle \\
&= i \begin{pmatrix} \sin\left(\frac{\theta}{2}\right) & -\cos\left(\frac{\theta}{2}\right) e^{-i\varphi} \end{pmatrix} \left[\hat{R} \frac{\partial}{\partial R} + \hat{\theta} \frac{1}{R} \frac{\partial}{\partial \theta} + \hat{\varphi} \frac{1}{R \sin\theta} \frac{\partial}{\partial \varphi} \right] \begin{pmatrix} \sin\left(\frac{\theta}{2}\right) \\ -\cos\left(\frac{\theta}{2}\right) e^{i\varphi} \end{pmatrix} \\
&= i \begin{pmatrix} \sin\left(\frac{\theta}{2}\right) & -\cos\left(\frac{\theta}{2}\right) e^{-i\varphi} \end{pmatrix} \begin{pmatrix} \hat{\theta} \frac{1}{2R} \cos\left(\frac{\theta}{2}\right) \\ -\hat{\theta} \frac{1}{2R} \sin\left(\frac{\theta}{2}\right) e^{i\varphi} + \hat{\varphi} \frac{i}{R\sin\theta} \cos\left(\frac{\theta}{2}\right) e^{i\varphi} \end{pmatrix} \\
&= i \left[\hat{\theta} \frac{1}{2R} \cos\left(\frac{\theta}{2}\right) \sin\left(\frac{\theta}{2}\right) - \cos\left(\frac{\theta}{2}\right) e^{-i\varphi} \left(-\hat{\theta} \frac{1}{2R} \sin\left(\frac{\theta}{2}\right) e^{i\varphi} + \hat{\varphi} \frac{i}{R\sin\theta} \cos\left(\frac{\theta}{2}\right) e^{i\varphi} \right) \right] \\
&= i \left[\hat{\theta} \frac{1}{2R} \left(\cos\left(\frac{\theta}{2}\right) \sin\left(\frac{\theta}{2}\right) - \cos\left(\frac{\theta}{2}\right) \sin\left(\frac{\theta}{2}\right) \right) - \hat{\varphi} \frac{i}{R\sin\theta} \cos^2\left(\frac{\theta}{2}\right) \right] \\
&= -i\hat{\varphi} \frac{i}{2R \sin\left(\frac{\theta}{2}\right) \cos\left(\frac{\theta}{2}\right)} \cos^2\left(\frac{\theta}{2}\right) \\
&= \hat{\varphi} \frac{1}{2R} \cot\left(\frac{\theta}{2}\right)
\end{aligned} \tag{17.13}
$$

Therefore, the Berry phase is

$$
\begin{aligned}
\gamma_+ &= i \int d\boldsymbol{R} \langle \phi_+ | \nabla_{\boldsymbol{R}} | \phi_+ \rangle \\
&= \int d\boldsymbol{R}\, A_+ \\
&= \int_0^{\omega t} R \sin\theta d\varphi \left(-\frac{1}{2R} \tan\left(\frac{\theta}{2}\right) \right) \\
&= -\frac{1}{2} \sin\theta \tan\left(\frac{\theta}{2}\right) \omega t \\
&= -\sin\left(\frac{\theta}{2}\right) \cos\left(\frac{\theta}{2}\right) \tan\left(\frac{\theta}{2}\right) \omega t \\
&= -\sin^2\left(\frac{\theta}{2}\right) \omega t
\end{aligned} \tag{17.14}
$$

$$
\begin{aligned}
\gamma_- &= i \int d\boldsymbol{R} \langle \phi_- | \nabla_{\boldsymbol{R}} | \phi_- \rangle \\
&= \int d\boldsymbol{R}\, A_- \\
&= \int_0^{\omega t} R \sin\theta d\varphi \frac{1}{2R} \cot\left(\frac{\theta}{2}\right) \\
&= \frac{1}{2} \sin\theta \cot\left(\frac{\theta}{2}\right) \omega t \\
&= \sin\left(\frac{\theta}{2}\right) \cos\left(\frac{\theta}{2}\right) \cot\left(\frac{\theta}{2}\right) \omega t \\
&= \cos^2\left(\frac{\theta}{2}\right) \omega t
\end{aligned} \tag{17.15}
$$

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Question

Solve the Lippmann-Schwinger equation and find the scattering cross section for a so called separable potential in the momentum space $\langle \boldsymbol{k}| V |\boldsymbol{k}'\rangle = \lambda v(k) v(k')$ where λ and $v(k)$ are real. Consider the solutions of the Schrodinger equation for such a potential and discuss when does it have bound states (hint: bound states are solutions of the L-S eq. for negative energies and thus without the free term). Show that the energies of the bound states are given by the poles of the T operator (for the definition of T cf., Sakurai).

Solution Outline

1. Get the expression for the transition operator T, and find poles. $T = \sum_{n=0}^{\infty} V \left(\frac{1}{E-H_0+i\epsilon} V\right)^n$.

2. Find the matrix elements $\langle \boldsymbol{k}| T |\boldsymbol{k}'\rangle$.

3. Solving Lippmann-Schwinger equation: Multiply LS equation by $\langle \boldsymbol{k}|$ from the left and get $\langle \boldsymbol{k}|\psi\rangle = \psi(\boldsymbol{k}) = \delta(\boldsymbol{k}-\boldsymbol{k}_0) + \frac{1}{E-\frac{\hbar^2 k^2}{2m}+i\epsilon} \langle \boldsymbol{k}| T |\boldsymbol{k}_0\rangle$

4. Scattering cross section: Calculate $f(\boldsymbol{k}_0, \boldsymbol{k}') = -\frac{1}{4\pi}(2\pi)^3 \frac{2m}{\hbar^2} \langle \boldsymbol{k}'| T |\boldsymbol{k}_0\rangle$, and get $\frac{d\sigma}{d\Omega} = \left|f(\boldsymbol{k}_0, \boldsymbol{k}')\right|^2$.

5. Solving Schrodinger equation: Multiply Sch. equation by $\langle \boldsymbol{k}|$ from the left, set $\alpha \equiv \int d^3k'\, v(k')\, \psi(\boldsymbol{k}') =$ const and insert the expression of $\psi(\boldsymbol{k})$ (now depends on α) back into the same equation (iterative solution). Find poles.

Solution

The Lippmann-Schwinger equation is

$$|\psi\rangle = |\phi\rangle + \frac{1}{E-H_0+i\epsilon} V |\psi\rangle \tag{18.1}$$

where $|\phi\rangle$ is a plane-wave state with momentum $\boldsymbol{k}_0$ ($|\phi\rangle = |\boldsymbol{k}_0\rangle$), H_0 stands for the kinetic-energy operator, and E denotes as the energies of the full Hamiltonian $H = H_0 + V$.

The transition operator T

For convenience, let us introduce the transition operator T which defined as

$$V|\psi\rangle = T|\phi\rangle \tag{18.2}$$

Using the Lippmann-Schwinger equation, we get

$$V|\psi\rangle = V|\phi\rangle + V\frac{1}{E-H_0+i\epsilon} V|\psi\rangle = \underbrace{\left[V + V\frac{1}{E-H_0+i\epsilon} T\right]}_{=T} |\phi\rangle \tag{18.3}$$

therefore,

$$T = V + V\frac{1}{E-H_0+i\epsilon} T \tag{18.4}$$

We can obtain an iterative solution for T as follows,

$$
\begin{aligned}
T &= V + V\frac{1}{E-H_0+i\epsilon}\left(V + V\frac{1}{E-H_0+i\epsilon}\left(V + V\frac{1}{E-H_0+i\epsilon}\dots\right)\right) \\
&= V + V\frac{1}{E-H_0+i\epsilon}V + V\frac{1}{E-H_0+i\epsilon}V\frac{1}{E-H_0+i\epsilon}V + \dots \\
&= \sum_{n=0}^{\infty} V\left(\frac{1}{E-H_0+i\epsilon}V\right)^n
\end{aligned} \tag{18.5}
$$

Let us calculate the matrix elements of T, as follows,

$$
\begin{aligned}
\langle \boldsymbol{k}| T \left|\boldsymbol{k}'\right\rangle &= \langle \boldsymbol{k}| \sum_{n=0}^{\infty} V\left(\frac{1}{E-H_0+i\epsilon}V\right)^n \left|\boldsymbol{k}'\right\rangle \\
&= \langle \boldsymbol{k}| V \left|\boldsymbol{k}'\right\rangle + \langle \boldsymbol{k}| V\frac{1}{E-H_0+i\epsilon}V\left|\boldsymbol{k}'\right\rangle + \dots \\
&= \langle \boldsymbol{k}| V \left|\boldsymbol{k}'\right\rangle + \int dk''\ \langle \boldsymbol{k}| V \left|\boldsymbol{k}''\right\rangle \left\langle \boldsymbol{k}''\right| \frac{1}{E-H_0+i\epsilon}\left|\boldsymbol{k}''\right\rangle \left\langle \boldsymbol{k}''\right| V \left|\boldsymbol{k}'\right\rangle + \dots \\
&= \langle \boldsymbol{k}| V \left|\boldsymbol{k}'\right\rangle + \int dk''\ \langle \boldsymbol{k}| V \left|\boldsymbol{k}''\right\rangle \frac{1}{E-\frac{\hbar^2 k''^2}{2m}+i\epsilon}\left\langle \boldsymbol{k}''\right| V \left|\boldsymbol{k}'\right\rangle + \dots
\end{aligned} \tag{18.6}
$$

Using the given potential,

$$
\langle \boldsymbol{k}| V \left|\boldsymbol{k}'\right\rangle = \lambda v(k)\, v(k') \tag{18.7}
$$

we get

$$
\begin{aligned}
\langle \boldsymbol{k}| T \left|\boldsymbol{k}'\right\rangle &= \lambda v(k)\, v(k') + \int dk''\, \lambda v(k)\, v(k'')\frac{1}{E-\frac{\hbar^2 k''^2}{2m}+i\epsilon}\lambda v(k'')\, v(k') + \dots \\
&= \lambda v(k)\, v(k') + \lambda v(k)\, v(k')\int dk''\ \frac{\lambda v^2(k'')}{E-\frac{\hbar^2 k''^2}{2m}+i\epsilon} + \dots \\
&= \lambda v(k)\, v(k')\left[1 + \int dk''\ \frac{\lambda v^2(k'')}{E-\frac{\hbar^2 k''^2}{2m}+i\epsilon} + \dots\right]
\end{aligned} \tag{18.8}
$$

Solving the Lippmann-Schwinger equation

Calculating $\psi(\boldsymbol{k})$ by multiplying LS equation by $\langle \boldsymbol{k}|$ from the left,

$$
\begin{aligned}
\langle \boldsymbol{k}|\psi\rangle &= \langle \boldsymbol{k}|\phi\rangle + \langle \boldsymbol{k}| \frac{1}{E-H_0+i\epsilon} V|\psi\rangle \\
&= \langle \boldsymbol{k}|\phi\rangle + \langle \boldsymbol{k}| \frac{1}{E-H_0+i\epsilon} T|\phi\rangle \\
&= \langle \boldsymbol{k}|\boldsymbol{k}_0\rangle + \langle \boldsymbol{k}| \frac{1}{E-H_0+i\epsilon} T|\boldsymbol{k}_0\rangle \\
&= \delta(\boldsymbol{k}-\boldsymbol{k}_0) + \int d^3k' \, \langle \boldsymbol{k}| \frac{1}{E-H_0+i\epsilon} \left|\boldsymbol{k}'\right\rangle \left\langle \boldsymbol{k}'\right| T|\boldsymbol{k}_0\rangle \\
&= \delta(\boldsymbol{k}-\boldsymbol{k}_0) + \int d^3k' \, \langle \boldsymbol{k}| \frac{1}{E-\frac{\hbar^2k'^2}{2m}+i\epsilon} \left|\boldsymbol{k}'\right\rangle \left\langle \boldsymbol{k}'\right| T|\boldsymbol{k}_0\rangle \\
&= \delta(\boldsymbol{k}-\boldsymbol{k}_0) + \int d^3k' \, \frac{1}{E-\frac{\hbar^2k'^2}{2m}+i\epsilon} \left\langle \boldsymbol{k}|\boldsymbol{k}'\right\rangle \left\langle \boldsymbol{k}'\right| T|\boldsymbol{k}_0\rangle \\
&= \delta(\boldsymbol{k}-\boldsymbol{k}_0) + \int d^3k' \, \frac{1}{E-\frac{\hbar^2k'^2}{2m}+i\epsilon} \delta_{\boldsymbol{k}\boldsymbol{k}'} \left\langle \boldsymbol{k}'\right| T|\boldsymbol{k}_0\rangle \\
&= \delta(\boldsymbol{k}-\boldsymbol{k}_0) + \frac{1}{E-\frac{\hbar^2k^2}{2m}+i\epsilon} \langle \boldsymbol{k}| T|\boldsymbol{k}_0\rangle
\end{aligned} \tag{18.9}
$$

Therefore, the solution of the LS equation is

$$
\psi(\boldsymbol{k}) = \delta(\boldsymbol{k}-\boldsymbol{k}_0) + \frac{1}{E-\frac{\hbar^2k^2}{2m}+i\epsilon} \lambda v(k)\, v(k_0) \left[1 + \int dk'' \, \frac{\lambda v^2(k'')}{E-\frac{\hbar^2k''^2}{2m}+i\epsilon} + \dots\right] \tag{18.10}
$$

For $\psi(\boldsymbol{r})$ we can use Fourier transform or use

$$
\psi(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}} \left[e^{i\boldsymbol{k}_0\boldsymbol{r}} + \frac{e^{ik_0r}}{r} f\left(\boldsymbol{k}_0, \boldsymbol{k}'\right)\right] \tag{18.11}
$$

for large r, with the scattering amplitude $f\left(\boldsymbol{k}_0, \boldsymbol{k}'\right)$ we will calculate in a moment.

Scattering cross section

The differential cross section is

$$
\frac{d\sigma}{d\Omega} = \left|f\left(\boldsymbol{k}_0, \boldsymbol{k}'\right)\right|^2 \tag{18.12}
$$

where $\boldsymbol{k}'$ represents the propagation vector for waves reaching observation point $\boldsymbol{r}$. The scattering amplitude is

$$
\begin{aligned}
f\left(\boldsymbol{k}_0, \boldsymbol{k}'\right) &= -\frac{1}{4\pi}(2\pi)^3 \frac{2m}{\hbar^2} \left\langle \boldsymbol{k}'\right| V|\psi\rangle \\
&= -\frac{1}{4\pi}(2\pi)^3 \frac{2m}{\hbar^2} \left\langle \boldsymbol{k}'\right| T|\phi\rangle \\
&= -\frac{1}{4\pi}(2\pi)^3 \frac{2m}{\hbar^2} \left\langle \boldsymbol{k}'\right| T|\boldsymbol{k}_0\rangle
\end{aligned} \tag{18.13}
$$

Correspondingly, we can expand $f\left(\boldsymbol{k}, \boldsymbol{k}'\right)$ as follows,

$$
f\left(\boldsymbol{k}, \boldsymbol{k}'\right) = \sum_{n=1}^{\infty} f^{(n)}\left(\boldsymbol{k}, \boldsymbol{k}'\right) \tag{18.14}
$$

where n is the number of times the V operator enters. Namely,

$$f^{(1)}\left(\boldsymbol{k},\boldsymbol{k}'\right) = -\frac{1}{4\pi}\left(2\pi\right)^3\frac{2m}{\hbar^2}\left\langle\boldsymbol{k}'\right|T^{(1)}\left|\boldsymbol{k}\right\rangle = -\frac{1}{4\pi}\left(2\pi\right)^3\frac{2m}{\hbar^2}\left\langle\boldsymbol{k}'\right|V\left|\boldsymbol{k}\right\rangle \tag{18.15}$$

$$f^{(2)}\left(\boldsymbol{k},\boldsymbol{k}'\right) = -\frac{1}{4\pi}\left(2\pi\right)^3\frac{2m}{\hbar^2}\left\langle\boldsymbol{k}'\right|T^{(2)}\left|\boldsymbol{k}\right\rangle = -\frac{1}{4\pi}\left(2\pi\right)^3\frac{2m}{\hbar^2}\left\langle\boldsymbol{k}'\right|V\frac{1}{E-H_0+i\epsilon}V\left|\boldsymbol{k}\right\rangle \tag{18.16}$$

$$\vdots$$

Since already know we know $\left\langle\boldsymbol{k}\right|T\left|\boldsymbol{k}'\right\rangle$ we can write the full expression,

$$f\left(\boldsymbol{k},\boldsymbol{k}'\right) = -\frac{1}{4\pi}\left(2\pi\right)^3\frac{2m}{\hbar^2}\left\langle\boldsymbol{k}'\right|T\left|\boldsymbol{k}\right\rangle = -\frac{1}{4\pi}\left(2\pi\right)^3\frac{2m}{\hbar^2}\lambda v\left(k\right)v\left(k'\right)\left[1+\int dk''\,\frac{\lambda v^2\left(k''\right)}{E-\frac{\hbar^2k''^2}{2m}+i\epsilon}+\ldots\right] \tag{18.17}$$

and get

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \left|f\left(\boldsymbol{k}_0,\boldsymbol{k}'\right)\right|^2\\ &= 4\pi^4\left(\frac{2m}{\hbar^2}\right)^2\left|\left\langle\boldsymbol{k}'\right|T\left|\boldsymbol{k}_0\right\rangle\right|^2\\ &= 4\pi^4\left(\frac{2m}{\hbar^2}\right)^2\left|\lambda v\left(k_0\right)v\left(k'\right)\left[1+\int dk''\,\frac{\lambda v^2\left(k''\right)}{E-\frac{\hbar^2k''^2}{2m}+i\epsilon}+\ldots\right]\right|^2\\ &= 4\pi^4\left(\frac{2m}{\hbar^2}\right)^2\lambda^2v^2\left(k_0\right)v^2\left(k'\right)\left|1+\int dk''\,\frac{\lambda v^2\left(k''\right)}{E-\frac{\hbar^2k''^2}{2m}+i\epsilon}+\ldots\right|^2\end{aligned} \tag{18.18}$$

Alternatively, we can use the first and second (or any other) order Born approximation,

$$f^{(1)}\left(\boldsymbol{k},\boldsymbol{k}'\right) = -\frac{1}{4\pi}\left(2\pi\right)^3\frac{2m}{\hbar^2}\left\langle\boldsymbol{k}\right|T^{(1)}\left|\boldsymbol{k}'\right\rangle = -\frac{1}{4\pi}\left(2\pi\right)^3\frac{2m}{\hbar^2}\lambda v\left(k\right)v\left(k'\right) \tag{18.19}$$

$$f^{(2)}\left(\boldsymbol{k},\boldsymbol{k}'\right) = -\frac{1}{4\pi}\left(2\pi\right)^3\frac{2m}{\hbar^2}\left\langle\boldsymbol{k}\right|T^{(2)}\left|\boldsymbol{k}'\right\rangle = -\frac{1}{4\pi}\left(2\pi\right)^3\frac{2m}{\hbar^2}\lambda v\left(k\right)v\left(k'\right)\int dk''\,\frac{\lambda v^2\left(k''\right)}{E-\frac{\hbar^2k''^2}{2m}+i\epsilon} \tag{18.20}$$

and get,

$$\frac{d\sigma}{d\Omega}\approx\left|f^{(1)}\left(\boldsymbol{k}_0,\boldsymbol{k}'\right)+f^{(2)}\left(\boldsymbol{k}_0,\boldsymbol{k}'\right)\right|^2 = 4\pi^4\left(\frac{2m}{\hbar^2}\right)^2\lambda^2v^2\left(k_0\right)v^2\left(k'\right)\left|1+\int dk''\,\frac{\lambda v^2\left(k''\right)}{E-\frac{\hbar^2k''^2}{2m}+i\epsilon}\right|^2 \tag{18.21}$$

Schrodinger equation

The Schrodinger equation is

$$\left(H_0+V\right)\left|\psi\right\rangle = E\left|\psi\right\rangle \tag{18.22}$$

multiplying by $\langle \boldsymbol{k}|$ from the left,

$$\begin{aligned}
\langle \boldsymbol{k}| H_0 |\psi\rangle + \langle \boldsymbol{k}| V |\psi\rangle &= E \langle \boldsymbol{k}|\psi\rangle \\
\frac{\hbar^2 k^2}{2m} \langle \boldsymbol{k}|\psi\rangle + \langle \boldsymbol{k}| V |\psi\rangle &= E\psi(\boldsymbol{k}) \\
\frac{\hbar^2 k^2}{2m}\psi(\boldsymbol{k}) + \int d^3k' \, \langle \boldsymbol{k}| V \left|\boldsymbol{k}'\right\rangle \left\langle \boldsymbol{k}'\right|\psi\rangle &= E\psi(\boldsymbol{k}) \\
\frac{\hbar^2 k^2}{2m}\psi(\boldsymbol{k}) + \int d^3k' \, \lambda v(k) \, v(k') \, \psi\left(\boldsymbol{k}'\right) &= E\psi(\boldsymbol{k}) \\
\frac{\hbar^2 k^2}{2m}\psi(\boldsymbol{k}) + \lambda v(k) \int d^3k' \, v(k') \, \psi\left(\boldsymbol{k}'\right) &= E\psi(\boldsymbol{k})
\end{aligned} \tag{18.23}$$

Assuming

$$\alpha \equiv \int d^3k' \, v(k') \, \psi\left(\boldsymbol{k}'\right) = \text{const} \tag{18.24}$$

we get

$$\psi(\boldsymbol{k}) = \alpha\lambda v(k) \frac{1}{E - \frac{\hbar^2 k^2}{2m}} \tag{18.25}$$

For iterative solution, plug back $\psi(\boldsymbol{k})$ into Sch. equation,

$$\begin{aligned}
\frac{\hbar^2 k^2}{2m}\alpha\lambda v(k) \frac{1}{E - \frac{\hbar^2 k^2}{2m}} + \lambda v(k) \int d^3k' \, v(k') \left(\alpha\lambda v(k') \frac{1}{E - \frac{\hbar^2 k'^2}{2m}}\right) &= E\alpha\lambda v(k) \frac{1}{E - \frac{\hbar^2 k^2}{2m}} \\
\int d^3k' \, \frac{\lambda v^2(k')}{E - \frac{\hbar^2 k'^2}{2m}} &= 1
\end{aligned} \tag{18.26}$$

The poles are at

$$k' = \pm\sqrt{\frac{2mE}{\hbar^2}} \tag{18.27}$$

which are the same as the poles of the T operator.

19

Question

Calculate the first Born approximation for a spherical potential well of depth V_0 and radius a. What happens in the limit of very deep well? What happens if the sign of V_0 is reversed? Compare the resulting cross section with the classical result (cf. Classical Mechanics of Landau and Lifshits) and give qualitative explanations of both results.

Solution Outline

1. Calculate the Fourier transform of the potential $V_{\boldsymbol{k}} = \int d^3r \, V(\boldsymbol{r}) \, e^{-i\boldsymbol{k}\boldsymbol{r}}$.
2. Denote $\boldsymbol{q} \equiv \boldsymbol{k} - \boldsymbol{k}'$ (so $q = 2k \sin\left(\frac{\theta}{2}\right)$), and calculate $f^{(1)}\left(\boldsymbol{k}, \boldsymbol{k}'\right) = f^{(1)}(\theta) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3r \, e^{i\boldsymbol{q}\boldsymbol{r}} V(\boldsymbol{r})$.
3. Calculate the differential cross section $\frac{d\sigma}{d\Omega} = \left|f^{(1)}(\theta)\right|^2$. The same as the classical result.
4. Explore the validity of the Born approximation: $\left|\frac{f\left(\boldsymbol{k},\boldsymbol{k}'\right)}{r}\right| \ll 1$. On $|V_0| \to \infty$ the approximation does not holds. The sign does not matter. Classical: for $V_0 < 0$ the incident particle will be transmitted.
5. Expand the first order $f^{(1)}(\theta)$ for $qa \ll 1$ and show that the angular dependence is vanish.

Solution

The spherical potential is

$$V(\boldsymbol{r}) = \begin{cases} V_0 & r \le a \\ 0 & r > a \end{cases} \tag{19.1}$$

The Fourier transform of $V(\boldsymbol{r})$ is

$$
\begin{aligned}
V_{\boldsymbol{k}} &= \int d^3 r\, V(\boldsymbol{r})\, e^{-i\boldsymbol{k}\boldsymbol{r}} \\
&= \int\limits_0^{\infty} dr \int\limits_0^{\pi} d\theta \int\limits_0^{2\pi} d\varphi\, r^2 \sin\theta V(\boldsymbol{r})\, e^{-ikr\cos\theta} \\
&= 2\pi \int\limits_0^{a} dr \int\limits_0^{\pi} d\theta\, r^2 \sin\theta V_0 e^{-ikr\cos\theta} \\
&= -2\pi V_0 \int\limits_0^{a} dr \int\limits_1^{-1} d(\cos\theta)\; r^2 e^{-ikr\cos\theta} \\
&= -2\pi V_0 \int\limits_0^{a} dr\, r^2 \left(-\frac{1}{ikr} e^{-ikr\cos\theta} \right)\Bigg|_{\cos\theta=1}^{\cos\theta=-1} \\
&= 2\pi V_0 \int\limits_0^{a} dr\, r^2 \frac{1}{ikr}\left(e^{ikr} - e^{-ikr}\right) \\
&= \frac{4\pi V_0}{k} \int\limits_0^{a} dr\, r \sin(kr) \\
&= \frac{4\pi V_0}{k} \left[-\frac{r}{k}\cos(kr)\Big|_{r=0}^{r=a} + \int\limits_0^{a} dr\, \frac{1}{k}\cos(kr) \right] \\
&= \frac{4\pi V_0}{k} \left[-\frac{a}{k}\cos(ka) + \frac{1}{k^2}\sin(kr)\Big|_{r=0}^{r=a} \right] \\
&= \frac{4\pi a V_0}{k^2} \left[\frac{1}{ka}\sin(ka) - \cos(ka) \right]
\end{aligned} \tag{19.2}
$$

The first order Born approximation is

$$
f^{(1)}\left(\boldsymbol{k}, \boldsymbol{k}'\right) = -\frac{1}{4\pi}\frac{2m}{\hbar^2} \int d^3 r'\, e^{i\left(\boldsymbol{k}-\boldsymbol{k}'\right)\boldsymbol{r}'} V\left(\boldsymbol{r}'\right) \tag{19.3}
$$

where $\boldsymbol{k}$ is propagation direction of the original plane wave and $\boldsymbol{k}'$ is the propagation vector for waves reaching observation point $\boldsymbol{r}$. We will denote $\boldsymbol{q}$ as

$$
\boldsymbol{q} \equiv \boldsymbol{k} - \boldsymbol{k}' \tag{19.4}
$$

For a spherically symmetric potential, $f^{(1)}\left(\boldsymbol{k}, \boldsymbol{k}'\right)$ is a function of $\left|\boldsymbol{k} - \boldsymbol{k}'\right|$, given by

$$
q = \left|\boldsymbol{k} - \boldsymbol{k}'\right| = \left| |\boldsymbol{k}|\, \hat{k} - \left|\boldsymbol{k}'\right| \hat{k}' \right| = |\boldsymbol{k}| \left|\hat{k} - \hat{k}'\right| = |\boldsymbol{k}|\, 2\sin\left(\frac{\theta}{2}\right) = 2k\sin\left(\frac{\theta}{2}\right) \tag{19.5}
$$

where $|\boldsymbol{k}| = |\boldsymbol{k}'|$ for elastic scattering. Therefore,

$$\begin{aligned} f^{(1)}\left(\boldsymbol{k},\boldsymbol{k}'\right) &= f^{(1)}\left(\theta\right) \\ &= -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3r'\, e^{i\boldsymbol{q}\boldsymbol{r}'}V\left(\boldsymbol{r}'\right) \\ &= -\frac{1}{4\pi}\frac{2m}{\hbar^2}V_{\boldsymbol{q}} \\ &= -\frac{1}{4\pi}\frac{2m}{\hbar^2}\frac{4\pi a V_0}{q^2}\left[\frac{1}{qa}\sin\left(qa\right)-\cos\left(qa\right)\right] \\ &= \frac{2ma}{\hbar^2 q^2}V_0\left[\cos\left(qa\right)-\frac{1}{qa}\sin\left(qa\right)\right] \end{aligned} \tag{19.6}$$

and the differential cross section is

$$\frac{d\sigma}{d\Omega} = \left|f^{(1)}\left(\theta\right)\right|^2 = \frac{4m^2a^2}{\hbar^4 q^4}V_0^2\left|\cos\left(qa\right)-\frac{1}{qa}\sin\left(qa\right)\right|^2 \tag{19.7}$$

As we can see, the sign of V_0 does not affect the result. The resulting are coincide with the classical result for $V_0 > 0$, however for $V_0 < 0$ the incident particle will be transmitted.

Validity of the Born approximation

The applicability condition for the Born approximation is that the change of the wave-function will be small in comparison to the incident wave. Namely,

$$\left|\frac{f\left(\boldsymbol{k},\boldsymbol{k}'\right)}{r}\right| \ll 1 \tag{19.8}$$

and using the expression for $f^{(1)}\left(\boldsymbol{k},\boldsymbol{k}'\right)$ in our problem,

$$|V_0| \ll \frac{\hbar^2 q^2 r}{2ma} \tag{19.9}$$

Observation is always made by a detector placed very far away from the scatterer at $\boldsymbol{r}$ greatly larger than the range of the potential, so $r \gg a$. Therefore, a sufficient (more strict) condition will be

$$|V_0| \ll \frac{\hbar^2 q^2}{2m} \tag{19.10}$$

For $ka \gg 1$ (fast particles, $qa \gg 1$), we can have the condition

$$|V_0| \ll \frac{\hbar^2}{2ma^2} \tag{19.11}$$

This can be thought of as saying that the potential energy is much smaller than the kinetic energy associated with the particle being localized in the potential. (weakness condition). For $ka \ll 1$ (slow particles, $qa \ll 1 \implies q \sim 1/r$), using (19.9), we can have the condition

$$|V_0| \ll \frac{\hbar^2 q}{2ma} = \frac{\hbar^2}{2ma^2}qa \tag{19.12}$$

To conclude,

$$|V_0| \ll \frac{\hbar^2}{2ma^2} \qquad \text{fast particle} \tag{19.13}$$

$$|V_0| \ll \frac{\hbar^2}{2ma^2}ka \qquad \text{slow particle} \tag{19.14}$$

In the limit of a very deep well (where the conditions are not met), we have to consider higher and higher orders of the approximation (or simply not to conduct it). However, $f \sim aV_0/q^2$ so taking $|V_0| \to \infty$ is equivalent to taking $q \to 0$ which means the incident particle has low energy. In this regime, there will be no angular dependence (S-wave scattering). If $|V_0|$ is not large enough, one can expand the first order $f^{(1)}(\theta)$ for $qa \ll 1$ and see that the angular dependence is vanish, as follows,

$$\begin{aligned} f^{(1)}(\theta) &\approx \frac{2ma}{\hbar^2 q^2} V_0 \left[\left(1 - \frac{1}{2}(qa)^2\right) - \frac{1}{qa}\left(qa - \frac{1}{6}(qa)^3\right) \right] \\ &= \frac{2ma}{\hbar^2 q^2} V_0 \left[-\frac{1}{2}(qa)^2 + \frac{1}{6}(qa)^2 \right] \\ &= -\frac{2ma}{3\hbar^2 q^2} V_0 (qa)^2 \\ &= -\frac{2ma^3}{3\hbar^2} V_0 \end{aligned} \tag{19.15}$$

we get no dependence on q, which means no dependence in θ, so $f^{(1)}(\theta)$ is isotropic (S-wave).