7 Work

Monday, February 19, 2024 5:28 PM

Extension: 48 Hours

25. Let's continue a bit further with the dipole interaction of problem 24. You obtained, I hope, an expression for the "electric dipole Hamiltonian". But it might look a bit mysterious. If this really describes an electric dipole interaction with a uniform external field, we might expect the Hamiltonian to look something like

$$H'_D = -qEZ\sin\omega t. \tag{1}$$

That is, qZ looks like a dipole moment. Consider the expectation value $\langle n|P_z|0\rangle$ with respect to two eigenstates of H_0. Show that this can be written in terms of an expectation value $\langle n|Z|0\rangle$ and quantities such as the electron mass, m, and the energy difference between the states. Rewrite H_D using this relation. Does it look more intuitive now?

$H_0 = \frac{P^2}{2m} + V(R)$ $\qquad H_0|m\rangle = E_m|m\rangle$ thm

We know that

$[z, p_z] = i\hbar$

Notice $\qquad AB - BA = [A, B]$

$[A, B^2] = AB^2 - B^2A = (BA + [A,B])B$

$- B(AB - [A,B]) = B[A,B] + [A,B]B$

Thus,

$[z, p_z^2] = p_z \cdot i\hbar + i\hbar p_z = 2i\hbar p_z$

Since we have z commutes with p_x^2, p_y^2 and $V(R)$,

$[z, H_0] = \frac{1}{2m}[z, p_z^2] = i\hbar\frac{p_z}{m}$

Further, notice

$\langle n|[z, H_0]|0\rangle = \langle n|H_0 z - zH_0|0\rangle$

$= \langle n|E_n z - zE_0|0\rangle$

$$= \langle n | (E_n - E_0) z | 0 \rangle = (E_n - E_0) \langle n | z | 0 \rangle$$

$$= \langle n | \frac{i\hbar}{m} p_z | 0 \rangle$$

$$\Rightarrow \boxed{\langle n | z | 0 \rangle = \frac{i\hbar}{m(E_n - E_0)} \langle n | p_z | 0 \rangle \equiv \alpha}$$

$$\left(\text{or} \quad \boxed{\langle n | p_z | 0 \rangle = \frac{m(E_n - E_0)}{i\hbar} \langle n | z | 0 \rangle} \right)$$

Let $\omega = E_n - E_0$. Since the above expression holds for any n in general, we have

$$H_p = \frac{q E_0}{m\omega} p_z \sin\omega t = -q(iE_0) z \sin\omega t \qquad \text{(natural units)}$$

$$\equiv -q_e E z \sin\omega t.$$

which is the desired form.

26. When we continue to apply our dipole approximation to an atom, we'll find that the dipole operator produces transitions from the ground state $|0\rangle$ to other eigenstates, $|n\rangle$, of H_0. The relative strengths of these transitions is given by an "oscillator strength":

$$f_{n0} = 2m\omega_{n0}|\langle n|Z|0\rangle|^2, \tag{2}$$

where $\omega_{n0} = E_n - E_0$ is the energy difference between the states. Note that f_{n0} is dimensionless. Demonstrate the oscillator strength "sum rule":

$$\sum_n f_{n0} = 1 \tag{3}$$

The work you have done in problem 25 will likely come in handy here.

Let $\alpha_n = \frac{i\hbar}{m(E_n - E_0)}$

Notice that

$$|\langle n|z|0\rangle|^2 = \langle n|z|0\rangle \cdot \langle n|z|0\rangle^*$$

$$= \langle n|z|0\rangle\langle 0|z|n\rangle = \alpha\langle n|z|0\rangle\langle 0|p_z|n\rangle$$

$$= \frac{1}{2}\left(\alpha^*\langle n|z|0\rangle\langle 0|p_z|n\rangle + \alpha\langle n|p_z|0\rangle\langle 0|z|n\rangle\right)$$

$$= -\frac{\alpha}{2}\left(\langle n|z|0\rangle\langle 0|p_z|n\rangle - \langle n|p_z|0\rangle\langle 0|z|n\rangle\right)$$

Then, we have

$$f_{n0} = \frac{m\omega_{n0}}{2}|\alpha|\left|{}_n\langle z\rangle_0\langle p_z\rangle_0 + \langle p_z\rangle_0\langle z\rangle_0\right| \qquad (\alpha \equiv C_0)$$

$$\sum_n f_{n0} = C_0\sum_n\left(\langle n|z|0\rangle\langle 0|p_z|n\rangle - \langle n|p_z|0\rangle\langle 0|z|n\rangle\right)$$

$$= C_0\sum_n \langle n|zp_z|0\rangle - \langle n|p_z z|0\rangle$$

$$= C_0\sum_n \langle n|zp_z - p_z z|0\rangle$$

$$= c_0 \sum_n \langle n | [Z, P_z] | 0 \rangle$$

$$= c_0 \sum_n \langle n | i\hbar | 0 \rangle = c_0 \langle 0 | i\hbar | 0 \rangle = i\hbar c_0$$

(By orthogonality)

Since

$$c_0 = 2m\omega_{n0} \cdot \frac{-a_n}{2} = -m(E_n - E_0)\left(\frac{i\hbar}{m(E_n - E_0)}\right)$$

$$= -i\hbar ,$$

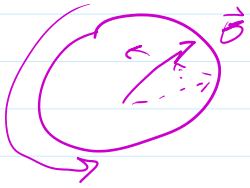
we have

$$\sum_n f_{n0} = i\hbar \cdot -i\hbar = \hbar^2 = 1 \qquad \text{(natural units)}$$

□

27. We discussed Berry's phase in class, including the example of the Aharonov-Bohm effect. Let us try another example.

Consider a spin-1/2 particle of magnetic moment μ in a magnetic field, **B**. Let the strength of the magnetic field be a constant, but suppose that its direction is slowly changing. Suppose the magnetic field vector is swept through a closed curve (*i.e.*, think of the tip of its vector as being varied along a closed curve on the surface of a sphere). Thus, two parameters describing the direction of the field are being varied, which we might take to be the polar angles (θ, ϕ).



(a) What does "slow" mean? That is, on what time scale should the variation be slow, in order for the adiabatic approximation to be reasonable?

(b) What is the expectation value of the spin vector in the adiabatic ground state?

(c) Express the adiabatic ground state wave function, $\psi^{(0)}_{\theta\phi}$, in terms of the adiabatically-varied parameters. You can in principle achieve this from your result to part (b), but it will probably be easier to accomplish by performing a rotation on a vector to the desired polar angles. The text pages 329-333 discuss finite rotations. The discussion of spin-1/2 in Chapter 14 of the text may also be helpful. I have also uploaded to module 7 the supplementary note on angular momentum from Ph 125a.

(d) Suppose we let the **B** field direction rotate slowly around the 3-axis at constant θ. Calculate Berry's phase for this situation. [Recall that Berry's phase is the change in the phase of the adiabatic wave function (ground state here) over one complete circuit in parameter space. We found that the Berry phase is given by:

$$\gamma_B = i \oint d\boldsymbol{\alpha} \cdot \langle \psi^{(0)}_{\boldsymbol{\alpha}} | \nabla_{\boldsymbol{\alpha}} \psi^{(0)}_{\boldsymbol{\alpha}} \rangle, \tag{4}$$

where $\boldsymbol{\alpha}$ is a vector in parameter space.] See if you can give a geometric

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where $\boldsymbol{\alpha}$ is a vector in parameter space.] See if you can give a geometric interpretation to your answer, in terms of an amount of solid angle swept out by the circuit in parameter space.

$\vec{\alpha} = (\phi)$

$H = -\mu \vec{S} \cdot \vec{B}$ $\quad \therefore \oint d\phi \langle \psi_{\theta\phi} | \nabla_\phi \psi_{\theta\phi} \rangle$

As explained in the lecture notes, "slowly" means that the difference in energy between the ground state and the first excited state, Δ, is much larger than the reciprical of the characteristic time scale of the process, T. In this case, Δ is the difference between the energy of a particle perfectly aligned with the magnetic field and the energy of a particle perfectly antialigned. We see that the ground and first excited state energies are given by

$E_0 = -\mu|B|, E_1 = \mu|B|$
$\Rightarrow \Delta = \mu|B| - (-\mu|B|) = 2\mu|B|$

T is the time it takes the magnetic field vector to make one full rotation.

Thus, we must have
$T \gg \frac{1}{2\mu|B|}$

b.) When the initial state is oriented with $\theta = 0$, we know from Shankar page 380 that

$\langle \psi^{(0)}_{\theta=0} | \vec{S} | \psi^{(0)}_{\theta=0} \rangle = \frac{\hbar}{2} \hat{e}_z$ $\quad (14.3.29)$

Therefore, by symmetry, we have

$$\langle \psi_{\theta\phi}^{(0)} | \vec{S} | \psi_{\theta\phi}^{(0)} \rangle = \pm \frac{\hbar}{2} \hat{e}_{\theta,\phi}$$

where

$$\hat{e}_{\theta\phi} = \sin\theta\cos\phi\,\hat{x} + \sin\theta\sin\phi\,\hat{y} + \cos\theta\,\hat{z}$$

c.) The $|n+\rangle$ ground state corresponds to on Shankar p. 378. From 14.3.28a, we see the form of $|n+\rangle$. We multiply it by $e^{i\phi/2}$ (a scale factor) so that $|n+\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ when $\theta = 0$:

$$|\psi_{\theta\phi}^{(0)}\rangle = \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2)\, e^{i\phi} \end{bmatrix}$$

d.) First notice that $\alpha = \phi$ since all else is held constant. Moreover, we see that

$$|\nabla_\phi \psi_{\theta\phi}^{(0)}\rangle = \frac{\partial}{\partial\phi} \psi_{\theta\phi}^{(0)} = \begin{bmatrix} \cos(\theta/2) \\ i\sin(\theta/2)\, e^{i\phi} \end{bmatrix}$$

and

$$\langle \psi_{\theta\phi}^{(0)}| = \begin{bmatrix} 0 \\ \sin(\theta/2) e^{-i\phi} \end{bmatrix}^\dagger$$

Thus,

$$\langle \psi_{\theta\phi}^{(0)} | \nabla_\phi \psi_{\theta\phi}^{(0)} \rangle = i\sin^2(\theta/2)$$

Since γ_B

$$\gamma_B = i \oint d\phi \sin^2(\theta/2)$$

$$= -\int_0^{2\pi} d\phi \sin^2(\theta/2) = -\pi\sin^2(\theta/2) \times$$

$$= -\int_0^{2\pi} d\phi \sin^2(\theta/2) = -2\pi \sin^2(\theta/2) \simeq \gamma_B$$

Geometrically, this answer makes sense because this is proportional to the solid angle of a cone for fixed theta. It also makes sense because for larger theta, it sweeps out a larger path and sin^ 2(theta/2) also increases with increasing theta (and is zero at zero theta, which also aligns with this geometric explanation).

28. Let us investigate our quantum electromagnetic field operators and in particular think about a notion for the energy density in the vacuum. We defined the quantum mechanical electromagnetic field operators $\hat{A}_{\mathbf{k}\boldsymbol{\epsilon}}$ and $\hat{A}^\dagger_{\mathbf{k}\boldsymbol{\epsilon}}$:

$$\hat{A}_{\mathbf{k}\boldsymbol{\epsilon}}|N_{\mathbf{k}_1\boldsymbol{\epsilon}_1},\ldots,N_{\mathbf{k}\boldsymbol{\epsilon}},\ldots\rangle = \sqrt{\frac{2\pi}{\omega}}\sqrt{N_{\mathbf{k}\boldsymbol{\epsilon}}}|N_{\mathbf{k}_1\boldsymbol{\epsilon}_1},\ldots,N_{\mathbf{k}\boldsymbol{\epsilon}}-1,\ldots\rangle \quad (5)$$

$$\hat{A}^\dagger_{\mathbf{k}\boldsymbol{\epsilon}}|N_{\mathbf{k}_1\boldsymbol{\epsilon}_1},\ldots,N_{\mathbf{k}\boldsymbol{\epsilon}},\ldots\rangle = \sqrt{\frac{2\pi}{\omega}}\sqrt{N_{\mathbf{k}\boldsymbol{\epsilon}}+1}|N_{\mathbf{k}_1\boldsymbol{\epsilon}_1},\ldots,N_{\mathbf{k}\boldsymbol{\epsilon}}+1,\ldots\rangle. \quad (6)$$

(a) Determine the commutation relations among these operators.

(b) We may define the quantum mechanical electric field operator according to:

$$\hat{\mathbf{E}}(\mathbf{x}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}\boldsymbol{\epsilon}}\left(-i\omega\hat{A}_{\mathbf{k}\boldsymbol{\epsilon}}\boldsymbol{\epsilon}e^{i\mathbf{k}\cdot\mathbf{x}} + i\omega\hat{A}^\dagger_{\mathbf{k}\boldsymbol{\epsilon}}\boldsymbol{\epsilon}^* e^{-i\mathbf{k}\cdot\mathbf{x}}\right). \quad (7)$$

Make sure this definition makes sense to you. We know that classically we can compute the energy density in an electromagnetic field as proportional to the squared electric (plus squared magnetic) fields. Compute the expectation value:

$$\langle\Omega|\hat{\mathbf{E}}(\mathbf{x})\cdot\hat{\mathbf{E}}(\mathbf{x}')|\Omega\rangle \quad (8)$$

Try to express your answer in terms of a dimensionless integral in one dimension (which will perhaps look divergent). Make sure the dimension of the coefficient is what you expect.

(c) Now let's consider the average, $\hat{\bar{\mathbf{E}}}(\mathbf{x})$, of $\hat{\mathbf{E}}(\mathbf{x})$ over a small volume $\mathcal{V}$. That is, we are interested in the average energy density in a small volume. What is

$$\langle\Omega|\left[\hat{\bar{\mathbf{E}}}(\mathbf{x})\right]^2|\Omega\rangle, \quad (9)$$

and what happens as $\mathcal{V}\to 0$? You may wish to think about your result in terms of harmonic oscillators and zero point energies.

a.) First, we consider the case where the $k\vec{e}$ subcript is different for the two operators. Since they independently change different components of the state vector, we have

components of the state vector, we have

$$[A_{k_1 e_1}, A_{k_2 e_2}] \equiv [A_1, A_2] = A_1 A_2 - A_2 A_1 = 0$$
$$[A_1^\dagger, A_2^\dagger] = 0$$
$$[A_1, A_2^\dagger] = 0 \qquad [A_1^\dagger, A_2] = 0$$

(when $k_1 \neq k_2$ or $e_1 \neq e_2$)

Now we consider the commutation relations when both operators have the same subscript (i.e., they act on the same component of the state vector). If the two operators are *identical*, the commutator is trivially zero since for any operator Ω, $[\Omega, \Omega] = \Omega^2 - \Omega^2 = 0$. Thus,

$$[A_{ke}, A_{ke}] = [A_{ke}^\dagger, A_{ke}^\dagger] = 0$$

However, if they are not the same exact operator, this is not the case. We show this by calculating the effect of the commutator on a state vector:

$$[A_{ke}, A_{ke}^\dagger] = [A, A^\dagger] = AA^\dagger - A^\dagger A$$

Notice

$$AA^\dagger |\psi\rangle = A \sqrt{\frac{2\pi}{\omega}} \sqrt{N_{ke}+1}\, |\psi+1\rangle$$

("+1" in the ke component; I am oversimplifying notation for convenience)

$$= \frac{2\pi}{\omega} \sqrt{(N_{ke}+1)^2}\, |\psi\rangle \rightarrow AA^\dagger = (N+1)\frac{2\pi}{\omega}$$

$$A^\dagger A |\psi\rangle = A^\dagger \sqrt{\frac{2\pi}{\omega}} \sqrt{N_{ke}}\, |\psi-1\rangle = \frac{2\pi}{\omega} N_{ke} |\psi\rangle$$

$$\Rightarrow A^\dagger A = N \frac{2\pi}{\omega}$$

$$\Rightarrow [A, A^\dagger] = (N - N + 1)\frac{2\pi}{\omega} = \frac{2\pi}{\omega}$$

$$\Rightarrow \boxed{[A_{k_1 e_1}, A_{k_2 e_2}^\dagger] = \frac{2\pi}{\omega} \delta_{k_1 k_2} \delta_{e_1 e_2}} \quad \text{(All others are 0).}$$

$$\Rightarrow \left[A_{k_1 \varepsilon_1}, A^{\dagger}_{k_2 \varepsilon_2} \right] = \frac{2\pi}{\omega} \delta_{k_1 k_2} \delta_{\varepsilon_1 \varepsilon_2} \quad \text{(All others are 0).}$$

b) We know that $|\Omega\rangle$ is the Fock state of the vacuum.

We see that

$$\langle \Omega | \hat{E} \cdot \hat{E}' | \Omega \rangle = \frac{-\omega^2}{V} \langle \Omega | \sum_{k_1,\varepsilon_1} \sum_{k_2,\varepsilon_2} \left(-A_1 \varepsilon_1 e^{ik_1 \cdot x} + A_1^{\dagger} \varepsilon_1^* e^{-ik_1 \cdot x} \right) \left(-A_2 \varepsilon_2 e^{ik_2 \cdot x'} + A_2^{\dagger} \varepsilon_2^* e^{-ik_2 \cdot x'} \right) | \Omega \rangle = \Gamma$$

In the expression that we label by Γ above, we see that the terms with a A^+ in the back or a A in the front vanish since we are acting on the vacuum (Fock) state. This leaves us with only AA^+ terms. However, unless these are acting on the component of the state vector, that term will go to zero by orthogonality. Thus, we may reduce the sum as following:

$$\langle \Omega | E \cdot E' | \Omega \rangle = \langle \Omega | \sum_{k\varepsilon} \frac{-\omega^2}{V} \cdot A A^+ \varepsilon \varepsilon^* e^{ik(x-x')} | \Omega \rangle$$

$$= \frac{1}{V} \sum_{k\varepsilon} |\varepsilon|^2 \omega^2 \langle \Omega | A A^+ e^{ik(x-x')} | \Omega \rangle$$

$$= \frac{1}{V} \sum_{k\varepsilon} |\varepsilon|^2 \omega^2 \langle \Omega | \frac{2\pi}{\omega} e^{ik(x-x')} | \Omega \rangle$$

$$= \frac{2\pi}{V} \sum_{k\varepsilon} |\varepsilon|^2 \omega \langle \Omega | e^{ik(x-x')} | \Omega \rangle$$

$$= \frac{2\pi}{V} \sum |\varepsilon|^2 \omega e^{ik(x-x')}$$

$\omega = ck$

$$= \frac{2\pi}{V} \sum_{k\varepsilon} |\varepsilon|^2 \omega e^{ik(x-x')} \qquad \int d\Omega = 4\pi$$

$$= \frac{2\pi}{V} \int_0^\infty \omega \frac{k^2 dk\, d\Omega}{(2\pi)^3} e^{ik(x-x')}$$

$$= \boxed{\frac{c}{V} \int_0^\infty k^3 e^{ik(x-x')} dk}$$

c.) We know that

$$E = \frac{1}{\nu} \int_{\nu'} \frac{i\omega}{\sqrt{V}} \sum_{k\varepsilon} A\varepsilon e^{ikx} + A^\dagger \varepsilon^* e^{-ikx}$$

Let V' be the volume of a cube with side length 2L centered at position $\vec{x}$. To get the average electric field, we will calculate the average field inside this box and eventually take the side length (and thus the volume) to zero. Our expression for the average field looks like this:

$$E = \frac{i}{V'\sqrt{V}} \sum_{k\varepsilon} \omega \int_{V'} -A\varepsilon e^{ikx} + A^\dagger \varepsilon^* e^{-ikx} \hat{x}$$

We first calculate the integral in one dimension (i.e., the volume is a line, not a cube) and then generalize to 3D:

$$\int_{x-L}^{x+L} e^{ikx'} dx' = \frac{1}{ik} e^{ikx'} \Big|_{x'=x-L}^{x+L}$$

$$= \frac{1}{ik} \left(e^{ik(x+L)} - e^{ik(x-L)} \right)$$

$$= \frac{1}{ik} e^{ikx} \left(e^{ikL} - e^{-ikL} \right)$$

$$= \frac{2}{k} e^{ikx} \sin(kL)$$

Generalizing to 3D, we find

Thus,

$$\int_{V'} e^{i\vec{k}\cdot\vec{x}'} d^3x' = \delta\left(\prod_{i\in\{x,y,z\}} \frac{\sin(k_i L)}{k_i}\right) e^{i\vec{k}\cdot\vec{x}}$$

Since $V' = (2L)^3 = 8L^3$,

$$\hat{\vec{E}}(x) = \frac{1}{V}\sum_{ks}\left[\left(-A\varepsilon e^{i\vec{k}\vec{x}} - A^+\varepsilon^* e^{-i\vec{k}\cdot\vec{x}}\right)\omega \cdot \prod \frac{\sin(k_i L)}{k_i L}\right]$$

Using the same logic as in part (b), we have

$$\langle\Omega|\left[\hat{\vec{E}}(x)\right]^2|\Omega\rangle = \frac{-\omega}{\sqrt{V}}\sum_{ks}\left(\langle\Omega|AA^+|\Omega\rangle\omega^2 \cdot \prod\left(\frac{\sin(k_i L)}{k_i L}\right)^2\right)$$

$$= \frac{-1}{V}\sum_{ks}\omega^2\left[\left(\frac{2\pi}{\omega}\right)\prod\left(\frac{\sin(k_i L)}{k_i L}\right)^2\right]$$

$$= -\frac{2\pi}{V}\sum_{ks}\omega\prod_{i\in\{x,y,z\}}\left(\frac{\sin(k_i L)}{k_i L}\right)^2$$

Where we used the fact that

$$\langle\Omega|AA^+|\Omega\rangle = \langle\Omega|A^+A + [A, A^+]|\Omega\rangle$$

$$= \langle\Omega|A^+A|\Omega\rangle + \langle\Omega|[A, A^+]|\Omega\rangle$$

$$= 0 + 2\pi/\omega$$

Letting $V \to 0$, we have $L \to 0$ and

$$\frac{\sin(k_i L)}{k_i L} \to \frac{k_i \cos(k_i L)}{k_i} \to 1$$

$$\langle \Omega | \hat{\vec{E}}^2 | \Omega \rangle = \frac{2\pi}{V} \sum_{k_i} \omega = \frac{2\pi}{V} \int_0^\infty \omega \frac{k^2 dk d\hat{s}}{(2\pi)^3}$$

$$= \boxed{\frac{c}{V} \int_0^\infty k^3 dk}$$