Leo Radzihovsky, Spring 2016

PHYS 5260: Quantum Mechanics - II

Homework Set 4

Issued February 22, 2016
Due March 14, 2016

Reading Assignment: Shankar, Ch.18, 21

1. (15 points) NMR and Rabi oscillations

   Consider a spin 1/2 (for a localized electron) in the presence of a dc magnetic field $\mathbf{B}_0 = B_0\hat{\mathbf{z}}$ and subjected to a weak transverse magnetic field $\mathbf{B}_\perp = B_\perp\hat{\mathbf{n}}(t)$ rotating in the xy plane with $\hat{\mathbf{n}}(t) = \hat{\mathbf{x}}\cos\omega t + \hat{\mathbf{y}}\sin\omega t$.

   (a) Using the general Zeeman Hamiltonian for such system, show that it can be written as $H = \frac{1}{2}\epsilon\sigma_z + g(e^{-i\omega t}\sigma_+ + e^{i\omega t}\sigma_-)$, where $\sigma_\pm = 1/2(\sigma_x \pm i\sigma_y)$ are raising and lowering Pauli matrices. What are parameters ϵ and g in terms of B_0 and $B_\perp$?

   (b) For a system that starts out in a lower energy, spin down state $|\psi(0)\rangle = |\downarrow\rangle$, characterized by coefficients $c_i(0) = \delta_{i2} = (0, 1)$ (using $\hat{\mathbf{z}}$ quantization axis representation), compute the probabilities at time t of finding the spin in state up and in state down, and using these compute the average value of spin projection along $\hat{\mathbf{z}}$, i.e., $\langle\psi(t)|s_z|\psi(t)\rangle$. Sketch these as a function of time.

   More specifically:

   i. Compute from these the frequency and amplitude of oscillations of the probabilities.

   ii. Show in terms of a semiclassical precessional picture how the amplitude depends on magnitude of ϵ, g and ω, contrasting the on- and off-resonance pictures.

   iii. Argue qualitatively based on your answer above that if instead of a rotating transverse field, a more easily created oscillating field along $\hat{\mathbf{x}}$, $\mathbf{B}_\perp(t) = B_\perp\hat{\mathbf{x}}\cos\omega t$ is used that the answer does not change much near a resonance. (Hint: A linearly polarized field can be thought of as a sum of two oppositely circularly polarized fields)

   iv. Verify that total probability of finding the spin in either of the states ($1 = \uparrow, 2 = \downarrow$) $|c_1|^2 + |c_2|^2 = 1$ is indeed conserved.

Suggestions: To solve this problem exactly, it is convenient to perform a time dependent unitary transformation on the states and the Hamiltonian that transforms the system into a coordinate system rotating with the transverse magnetic field. In this coordinate system the Hamiltonian becomes time independent and can therefore be easily diagonalized to solve the full problem. To minimize algebra, it is convenient to develop (or just recall) and then take advantage of Pauli spin algebra.

(c) Use time dependent perturbation theory to lowest nontrivial order in g and compare your result with the exact solution above approximated for small g. Treat the cases of near resonance $\hbar\omega \approx \epsilon$ and far off resonance $|\hbar\omega - \epsilon| \gg g$ separately.

2. (30 points) Consider Jaynes-Cummings (JC) Hamiltonian

$$H_{JC} = \frac{1}{2}\epsilon\sigma_z + \hbar\omega_0 a^\dagger a + g(a^\dagger\sigma_- + a\sigma_+), \tag{1}$$

that can be thought of a generalization of above problem where the external transverse field is replaced by a quantum field a representing a single bosonic oscillation mode.

This is a beautiful model with a rich behavior and many physical realizations. For example it describes cavity quantum electrodynamics (QED) (an atom in a electomagnetic cavity) system, where one focusses on only two atomic levels $|1\rangle$, $|2\rangle$ (forming an effective pseudo-spin 1/2 system described by σ) and coupled to a single electromagnetic radiation mode with cavity frequency ω_0, whose excitations are described by a photon creation/annihilation fields $a^\dagger, a$.

Equivalently, it describes a recently realized (by Rob Schoelkopf at Yale) quantum circuit QED, a circuit version of a cavity QED consisting of a superconducting island coupled to a single microwave mode. In this latter case a 0 and a 1 unit of charge on the superconducting island correspond to the pseudo spin up and down, respectively (with energy cost being the difference in capacitive, electrostatic energy).

JC Hamiltonian also describes a microscopic cantilever coupled to a quantum dot on which electrons can hop on and off. In this case a describes a dominant (elastic) phonon field (modes of vibration of the cantilever) and eigenstates of σ_z correspond to for example charge 0 and 1 sitting on the quantum dot. The two degrees of freedom are coupled through electrostatic interaction.

So much for the background. Here we will explore some properties of the JC model.

(a) Write down the spectrum and eigenkets (Dirac notation is fine) for the decoupled case of $g = 0$? Using horizontal dash notation, draw the spectrum for a few lowest eigen-energies of the Hamiltonian for $g = 0$. Label each state with quantum numbers appropriate to the $g = 0$ case.

Hint: There are quantum numbers associated with the oscillator mode (phonon number) and the spin part of the system.

(b) For far off the resonance ($\Delta \equiv \epsilon - \hbar\omega_0 \neq 0$) use time independent perturbation theory to compute the modification of the spectrum to a lowest nontrivial order in g. You should get two contributions; one of these is the analog of the Lamb shift (coming from quantization of the oscillator field a) and another one that is an analog of the ac Stark effect used by your JILA colleagues to trap and confine atoms with a focussed laser field.

(c) Noting that because of the structure of H_{JC} and because spin-1/2 Hilbert space is just two-dimensional (i.e., σ_+, σ_- annihilate $|\uparrow\rangle$, $|\downarrow\rangle$ respectively), the full infinite dimensional Hilbert space for this system breaks up into two-dimensional subspaces that do not "talk" to each other even at finite g . Use this property to find the exact spectrum and eigenstates of H_{JC}.

Suggestion: To see how this goes, it is instructive to compute matrix elements of H_{JC} in the $g = 0$ basis, write out a few coupled time-independent Schrodinger equations for the coefficients c_{n,σ_z}, and also write these out in matrix form.

(d) Use the above exact solution to compute the probability of finding the system at time t in the spin-up state that started in a spin-down state with n excited oscillator quanta (phonons or photons, depending on the physical context) at time $t = 0$.

Hint: To do this, as usual you will need to expand the initial state in terms of the exact eigenstates found above and evolve each eigenstate according to the exact spectrum found above.

(e) Use time dependent perturbation theory to compute phonon absorption/spin-flip transition rate from a spin down state with n excited quanta (n phonons in the system). Also compute phonon emission/spin-flip transition rate from a spin up state with n phonons in the system. Note that the difference between these is what's called spontaneous emission due to quantum nature of the bosonic field a.

(f) Use the exact solution found in (c) to write down (in terms of an infinite sum, that you are welcome to evaluate with Mathematica if you wish, but don't have to) the average value of spin $\langle\psi(t)|\sigma_z|\psi(t)\rangle$ and the oscillator field $\langle\psi(t)|a|\psi(t)\rangle$ at time t, starting with a state of spin-down and coherence state of the oscillator labelled by α. To considerably simplify the algebra, please evaluate these expressions on resonance, i.e., for $\epsilon = \hbar\omega$.

3. (20 points) Dyson Expansion

(a) Use coordinate space path integral formulation to derive Dyson series expansion for the evolution operator $U(t)$. Demonstrate that in this formulation, path integral automatically produces a time-ordered evolution operator, and show that it agrees with expression derived in class and in the Shankar text.

Suggestion: Expand in powers of S_1, think about the discretized (in time) definition of a path integral and be careful to locate $H_1(t_i)$'s at the correct position

in the time sequence. Note that the advantage of the path integral formulation is that all fields are commuting classical fields, with quantum mechanics coming in from integration over these fields.

(b) Show that for a time independent Hamiltonian the Dyson series for the evolution operator $U(t)$ (e.g., from above derivation or derived by Shankar) simplifies considerably and show that its Fourier transform $U(E + i\epsilon)$ ($\epsilon \to 0^+$) reduces to a geometric series (in operator $U_0(E)H_1$) that can be resummed into $U(E) = i\hbar/(E - H)$, a result much more easily obtained by directly Fourier transforming $U(t) = e^{-i/\hbar Ht}\theta(t)$, where $\theta(t)$ function and ϵ were added to make the Fourier transform well-defined.

Suggestion: In manipulating the above series, make sure to take care of noncommutativity of operators (e.g., U_0 and H), i.e., be very careful not to interchange order of operators and to properly treat inverses of operators $1/O \equiv O^{-1}$. If it is not obvious how the series resums, try working backwards from the above given answer and Taylor expanding it in H_1, being careful about noncommutativity of operators.

4. (30 points) Quantum field theory: field quantization

This problem is a preview to our class discussion of quantum field theory. First let us recall what a classical field is. It is a generalization of a single degree of freedom, (e.g., position q of a single particle) to a field (e.g., electric field $E(\mathbf{r})$ that represents many (potentially infinite number of) degrees of freedom, one for each point in space $\mathbf{r}$. This latter thing is not easy to imagine, so to make things well-defined we always (at least in the back our minds) want to think about space as a discrete set of points $\mathbf{r}_i$ (i.e., a lattice), in which case a field $E(\mathbf{r}_i)$ is nothing more than a one (or a finite, in case of a vector field like electromagnetic field, or ion displacement) degree of freedom at each lattice point $\mathbf{r}_i$.

Now, in studying quantum mechanics we have learned how to quantize a single (or a small number of) degree of freedom q treating it as an operator $\hat{q}$, that does not commute with its canonically conjugate momentum $\hat{p}$, etc. Quantum field theory is nothing more than quantum mechanics for a field, $E(\mathbf{r})$, which once you think of space as discrete is nothing more than quantum mechanics for many (often coupled) degrees of freedom, that become operators $\hat{E}(\mathbf{r}_i)$ that do not commute with the canonically conjugate momenta fields $\hat{\Pi}(\mathbf{r}_i)$, i.e., $[\hat{E}(\mathbf{r}_i), \hat{\Pi}(\mathbf{r}_j)] = i\hbar\delta_{\mathbf{r}_i,\mathbf{r}_j}$. For example quantum electrodynamics (QED) is a quantization of electromagnetic fields $\mathbf{E}(\mathbf{r})$ and $\mathbf{B}(\mathbf{r})$ (and also of the electron field operator $\psi(\mathbf{r})$, but nevermind about this for now), that become noncommuting vector operators, at each point $\mathbf{r}$ in space. Now an understandable source of confusion is to think that $\mathbf{r}$ is an operator as it was in quantum mechanics. In quantum field theory $\mathbf{r}$ is most certainly *not* an operator, and is simply a *label* for quantum operators, $\hat{E}(\mathbf{r}_i)$, that make up the quantum field $\hat{E}(\mathbf{r})$. This is particularly clear in the above discretized form.

To illustrate these ideas let's look at a simplest example of a quantization of vibration of ions in a one-dimensional crystalline solid, i.e., at a quantum field theory of vibration of a crystal

(a) Recall that for a single oscillator with a Hamiltonian $H = \frac{1}{2m}\Pi^2 + \frac{1}{2}m\omega_0^2 u^2 = \hbar\omega_0(a^\dagger a + 1/2)$, where displacement is described by a single variable u and momentum Π, the eigenstates are labeled by single eigenvalues n of the number operator $\hat{n} = a^\dagger a$ and given by $|n\rangle$ and spectrum is given by $E_n = \hbar\omega_0(n + 1/2)$. In the (so called 2nd quantized) many-body language, n is the number of quanta of vibrations (called phonons) to which the oscillator is excited. For state $|n\rangle$ we say that we have n phonons in the system. For generalization of many oscillators, these phonons will be genuine bosonic particles (much like photons in the case of electromagnetic field quantization, QED) that can move around the system with a dispersion that you will derive below.

Now imagine a crystal of N ions with a displacement of ith ion given by u_i, a canonically conjugate momentum Π_i, and a Hamiltonian given by

$$H = \sum_{i=1}^{N}\left[\frac{1}{2m}\Pi_i^2 + \frac{1}{2}m\omega_0^2 u_i^2\right]. \tag{2}$$

Introduce creation and annihilation operators for this problem, expressing the Hamiltonian in terms of them, and write down the eigenstates and spectrum for this system.

Hint: Because ions are not coupled this is a trivial generalization of a single oscillator, and is referred to as Einstein's model of a solid, that he introduced to describe vibrational heat capacity of a solid.

Note: Just as a point of interest, note that in a slight generalization of notation, where one uses $x_i = ci$ (c is lattice spacing) to label ith ion (oscillator) above Hamiltonian can be rewritten as $H = \sum_{x_i=0}^{Nc}\left[\frac{1}{2m}\Pi(x_i)^2 + \frac{1}{2}m\omega_0^2 u(x_i)^2\right]$, which in the continuum becomes a true field theoretic Hamiltonian $H = \int_0^L \frac{dx}{c}[\frac{1}{2m}\Pi(x)^2 + \frac{1}{2}m\omega_0^2 u(x)^2]$, with $L = Nc$ the length of the system and $u(x)$ the phonon field.

(b) A slight generalization of Einstein model is one in which ion i has a natural frequency of vibration ω_i, that can be different. Write down the spectrum for this generalized Einstein model.

(c) Now consider the so called Debye model of a solid where the nearest neighbor ions are coupled together by "electromagnetic springs", with a Hamiltonian given by

$$H = \sum_{x_i=0}^{Nc}[\frac{1}{2m}\Pi(x_i)^2 + \frac{1}{2}B(u(x_{i+1}) - u(x_i))^2], \tag{3}$$

where B is solid's compressional modulus. Note that in the continuum the Hamiltonian for the corresponding field theory becomes $H = \int_0^L \frac{dx}{c}[\frac{1}{2m}\Pi(x)^2 + \frac{1}{2}Bc^2(\partial_x u(x))^2]$,

i. Show that these N harmonic oscillators can be decoupled using Fourier series transformation. That is, when one changes variables to normal modes given by Fourier series coefficients $\tilde{u}(k_n)$ of field $u(x_i) = \frac{1}{L}\sum_{k_n=-\pi/c}^{\pi/c} e^{ik_n x_i}\tilde{u}(k_n)$ (and same for the momentum field operator, $\Pi(x_i)$) show that in terms of $\tilde{u}(k_n)$ and $\tilde{\Pi}(k_n)$ the Hamiltonian decouples into N independent harmonic oscillators

$$H = \frac{1}{Lc}\sum_{k_n}\left[\frac{1}{2m}|\Pi_{k_n}|^2 + \frac{1}{2}m\omega_{k_n}^2|\tilde{u}_{k_n}|^2\right], \quad (4)$$

one for each value of Fourier wavevector $k_n = (2\pi/L)n$, with n integers in finite range $-N/2 < n \leq N/2$.
Hint: You will find previously discussed identity $\sum_{x_i=0}^{N} e^{-i(k_n+k_m)x_i} = N\delta_{k_n+k_m,0}$ (valid for large N) extremely useful.
What is the natural frequency ω_{k_n} for mode k_n? Plot it as function of k_n over the physical range $-\pi/c < k_n \leq \pi/c$. Why is k_n limited to this range rather than having infinite range?
Hint: Think about what happens to the Fourier coefficient $\tilde{u}_{k_n}$ when k_n falls outside of this range?

ii. Recalling what we did next for a single harmonic oscillator, introduce annihilation and creation operators $\hat{a}_{k_n}$, $\hat{a}^\dagger_{k_n}$ for each mode k_n, such that $\hat{u}_{k_n} = \frac{\delta_{k_n}}{\sqrt{2}}(\hat{a}_{k_n} + \hat{a}^\dagger_{-k_n})$, $\hat{\Pi}_{k_n} = \frac{-i\hbar}{\delta_{k_n}\sqrt{2}}(\hat{a}_{k_n} - \hat{a}^\dagger_{-k_n})$, and show that the Hamiltonian then reduces to a standard form

$$H = \frac{1}{Lc}\sum_{k_n}\left[\hbar\omega_{k_n}(\hat{a}^\dagger_{k_n}\hat{a}_{k_n} + Lc/2)\right]. \quad (5)$$

In above what is δ_{k_n}? If the commutation relation for the original displacement and its momentum fields $\hat{u}(x_i)$ and $\hat{\Pi}(x_i)$ is the standard canonical one, $[\hat{u}(x_i), \hat{\Pi}(x_i)] = i\hbar\delta_{x_i,x_j}$, show that the resulting commutation relation for the creation and annihilation operators is given by

$$[\hat{a}_{k_n}, \hat{a}^\dagger_{k_m}] = Lc\delta_{k_n,k_m} \quad (6)$$

iii. What are the quantum numbers that uniquely specify the eigenstates of the system and what is the spectrum, i.e., the total energy of the system for each such state?

5. (5 points) Electromagnetic field

We describe the electromagnetic field in terms of a vector potential field $\mathbf{A}(\mathbf{r}, t) = A_0\hat{\epsilon}\, 2\cos(\mathbf{k}\cdot\mathbf{r} - \omega t)$, where $\hat{\epsilon}$ is its polarization (that is required to be transverse to photon's momentum $\mathbf{k}$) and A_0 is the amplitude. Using the expression for the Poynting vector $\mathbf{S} = \frac{c}{4\pi}\mathbf{E}\times\mathbf{B}$, whose magnitude is the intensity, i.e., energy per unit of time

crossing a unit of area perpendicular to direction of propagation $\mathbf{k}$, determine A_0 for a field of one photon (energy $\hbar\omega_k = \hbar ck$) in a box of volume V. Equivalently, one can look at the total electromagnetic energy $H_{EM} = \frac{1}{8\pi}\int d^3r\,[\mathbf{E}^2 + \mathbf{B}^2]$.