Leo Radzihovsky, Spring 2016

PHYS 5260: Quantum Mechanics - II

Homework Set 2

Issued January 25, 2016
Due February 8, 2016

Reading Assignment: Shankar, Ch.17

1. Anharmonic oscillator

   Consider an anharmonic oscillator with a small quartic perturbing nonlinearity, $H_1 = \lambda x^4$.

   (a) Use time-independent perturbation theory to show that the lowest (nontrivial) order expression for the n-th excited state is given by $E_n = \hbar\omega(n + 1/2) + \frac{3\hbar^2\lambda}{4m^2\omega^2}[1 + 2n + 2n^2]$.

   (b) Argue that no matter how small λ is, the perturbation expansion will break down for some large enough n. What is the physical reason?

   Hint: You might find it useful to use the 2nd quantized notation of creation and annihilation operators (rather than working in the coordinate representation).

2. Consider a spin-1/2 particle with a gyromagnetic ratio γ in a magnetic field $\mathbf{B} = B_\perp \hat{\mathbf{r}}_\perp + B_0 \hat{\mathbf{z}}$, characterized by a purely Zeeman Hamiltonian $H = -\mu \cdot \mathbf{B}$ (ignore orbital degrees of freedom).

   (a) By using a convenient choice of quantization axis of $\mathbf{S}$, find the spectrum by solving this problem *exactly.* Also find the corresponding exact spinor eigenstates in the basis with $\hat{\mathbf{z}}$ as the quantization axis.

   Hint: You can do the latter by either directly diagonalizing H or by an appropriate unitary rotation from the eigenstates expressed in basis with quantization axis along $\mathbf{B}$ to the basis with quantization axis along $\hat{\mathbf{z}}$.

   (b) Treating $B_\perp$ as a perturbation calculate the first- and second-order shifts in the spectrum and first-order shift in the corresponding eigenstates.

   (c) Compare your results in (b) to the Taylor expansion (to appropriate order) of the exact results for the energy and the eigenstates found in (a).

   Hint: To simplify the algebra, it is convenient (but not necessary) to pick $\mathbf{B}_\perp$ along $\hat{\mathbf{x}}$, namely choose a vanishing azimuthal angle.

3. Prove the Thomas-Reiche-Kuhn sum rule

$$\sum_{n'}(E_{n'} - E_n)|\langle n'|x|n\rangle|^2 = \frac{\hbar^2}{2m}, \tag{1}$$

where $|n\rangle$ and $|n'\rangle$ are exact eigenstates of $H = p^2/2m + V(x)$.

Hint: Eliminate the $E_{n'} - E_n$ factor in favor of the Hamiltonian operator H. This should allow you to reverse our usual insertion of a complete set of states, thereby considerably simplifying the expression.

Test the sum rule on the nth state of a harmonic oscillator.

4. Band structure

A fairly good model of electrons in a crystalline solid is of independent particles confined to a macroscopic box, moving in the presence of a periodic potential of positively charged ions. The corresponding single-electron Hamiltonian is $H = p^2/2m + V_{ions}(x)$. For simple (e.g., alkali) metals, to zeroth order one can even simply ignore the periodic potential, approximating electron waves by plane-waves (with $L \to \infty$, and periodic boundary conditions with normalization $1/\sqrt{L}$), i.e., by familiar plane waves with a quadratic spectrum $E_k^0 = \hbar^2 k^2/2m$.

(a) Use a non-degenerate perturbation theory to compute the correction to this quadratic spectrum to second-order and the eigenfunctions to first-order in the periodic potential $V_{ions}(x)$. Write down your answer for a generic periodic potential $V_{ion}(x)$, expressing it in terms of the Fourier coefficients V_{Q_n} of the periodic potential; $Q_n = nQ_1$ is the nth Fourier wavevector, with n running over integers and Q_1 is the elementary smallest wavevector characterizing $V_{ion}(x)$.

You obviously need not compute the infinite sum (particularly that you do not know the Fourier coefficients), but please simplify the expression as much as possible.

(b) Specialize this result to a single harmonic periodic potential, i.e., with just two values of $Q_n = \pm Q_1$, e.g., just taking the periodic potential to be $V_{ions}(x) = V_1 \cos(Q_1 x)$.

(c) By examining your expression above, note that for some values of k, the above nondegenerate perturbation theory breaks down. Find these special values $k^*_\pm$ for which this breakdown happens.

Using the property of the nonperturbed, free particle spectrum, E_k^0, and the nature of the perturbing Hamiltonian, explain mathematically and physically why the breakdown takes place. Drawing pictures might be useful for the former, and thinking about interference of (electron) waves scattered by the periodic potential for the latter.

(d) Sketch the resulting E_k, indicating the location of special k points.

(e) Apply a lowest order (1st order in V_{ions}) degenerate perturbation theory to compute the perturbed energies and eigenstates right at these special k points, where the non-degenerate perturbation theory breaks down.

Hint: There are only two such k points.

(f) Now that you know exactly what happens right at these special k points and far away from them (where nondegenerate perturbation theory is valid), make an educated guess of what happens to the spectrum around the special k points, sketching it for all values of k.

Hint: The spectrum must be continuous away from these special values of k. For your "cultural" information the form of the resulting spectrum is sufficient to then explain why some materials are metals and some are insulations and the difference between their physical properties.

5. Consider a spin-1 particle characterized by a Hamiltonian $H = AS_z^2 + B(S_x^2 - S_y^2)$, with $B \ll A$.

   (a) Compute the spectrum and the eigenstates to 0th order in B. Sketch the spectrum.

   (b) Treating B term as a perturbation, compute its effects on all the eigenstates (spinors) and the spectrum to 1st order in B.

   Sketch the spectrum, showing how it changes from $A = B = 0$ to $A \neq 0$, $B = 0$, to $A \neq 0$, $B \neq 0$, labeling all the states, and the corresponding energies.

6. Anisotropic 2D harmonic oscillator

   (a) Consider a two-dimensional isotropic harmonic oscillator with $H_0 = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega^2(x^2 + y^2)$.

      i. Find its spectrum E_{n_x,n_y} and eigenfunctions $\psi_{n_x,n_y}(x, y)$.

      ii. Sketch the spectrum, labeling lowest few *states* (not just, possibly degenerate, energy levels) by unique quantum numbers.

   (b) Consider a rotational symmetry-breaking perturbation $H_1 = \lambda xy$ to the above Hamiltonian, such that the total $H = H_0 + H_1$.

      i. Use perturbation theory to compute the shifts in the energy of the ground state and the first excited states to 2nd and 1st orders in λ, respectively. Also compute the eigenstates for the ground state and the lowest excited states to 1st and 0th orders in λ, respectively.

      Hint: You might find it useful to use the 2nd quantized notation of creation and annihilation operators (rather than working in the coordinate representation).

      ii. Sketch the spectra for these lowest states for $\lambda \neq 0$, comparing them with the isotropic case of $\lambda = 0$, and clearly labeling them by corresponding quantum numbers.

iii. Find the *exact* spectrum $E_{n_x,n_y}(\lambda)$ and eigenfunctions $\psi_{n_x,n_y}(x,y)$. Verify the agreement of the Taylor expansion of $E_{n_x,n_y}(\lambda)$ to the appropriate order in λ with the above perturbative results.