Homework #1 — Phys623 — Spring 1999
Deadline: Friday, February 5, 1999.
Turn in homework in the class or put in
the box on the door of Phys 2314 by 5 p.m.

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Do not forget to write your name and the homework number!
Equation numbers with the period, like (3.25), refer to the equations of Schwabl.
Equation numbers without period, like (5), refer to the equations of this homework.

Time-Independent Perturbation Theory (Chapters 11.1 and 11.4)

1. [**3 points**] Schwabl's Problem 11.4. *Hints*: (*i*) Use raising and lowering operators to simplify the computations. (*ii*) Finding the exact result requires almost no labor because it amounts to a shift of the origin of the coordinate x.

2. [**2 points each part**] Consider a two-state quantum system described by the Hamiltonian

$$\hat{H} = \begin{pmatrix} E_0 + U & \Delta e^{i\phi} \\ \Delta e^{-i\phi} & E_0 - U \end{pmatrix}, \tag{1}$$

where E_0, U, Δ, and ϕ are all real. This is the most general Hermitian 2×2 matrix.

(a) Find the exact eigenvalues and normalized eigenvectors of $\hat{H}$.

(b) Sketch the eigenvalues of $\hat{H}$ as functions of U when U changes from $U \ll -\Delta$ to $U \gg \Delta$. Do the energy levels cross or "repel" in the region $U \approx 0$ where they would cross if Δ were zero?

(c) Considering the Δ terms of the Hamiltonian (1) as a perturbation, compute the first and second order energy level shifts using non-degenerate perturbation theory (assuming $U \neq 0$). Compare the result with the expansion of the exact eigenvalues to lowest nonvanishing order in Δ/U when $U \gg \Delta$.

(d) Is non-degenerate perturbation theory applicable in the opposite case $U \ll \Delta$? For which values of Δ/U the degenerate and non-degenerate versions the perturbation theory are appropriate?

(e) Describe how the eigenvectors evolve when U changes from $U \ll -\Delta$ to $U \gg \Delta$. What are the eigenvectors at $U = 0$?

3. *Adapted from Physics Qualifier, August 1987, II-1.*

A free particle of mass m, wave number k, momentum $\hbar k$, and kinetic energy

$$\epsilon(k) = \hbar^2 k^2 / 2m$$

moves one-dimensionally along the x-axis under the influence of the weak periodic potential

$$U(x) = 2V \cos(qx), \tag{2}$$

where $V \ll \epsilon(q/2)$.

(a) [**3 points**] While the spectrum of the problem is actually continuous, for solving the following problems, it may be convenient to discretize it by imposing the periodic boundary conditions $\psi(x) = \psi(x + L)$, where a big distance L will be taken to infinity at the end of calculations. This results in quantization the wave vector values: $k_n = 2\pi n/L$ (see pages 229–230 of Schwabl for a more detailed explanation). We may also assume that L is selected so that q also belongs to the set of values $2\pi n/L$.

Find the matrix elements of the perturbation (2) in the basis of unperturbed energy eigenstates.

(b) [**3 points**] The perturbation (2) modifies the energy relation of the particle:

$$E(k) = \epsilon(k) + E^{(2)}(k). \tag{3}$$

Calculate the energy shift $E^{(2)}(k)$ using the second-order perturbation theory in (2). Show that $E^{(2)}(k)$ diverges near $k = \pm q/2$ and interpret this result.

(c) [**5 points**] Show that $U(x)$ mixes a state of the wave vector $k = q/2 + \delta k$ close to $q/2$ with the state of the wave vector $k = -q/2 + \delta k$ close to $-q/2$. For a small δk, the unperturbed energies of these states are approximately equal to

$$\epsilon(k) \approx \epsilon(q/2) \pm v\delta k, \tag{4}$$

where $v = d\epsilon/dk$ taken at $k = q/2$.

Using these two states as a truncated basis, represent the Hamiltonian as a 2×2 matrix and find its eigenvalues $E(k)$. Sketch $E(k)$ versus k and comment on the appearance of an energy gap and on its magnitude.

4. [**5 points**] Let us consider the following Hamiltonian for a three-state system

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}_1, \qquad \hat{H}_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad \hat{H}_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{5}$$

Treating λ as a small perturbation, write and solve the modified secular equation given in Schwabl's Problem 11.9 for this problem. (Derivation of the modified secular equation can be found in the book by Landau and Lifshitz, Chapter 39.) Find the energy eigenstates and eigenvalues.

5. *Adapted from Qualifier, January 1997, II-1, August 1995, II-2, and August 1986, II-1.*

A diatomic molecule with moment of inertia I is constrained to rotate freely within the xy-plane with angular momentum $L_z = m\hbar$, where m is an integer. The molecule has a permanent electric dipole moment $\mathbf{d}$, which is parallel parallel to its axis and whose amplitude d is independent of the rotational motion or the external conditions. A weak uniform electric field $\mathcal{E}$ is applied along the x-axis.

(a) [**3 points**]

i. Write down the unperturbed ($\mathcal{E} = 0$) wave functions and energies.

ii. Then, write down the Hamiltonian in the presence of the electric field ($\mathcal{E} \neq 0$).

iii. Also write down the full Hamiltonian ($\mathcal{E} \neq 0$) as a matrix with respect to the unperturbed states.

(b) [**7 points**] Using perturbation theory up to the second order in $\mathcal{E}$,

i. Find the shifts and, perhaps, the splittings of the energy levels of the system. Discuss the difference between the cases of $m = 0$, $m = 1$, and $m > 1$. [Hint: You may need to use the results of Problem 4.] Qualitatively discuss a possibility of energy splitting of the levels with $m > 1$ in the higher orders of perturbation theory.

ii. Find the expectation value $\langle d_x \rangle$ of the x-component of the dipole moment and deduce the electric polarizability $\alpha = \langle d_x \rangle / \mathcal{E}$.

iii. Formulate the conditions of applicability of your calculation.

(c) [**5 points**] Consider a classical rotor with moment of inertia I, intrinsic dipole moment d, and suppose that in the absence of an electric field its angular velocity is ω_0. Using energy conservation, determine its angular velocity ω in the presence of a *weak* electric field and then calculate the time-averaged electric dipole moment $\langle d_x \rangle$. [Hint: note that $dt = d\theta/\omega$.] Compare the classical result to the quantum result in the limit of large m. Qualitatively explain the difference in the signs of the energy shifts found in Problem 5(b)i in terms of the classical picture of the spinning dipole.

(d) [**5 points**] Let's consider the quantum two-dimensional rotator again. Consider now the case of a strong electric field such that $Id\mathcal{E}/\hbar^2 \gg 1$. Find approximately the wave functions and the energy levels in the lower part of the energy spectrum.