Applied Quantum Mechanics

Chapter 8 problems

LAST NAME FIRST NAME

Problem 8.1

(a) Starting from the exact result (Eq. (8.18))

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}a_m(t) = \sum_n a_n(t)\langle m|\hat{W}(x,t)|n\rangle e^{i\omega_{mn}t},$$

for which eigenstates $|n\rangle$ and eigenvalues $\hbar\omega_n = E_n$ are known prior to application of perturbation $\hat{W}(x,t)$ at time $t \geq 0$, we seek the time-dependent coefficients $a_n(t)$ that describe the time-dependent state

$$|\psi(t)\rangle = \sum_n a_n(t)|n\rangle e^{-i\omega_n t}.$$

If $a_n(t)$ can be expressed as a power series in the perturbing potential then

$$\hat{W}(x,t) = \lambda\hat{W}(x,t)$$

and

$$a_n(t) = a_n^{(0)}(t) + \lambda a_n^{(1)}(t) + \lambda^2 a_n^{(2)}(t) + \lambda^3 a_n^{(3)}(t) + \ldots,$$

where λ is a dummy variable used to keep track of the order of terms in the power series and is set to unity at the end of the calculation. Substitute into Eq. (8.18) and evaluate zeroth-order, first-order, and k-th order terms.

(b) A particle initially in eigenstate $|n\rangle$ of the unperturbed Hamiltonian for all time $t < 0$ scatters into state $|m\rangle$ with probability $|a_m(t)|^2$ after the perturbation $\hat{W}$ is applied at time $t \geq 0$. Show using first-order time-dependent perturbation theory that the scattering amplitude is

$$a_m(t) = \frac{1}{i\hbar}\int_{t'=0}^{t'=t} W_{mn}e^{i\omega_{mn}t'}dt'$$

where the matrix element $W_{mn} = \langle m|\hat{W}(x,t)|n\rangle$ and $\hbar\omega_{mn} = E_m - E_n$ is the difference in eigenenergies of the states $|m\rangle$ and $|n\rangle$.

(c) A particle of mass m_0 is initially in the ground state of a one dimensional harmonic oscillator. At time $t = 0$ a perturbation $\hat{W}(x,t) = V_0 x^3 e^{-t/\tau}$ is applied where V_0 and τ are constants. Using the result in part (b), calculate the probability of transition to each excited state of the system in the long time limit, $t \to \infty$.

Problem 8.2

An electron is in the ground state of a one-dimensional rectangular potential well for which $V(x) = 0$ in the range $0 < x < L$ and $V(x) = \infty$ elsewhere. It is decided to control the state of the electron by applying a pulse of electric field $\mathbf{E}(t) = \mathbf{E}_0 e^{-t^2/\tau^2}$ in the x-direction starting at time $t = 0$, where τ is a constant and $|\mathbf{E}_0|$ is the maximum strength of the applied electric-field.

(a) Calculate the probability P_{12} that the particle will be found in the first excited state in the long time limit, $t \to \infty$.

(b) If the electron is in a semiconductor and has an effective mass $m^* = 0.07 \times m_0$, where m_0 is the bare electron mass, and the potential well is of width $L = 10\ \text{nm}$, calculate the value of $|\mathbf{E}_0|$ for which $P_{12} = 1$. Comment on your result.

You may wish to make use of the standard integral $\int\limits_{t'=0}^{t'=\infty} e^{-ax^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}$.

Problem 8.3

An electron is initially in the ground state of a one-dimensional rectangular potential well for which $V(x) = 0$ in the range $0 < x < L$ and $V(x) = \infty$ elsewhere. The ground state energy is E_1 and the first excited state energy is E_2. At time $t = 0$ the system is subject to a perturbation $\hat{W}(x, t) = V_0 x^2 e^{-t/\tau}$. Calculate analytically and then use a computer program to plot the probability of finding the particle in the first excited state as a function of time for $t \geq 0$. In your plot, normalize time to units of τ and consider the three values of $\omega_{21} = 1/2\pi$, $\omega_{21} = 1$, and $\omega_{21} = 2\pi$, where $\hbar\omega_{21} = E_2 - E_1$. Explain your result

Problem 8.4

Use the Einstein spontaneous emission coefficient $A = \frac{4\omega^3 e^2}{3\hbar c^3 4\pi\varepsilon_0} |\langle j|r|k\rangle|^2$ to estimate the numerical value of the spontaneous emission lifetime of the 2*p* excited state of atomic hydrogen. Use your results to estimate the spontaneous emission lifetime of the 2*p* transition of atomic He^+ ions. Describe the spontaneous emission spectral line-shape you expect to observe. Do you expect the He^+ ion 2*p* spontaneous emission line spectrum to have a larger or smaller full-width at half maximum compared to atomic hydrogen?

Problem 8.5

(a) A particle in a continuum system described by Hamiltonian $\hat{H}_0$ is prepared in eigenstate $|n\rangle$ with eigenvalue $E_n = \hbar\omega_n$. Consider the effect of a perturbation turned on at time $t = 0$ that is harmonic in time such that $\hat{W}(x, t) = V(x)\cos(\omega t)$, where $V(x)$ is the spatial part of the potential and ω is the frequency of oscillation. Start by writing down the Schrödinger equation for the complete system including the perturbation and then go on to show that the scattering rate in the static limit ($\omega \to 0$) is given by Fermi's golden rule $\frac{1}{\tau_n} = \frac{2\pi}{\hbar}|W_{mn}|^2 D(E)\delta(E_m - E_n)$, where the matrix element $W_{mn} = \langle m|\hat{W}(x, t)|n\rangle$ couples state $|n\rangle$ to state $|m\rangle$ via the static potential $V(x)$, the density of final continuum states is $D(E)$, and $\delta(E_m - E_n)$ ensures energy conservation.

(b) An electron of energy E moving in the x-direction in the conduction band of a semiconductor has effective electron mass $m^* = 0.07 \times m_0$ and is incident on two identical ionized impurities, one at position $x = 0$ nm and the other at $x = 20$ nm. The semiconductor has low frequency relative permitivity $\varepsilon_{r0} = 13.2$. Calculate the elastic scattering rate $1/\tau_n(E)$ and explain you results.

Problem 8.6

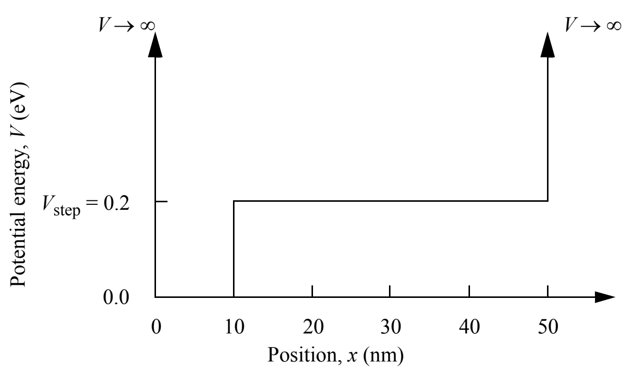
(a) In a uniform dielectric the dielectric function is a constant over space but depends on wave vector so that $\varepsilon = \varepsilon(\mathbf{q})$. Given an impurity potential at position $\mathbf{r}$ due to a charge e at position $\mathbf{R}_i$ is $\upsilon_q(\mathbf{r} - \mathbf{R}_i) = \frac{-e^2}{4\pi\varepsilon_q|\mathbf{r} - \mathbf{R}_i|}$, derive an expression for $\upsilon(\mathbf{q})$.

(b) Use the expression for $\upsilon(\mathbf{q})$ and Fermi's Golden rule to evaluate the total elastic scattering rate for an electron of initial energy $E(\mathbf{k})$ due to a single impurity in a dielectric with dielectric function $\varepsilon = \varepsilon(\mathbf{q})$. Describe any assumptions you have made. Outline how you might extend your calculations to include elastic scattering from n ionized impurities in a substitutionally doped crystalline semiconductor.

(c) What differences in scattering rate do you expect in (b) for the case of randomly positioned impurities and for the case of strongly correlated impurity positions?

Problem 8.7

(a) Using the method outlined in Exercise 3.7 as a starting point, calculate numerically the dipole matrix elements between the ground state and the first three excited states for an electron with effective mass $m_e^* = 0.07 \times m_0$ confined to the asymmetric potential well sketched in the following figure and bounded by barriers of infinite energy at $x < 0$ nm and $x > 50$ nm. The value of the step change in potential energy in the figure is $V_{\text{step}} = 0.2$ eV.



(b) Explain the difference in matrix elements you obtain.

(c) Calculate the spontaneous emission rate associated with each transition in a medium with refractive index $n_r = 3.3$.

Problem 8.8

An electron is initially in the ground state of a one dimensional harmonic oscillator characterized by frequency ω_0. At time $t = 0$ a uniform electric field $\mathbf{E}$ is applied in the x direction for time τ. Calculate the probability of transition to the first excited state of the oscillator and plot the result as a function of the electric field pulse duration τ.

Problem 8.9

A lattice vibration at frequency ω that lasts for a time t can result in an electron making a transition from an initial state $|\psi_i\rangle$ with eigenenergy E_i to a final state $|\psi_f\rangle$ with eigenenergy $E_f = E_i + \hbar\omega$ or $E_f = E_i - \hbar\omega$. The lattice vibration can be viewed as a harmonic perturbation of the form

$$\hat{W}(t') = W_0(\hat{b}e^{i\omega t'} + \hat{b}^{\dagger}e^{-i\omega t'})$$

where W_0 is a constant. According to first-order time-dependent perturbation theory and assuming that each scattering process is an independent parallel channel, the transition probability is

$$P(t) = \frac{1}{\hbar^2}\sum_f \left| \int_{t'=0}^{t'=t} \langle\psi_f|\hat{W}(t')|\psi_i\rangle e^{i\omega_{fi}t'}dt' \right|^2$$
$$= \frac{W_0^2}{\hbar^2}|\langle\psi_f|\hat{b}|\psi_i\rangle|^2 \left| \int_{t'=0}^{t'=t} e^{i(\omega_{fi}+\omega)t'}dt' \right|^2 + \frac{W_0^2}{\hbar^2}|\langle\psi_f|\hat{b}^{\dagger}|\psi_i\rangle|^2 \left| \int_{t'=0}^{t'=t} e^{i(\omega_{fi}-\omega)t'}dt' \right|^2$$

where $\hbar\omega_{fi} = (E_f - E_i)$.

(a) Show that

$$P(t) = \frac{4W_0^2}{\hbar^2}|\langle\psi_f|\hat{b}|\psi_i\rangle|^2 \frac{\sin^2((\omega_{fi}+\omega)t/2)}{(\omega_{fi}+\omega)^2 t}t + \frac{4W_0^2}{\hbar^2}|\langle\psi_f|\hat{b}^{\dagger}|\psi_i\rangle|^2 \frac{\sin^2((\omega_{fi}-\omega)t/2)}{(\omega_{fi}-\omega)^2 t}t$$

(b) In the limit $t \to \infty$ show that the transition rate is

$$\frac{1}{\tau} = \frac{2\pi}{\hbar}W_0^2|\langle\psi_f|\hat{b}|\psi_i\rangle|^2\delta(E_f - E_i + \hbar\omega) + \frac{2\pi}{\hbar}W_0^2|\langle\psi_f|\hat{b}^{\dagger}|\psi_i\rangle|^2\delta(E_f - E_i - \hbar\omega)$$

and explain the physical meaning of the result.

You may wish to make use of the relations $|e^{ix} - 1|^2 = 4\sin^2\left(\frac{x}{2}\right)$, $\delta(x) = \frac{1}{\pi}\lim_{\eta\to\infty}\frac{\sin^2(\eta x)}{\eta x^2}$, and $\delta(ax) = \frac{1}{|a|}\delta(x)$ so that $2\hbar\delta(\hbar\omega) = \delta\left(\frac{\omega}{2}\right)$

Problem 8.10

(a) A hydrogen atom excited in a $2p$ state is placed inside a cavity. At what temperature of the cavity are the spontaneous and induced photon emission rates equal?

(b) An electron in a GaAs quantum dot is modeled as a particle of mass $m^* = 0.07 \times m_0$ embedded in a medium with refractive index $n_r = 3.3$ and confined by a potential that is infinite everywhere except for the region $0 < x < L$, $0 < y < L$, and $0 < z < L$, where the potential is zero. The value of $L = 20$ nm. The electron is in the first excited state of the quantum dot. At what temperature are the spontaneous and induced photon emission rates equal? Comment on any assumptions you have made.

Problem 8.11

A two-level atom described by Hamiltonian $\hat{H}_0$ has eigenstates $|1\rangle$ and $|2\rangle$ with energy separation $\hbar\omega_{21} = E_2 - E_1$. The atom is initially in its ground state $|1\rangle$ and at time $t \geq 0$ it is illuminated with an electric field $\mathbf{E} = \mathbf{E}_0(e^{i\omega t} + e^{-i\omega t})$ in the x-direction. The electric field oscillates at frequency ω and has amplitude $|\mathbf{E}_0|$.

(a) Write down the Hamiltonian for time $t \geq 0$ in terms of $\hat{H}_0$ and a perturbation $\hat{W}$.

(b) The solution at time $t \geq 0$ is of the form $|x, t\rangle = a_1(t)e^{-i\omega_1 t}|1\rangle + a_2(t)e^{-i\omega_2 t}|2\rangle$ where $E_1 = \hbar\omega_1$ and $E_2 = \hbar\omega_2$. Substitute this into the time-dependent Schrödinger equation and show that

$$i\hbar\left(\frac{d}{dt}a_1(t)\right)e^{-i\omega_1 t}|1\rangle + i\hbar\left(\frac{d}{dt}a_2(t)\right)e^{-i\omega_2 t}|2\rangle = a_1(t)e^{-i\omega_1 t}\hat{W}|1\rangle + a_2(t)e^{-i\omega_2 t}\hat{W}|2\rangle$$

(c) If $|\mathbf{E}_0|$ is small and $\omega = \omega_{21}$, show that the probability that the atom will be in state $|2\rangle$ at time $t > 0$ is $|a_2(t)|^2 = \sin^2\left(\frac{W_{21}t}{\hbar}\right)$, where $W_{21} = |\mathbf{E}_0|\langle 2|\hat{x}|1\rangle$.

(d) How is your result in (c) modified if ω is slightly detuned from ω_{21}?

Problem 8.12

A conduction band electron is initially in the lowest energy state of a GaAs quantum well that has width $L = 10$ nm. The effective electron mass is $m^* = 0.07 \times m_0$, where m_0 is the bare electron mass, and the ground-state energy eigenvalue is E_1. An electric field pulse $\mathbf{E}(t) = \mathbf{E}_0 e^{-t^2/\tau^2}$ is applied in the x-direction across the quantum well starting at time $t = 0$, where τ is a constant and $|\mathbf{E}_0| = 1.17 \times 10^6$ V m^{-1} is the maximum strength of the applied electric-field.

(a) Modeling the quantum well as a rectangular potential well for which $V(x) = 0$ in the range $0 < x < L$ and $V(x) = \infty$ elsewhere, find the value of τ that maximizes the probability that the electron will be found in the first excited state in the long time limit, $t \to \infty$.

(b) The quantum well has an area 10×10 μm^2 and electron density 10^{12} cm^{-2}. Using the value of τ calculated in (a) and assuming any electron in the first excited state flows as current in an external circuit, how many electrons contribute to the current?

(c) Is it possible to operate this particular device at room temperature?

You may wish to make use of the standard integral $\int_{t'=0}^{t'=\infty} e^{-ax^2}dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}$.

Problem 8.13

Consider a time-dependent Hamiltonian $H(t)$ with state $|\psi(t)\rangle$ evolving from time t_0 that satisfies the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle. \tag{1}$$

If at any given instant in time the eigenstates $|\phi_n(t)\rangle$ and energy eigenvalues $E_n(t) = \hbar\omega_n(t)$ are known then they can be used as a basis to expand the time-evolving wave function

$$|\psi(t)\rangle = \sum_n a_n(t)|\phi_n(t)\rangle e^{-i\theta_n(t)} \tag{2}$$

where $\theta_n(t) = \int\limits_{t'=t_0}^{t'=t} \omega_n(t')dt'$, so that $\frac{\mathrm{d}}{\mathrm{d}t}\theta_n(t) \equiv \dot{\theta}_n(t) = \omega_n(t)$, and $a_n(t)$ is the occupation amplitude of the n-th state at time t.

(a) Substitute (2) into (1) and show that

$$i\hbar\sum_n e^{-i\theta_n(t)}(a_n(t)|\phi_n(t)\rangle - i\dot{\theta}_n(t)a_n(t)|\phi_n(t)\rangle + a_n(t)|\dot{\phi}_n(t)\rangle) = \sum_n E_n(t)a_n(t)|\phi_n(t)\rangle e^{-i\theta_n(t)}$$

(b) Multiply both sides of (a) by $\langle\phi_m(t)|$ and show that

$$\dot{a}_m(t)e^{-i\theta_m(t)} = -\sum_n a_n(t)\langle\phi_m(t)|\dot{\phi}_n(t)\rangle e^{-i\theta_n(t)}$$

(c) To find $\langle\phi_m(t)|\dot{\phi}_n(t)\rangle$ differentiate $H(t)|\phi_n(t)\rangle = E_n(t)|\phi_n(t)\rangle$ with respect to time and then show that

$$\dot{a}_m(t) = -a_m\langle\phi_m|\dot{\phi}_m\rangle + \sum_{n\neq m} a_n \frac{\langle\phi_m|\dot{H}(t)|\phi_n\rangle}{E_m - E_n} e^{i\omega_{mn}}$$

where $\omega_{mn} = \omega_m - \omega_n$.

Problem 8.14

An electron mass m free to move in one-dimension is incident from the left in state $\psi_i(x)$ with momentum p. At low temperatures the electron can excite a localized Einstein phonon at position $x = 0$ of energy $\hbar\omega$ and dispersion relation $\omega(q) = \text{constant}$. The matrix element coupling initial electron state $\psi_i(x)$ to final scattered electron state $\psi_f(x)$ is W_{if} measured in J m.

(a) Use first-order time-dependent perturbation theory to calculate the total electron transmission probability for $0 < E \leq 2.5\hbar\omega$ with no phonons initially in the system. Comment on your result.

(b) The Hamiltonian of the system can be written

$$\hat{H} = \frac{p^2}{2m} + W_{if}(\hat{b}^\dagger + \hat{b})\delta(x) + \hbar\omega\hat{b}^\dagger\hat{b}$$

where $\hat{b}^\dagger$ creates a phonon of energy $\hbar\omega$. The constant zero-point energy of the phonon is not included because it only contributes a $\hbar\omega/2$ shift in energy.

The total wave function Ψ of the coupled electron-phonon system can be expanded in the oscillator basis as

$$\langle x|\Psi\rangle = \sum_{n=0}^{n=\infty} \psi_n(x)|n\rangle$$

For $x \neq 0$ the wave function coefficients are superpositions of plane waves if E is above threshold for the n-th phonon energy, then $E > n\hbar\omega$, $k_n = \sqrt{2m(E - n\hbar\omega)}/\hbar$, and

$$\psi_n(x<0) = a_n e^{ik_n x} + b_n e^{-ik_n x}$$

$$\psi_n(x>0) = c_n e^{ik_n x}$$

If $E < n\hbar\omega$, then $\kappa_n = \sqrt{2m(n\hbar\omega - E)}/\hbar$, and

$$\psi_n(x<0) = b_n e^{\kappa_n x}$$

$$\psi_n(x>0) = c_n e^{-\kappa_n x}$$

At low temperatures the phonon is initially in its ground state so that $a_n = \delta_{n,0}$ (meaning $a_0 = 1$ and $a_{n \neq 0} = 0$). Integrate the time-independent Schrödinger equation around $x = 0$ and show that continuity in $\psi_n(x)$ requires

$$a_n + b_n = c_n$$

and

$$\frac{2m}{\hbar^2} W_{if} \sqrt{n} c_{n-1} - 2i\gamma_n c_n + \frac{2m}{\hbar^2} W_{if} \sqrt{n+1} c_{n+1} = -2i\gamma_n \delta_{n,0} \qquad (1)$$

where $\gamma_n = k_n \theta(E - n\hbar\omega) + i\kappa_n \theta(n\hbar\omega - E)$ and θ is the heavyside step function.

(c) The total transmission coefficient as a function of incident electron energy E is the sum over all *propagating states* in which k_n remains *real*, so that

$$T(E) = \sum_{n=0}^{n = E/\hbar\omega} \frac{k_n(E)}{k_0(E)} |c_n(E)|^2$$

The transmission amplitudes can be determined from the matrix equation

$$\mathbf{Mc} = \mathbf{a}$$

where $\mathbf{c}^{\mathrm{T}} = \begin{bmatrix} c_0 & c_1 & \ldots & c_{N-1} \end{bmatrix}$, $\mathbf{a}^{\mathrm{T}} = \begin{bmatrix} -2i\gamma_0 & 0 & \ldots & 0 \end{bmatrix}$, and $\mathbf{M}$ is a $N \times N$ tri-diagonal matrix given by Eqn. (1) in part (b). Let $N = 10$ and write MATLAB code to invert the matrix. Evaluate and plot $T(E)$ for $0 < E \leq 2.5\hbar\omega$ when $W_{if} = 0.04$ and $W_{if} = 0.4$ in units where $\hbar = 2m = 1$. Comment on your results and explain why they differ from (a).

(d) If there is a delta function barrier of strength W_0 at position $x = 0$, the Hamiltonian in (b) becomes $\hat{H} = \frac{\hat{p}^2}{2m} + (W_0 + W_{if}(\hat{b}^\dagger + \hat{b}))\delta(x) + \hbar\omega\hat{b}^\dagger\hat{b}$. Write down the new matrix $\mathbf{M}$. Evaluate and plot $T(E)$ for $0 < E \leq 2.5\hbar\omega$ when $W_0 = 1$ and $W_{if} = 0.4$ in units where $\hbar = 2m = 1$. What happens if $W_0 = -1$? Explain your results.