Applied Quantum Mechanics

Chapter 9 problems

Problem 9.1

Consider a three-dimensional potential $V(x, y, z)$ that is infinite except in a region $0 < x < L$, $0 < y < L$, and $0 < z < L$ where $V(x, y, z) = 0$.

(a) Write down the time-independent Schrödinger equation for a particle mass m confined to motion in the potential and solve for the eigenfunctions.

(b) Show that the eigenenergies are $E^{(0)}_{n_x, n_y, n_z} = \frac{\pi^2 \hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$, where n_x, n_y, and n_z are non-zero positive integers. What is the degeneracy of the ground state and what is the degeneracy of the first excited state?

(c) The system is perturbed by introducing a potential $\hat{W} = V_0$ in a region for which $0 < x < \frac{L}{2}$, $0 < y < \frac{L}{2}$, and $0 < z < L$. The perturbation $\hat{W} = 0$ elsewhere and V_0 is a constant. Use first-order perturbation theory to find the new ground state energy.

(d) What are the new eigenenergies and eigenfunctions of the first excited state?

Problem 9.2

A particular unperturbed Hamiltonian expressed in matrix form is

$$\boldsymbol{H}^{(0)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

The system is subject to the perturbation

$$\mathbf{W} = \begin{bmatrix} 0 & \Delta & 0 \\ \Delta & 0 & 0 \\ 0 & 0 & \Delta \end{bmatrix}$$

where $\Delta \ll 1$.

(a) Find the exact eigenvalues of $\boldsymbol{H} = \boldsymbol{H}^{(0)} + \mathbf{W}$.

(b) Find the eigenvalues to second-order using time-independent non-degenerate perturbation theory.

(c) Compare the results obtained in (a) and (b).

Problem 9.3

(a) An electron moves in a one-dimensional box of length *X*. Apply the periodic boundary conditions and find the electron eigenfunction and eigenvalues.

(b) Now apply a weak periodic potential $V(x) = V(x + L)$ to the system, where $X = NL$ and N is a large positive integer. Using nondegenerate perturbation theory, find the first order correction to the wave functions and the second order correction to the eigenenergies.

(c) When wave vector *k* is close to $n\pi/L$, where n is an integer, the result in (b) is no longer valid. Use two-state degenerate perturbation theory to find the corrected energy values for $k = n\pi((1 + \Delta)/L)$, and $k' = n\pi((1 - \Delta)/L)$ where Δ is small compared with π/L.

(d) Use the results of (b) an (c) to draw the electron dispersion relation, $E(k)$.

(e) If the lowest-frequency Fourier component of the perturbative periodic potential is chosen in part (b), then $V(x) = V_1\cos(\pi x/L)$. Repeat (b), (c), and (d) using this potential.

Hint: $V(x) = V_0 + \sum_{n\neq 0} V_n e^{i2\pi nx/L}$, and choose $V_0 = 0$.

Problem 9.4

A semiconductor quantum dot is modeled as a three-dimensional box of side L and infinite barrier energy. An electron in the quantum dot has energy $E = \frac{3\pi^2\hbar^2}{m_e^* L^2}$, where m_e^* is the effective electron mass.

(a) Calculate the first-order correction to the electron energy when a uniform electric field **E** is applied in the *z*-direction.

(b) If $L = 20$ nm, the effective electron mass is $m_e^* = 0.07 \times m_0$, and the strength of the applied electric field is $\mathbf{E} = 10^4$ V cm^{-1}, what is the value of the new electron energy level?

(c) Explain the degeneracy of the system after the perturbation is applied.

Problem 9.5

The first four lowest energy states of a one-dimensional harmonic oscillator with characteristic frequency ω_0 are subject to the perturbation

$$\mathbf{W} = \begin{bmatrix} W_{00} & W_{01} & W_{02} & W_{03} \\ W_{10} & W_{11} & W_{12} & W_{13} \\ W_{20} & W_{21} & W_{22} & W_{23} \\ W_{30} & W_{31} & W_{32} & W_{33} \end{bmatrix} = \Delta\hbar\omega_0 \begin{bmatrix} 1 & 0 & \frac{-1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 \\ \frac{-1}{\sqrt{2}} & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

where $\Delta \ll 1$.

(a) Find the new eigenenergies to first-order in time-independent perturbation theory.

(b) Find the new eigenenergies to second-order in time-independent perturbation theory.

Problem 9.6

An electron is confined in a one-dimensional rectangular potential well of width $2L$ such that $V(x) = 0$ for $0 < x < 2L$ and $V(x) = \infty$ elsewhere. The system is subject to a constant uniform electric field **E** in the *x* direction.

(a) Write down an analytic expression for the new eigenfunctions and energy eigenvalues evaluated to first-order in time-independent perturbation theory.

(b) For an electron with effective electron mass $m_e^* = 0.07 \times m_0$, where m_0 is the bare electron mass, well width $2L = 10$ nm, and electric field of 2×10^5 V cm^{-1}, use the result from (a) to find the new eigenfunctions and energy eigenvalues.

(c) Sketch and explain how, according to first-order time-independent perturbation theory, the unperturbed ground-state wave function is modified under the influence of the perturbation. Under what circumstances are the results of first-order time-independent perturbation theory are expected to be valid?

Problem 9.7

An electron mass m_0 confined to motion in a one-dimensional harmonic potential with characteristic frequency ω is subject to a perturbing potential

$\hat{W} = \xi x^3 \hbar\omega(m_0\omega/\hbar)^{3/2}$.

(a) Write down the Hamiltonian for the system.

(b) Calculate to second-order the eigenenergies of the perturbed system.

(c) Calculate to first-order the eigenstates for the perturbed system.

Problem 9.8

The unperturbed Hamiltonian for a particle of mass m_e^* with kinetic energy $T = \frac{\hat{p}_x^2 + \hat{p}_y^2}{2m_e^*}$ in a two-dimensional harmonic potential $V(x, y) = \frac{\kappa}{2}(\hat{x}^2 + \hat{y}^2)$ is $\hat{H}^{(0)} = \hat{T} + \hat{V}$ where $\kappa = m_e^*\omega^2$. The eigenstates associated with $\hat{H}^{(0)}\phi_{nm} = E_{nm}\phi_{nm}$ are of the form $\phi_{nm} = \phi_n(x)\phi_m(y) = |nm\rangle$ with $n, m = 0, 1, 2, \ldots$. The eigenstates are $(n + m + 1)$-fold degenerate with eigenenergies $E_{nm} = \hbar\omega(n + m + 1)$.

(a) Find the position of minimum potential and the amount by which any perturbing potential $\hat{W} = \frac{\kappa'}{2}\hat{x}$ or $\hat{W} = \frac{\kappa'}{2}(\hat{x} + \hat{y})$ shifts eigenenergy values and show that the perturbation does not break the degeneracy of the states.

(b) Create a contour plot of the potential $V(x, y)$ in the range $-2\text{ nm} < x < 2\text{ nm}$ and $-2\text{ nm} < y < 2\text{ nm}$ for $\kappa = 2\text{ eV nm}^{-2}$ and overlay a contour plot of $\hat{V}(x, y) + \hat{W}(x) = \frac{\kappa}{2}(\hat{x}^2 + \hat{y}^2) + \frac{\kappa'}{2}\hat{x}$ for $\kappa' = 1\text{ eV nm}^{-1}$. Use the contour plots to explain why the perturbing potential fails to break the degeneracy of the states.

(c) Create a contour plot of the potential $V(x, y)$ in the range $-2\text{ nm} < x < 2\text{ nm}$ and $-2\text{ nm} < y < 2\text{ nm}$ for $\kappa = 2\text{ eV nm}^{-2}$ and overlay a contour plot of $\hat{V}(x, y) + \hat{W}(x, y) = \frac{\kappa}{2}(\hat{x}^2 + \hat{y}^2) + \frac{\kappa'}{2}\hat{x}\hat{y}$ for $\kappa' = 1\text{ eV nm}^{-2}$. Use the contour plots to explain why in this case the perturbing potential breaks the degeneracy of the states.

Problem 9.9

Consider a system such that

$\hat{H}|\psi_n\rangle = (\hat{H}_0 + \lambda\hat{W})|\psi_n\rangle = E|\psi_n\rangle$

for which

$$(H_0 + \lambda W)(|\phi_n^{(0)}\rangle + \lambda|\phi_n^{(1)}\rangle + \lambda^2|\phi_n^{(2)}\rangle + \ldots)$$
$$= (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots)(|\phi_n^{(0)}\rangle + \lambda|\phi_n^{(1)}\rangle + \lambda^2|\phi_n^{(2)}\rangle + \ldots)$$

where the unperturbed Hamiltonian is $\hat{H}_0$ with known eigenstates $|\phi_n^{(0)}\rangle$, the perturbation is $\hat{W}$, and λ is a dummy variable of unit magnitude used to keep track of the order of terms in the perturbative expansion. The energy eigenstate to first-order in time-independent nondegenerate perturbation theory is normalized to unity so that

$$\int \psi_n^* \psi_n \mathrm{d}^3 r = 1 + \lambda a_m^{(1)} + \lambda a_m^{(1)*} + 0(\lambda^2) = 1$$

with $\psi_n = \phi_n^{(0)} + \phi_n^{(1)}$ and $a_m^{(1)} = 0$ as one possible solution. Another solution is $a_m^{(1)}$ pure imaginary so that $a_m^{(1)} = \mathrm{i}a = a\mathrm{e}^{\mathrm{i}\pi/2}$ with a real.

(a) Show that for $a_m^{(1)}$ pure imaginary the terms $\phi_m^{(0)} + a_m^{(1)}\phi_m^{(0)}$ may be written $\mathrm{e}^{\mathrm{i}a}\phi_m^{(0)}$.

(b) The phase term $e^{\mathrm{i}a}$ in (a) may be chosen arbitrarily. Choose the value of a so that $\langle\phi_m^{(0)}|\phi_m^{(1)}\rangle = 0$ and comment on the result.

Problem 9.10

An electron of mass m_0 with motion confined to one-dimension in a potential $V(x)$ has lowest energy (ground state) wave function

$$\psi_0(x) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} \mathrm{e}^{-x^2/2\sigma^2}$$

(a) Find an expression for the potential $V(x)$ and the numerical value of the ground-state energy in units of eV if $\sigma = 1.4$ nm.

(b) Calculate to first-order the change in ground-state energy when the system is subject to a perturbation

$$\hat{W} = \frac{\lambda}{x^2 + \gamma^2}$$

when $\gamma \ll \sigma$.

(c) Repeat the calculation (b) for the case when $\gamma \gg \sigma$.

Note $\int_{-\infty}^{\infty} \frac{1}{x^2 + \gamma^2}\mathrm{d}x = \frac{\pi}{\gamma}$ and $\int_{-\infty}^{\infty} \mathrm{e}^{ax^2}\mathrm{d}x = \sqrt{\frac{\pi}{a}}$.