Solution 8.1

(a) Consider a quantum mechanical system described by Hamiltonian $\hat{H}_0$ and for which we know the solutions to the time-independent Schrödinger equation $\hat{H}_0|n\rangle = E_n|n\rangle$ and the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|n\rangle e^{-i\omega_n t} = \hat{H}_0|n\rangle e^{-i\omega_n t}$$

At time $t = 0$ we apply a time-dependent change in potential $\hat{W}(t)$ so the new Hamiltonian is $\hat{H} = \hat{H}_0 + \hat{W}(t)$ and the state $|\psi(t)\rangle$ evolves in time according to

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = (\hat{H}_0 + \hat{W}(t))|\psi(t)\rangle$$

where $|\psi(t)\rangle = \sum_n a_n(t)|n\rangle e^{-i\omega_n t}$ and $a_n(t)$ are time dependent coefficients.

Substitution of the state $|\psi(t)\rangle$ in to the time-dependent Schrödinger equation gives

$$i\hbar\frac{d}{dt}\sum_n a_n(t)|n\rangle e^{-i\omega_n t} = (\hat{H}_0 + \hat{W}(t))\sum_n a_n(t)|n\rangle e^{-i\omega_n t}$$

Using the product rule for differentiation ($(fg)' = (f'g + fg')$), one may rewrite the left-hand-side as

$$i\hbar\sum_n\left(\left(\frac{\partial}{\partial t}a_n(t)\right)|n\rangle e^{-i\omega_n t} + a_n(t)\left(\frac{\partial}{\partial t}|n\rangle e^{-i\omega_n t}\right)\right) = (\hat{H}_0 + \hat{W}(t))\sum_n a_n(t)|n\rangle e^{-i\omega_n t}$$

and remove the term

$$i\hbar\sum_n a_n(t)\frac{\partial}{\partial t}|n\rangle e^{-i\omega_n t} = \sum_n a_n(t)\hat{H}_0|n\rangle e^{-i\omega_n t}$$

to leave

$$i\hbar\sum_n |n\rangle e^{-i\omega_n t}\frac{\partial}{\partial t}a_n(t) = \sum_n a_n(t)\,\hat{W}(t)|n\rangle e^{-i\omega_n t}$$

Multiplying both sides by $\langle m|$ and using the orthonormal relationship $\langle m|n\rangle = \delta_{mn}$ gives

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

However, since

$$\langle m|\,\hat{W}(t)|n\rangle = \int\phi_m^*(x)e^{i\omega_m t}W\phi_n(x)e^{-i\omega_n t}dx = W_{mn}e^{i\omega_{mn}t}$$

where $\hbar\omega_{mn} = E_m - E_n$ and W_{mn} is defined as the matrix element $\int\phi_m^*(x)\,\hat{W}\phi_n(x)\,dx$, we may write

$$i\hbar\frac{d}{dt}a_m(t) = \sum_n a_n(t)\,W_{mn}e^{i\omega_{mn}t}$$

If the system is initially in an eigenstate $|n\rangle$ of the Hamiltonian $\hat{H}_0$ then $a_n(t = -\infty) = 1$ and $a_m(t = -\infty) = 0$ for $m \neq n$. Using first order perturbation theory in which we approximate $a_n(t)$ with its initial value such that $a_n(t) = 1$, we may write

$$i\hbar \frac{d}{dt} a_m(t) = W_{mn} e^{i\omega_{mn} t}$$

Integration from the time when the perturbation is applied at $t = 0$ gives

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

(b) The transition probability from state $|n\rangle$ to state $|m\rangle$ is $P_{nm} = |a_m(t)|^2$. Using our solution in part (a) we have

$$P_{nm} = \frac{1}{\hbar^2} \left| \int_{t'=0}^{t'=t} \langle m| V(x,t) |n\rangle e^{i\omega_{mn} t'} dt' \right|^2 = \frac{V_0^2}{\hbar^2} \left| \int_{t'=0}^{t'=t} \langle m|\hat{x}^3|n\rangle e^{(i\omega_{mn} - 1/\tau)t'} dt' \right|^2$$

In the problem we have initial state $|n = 0\rangle$ and we consider the long time limit, $t \rightarrow \infty$, this allows us to write

$$P_{nm} = \frac{V_0^2}{\hbar^2} |\langle m|\hat{x}^3|0\rangle|^2 \left| \int_{t'=0}^{t'=\infty} e^{(im\omega - 1/\tau)t'} dt' \right|^2$$

where, for the harmonic oscillator, the non-zero positive integer m multiplied by the frequency ω is related to the difference in energy eigenvalue by $m\omega = (E_m - E_0)/\hbar$. The time integral is

$$\left| \int_{t'=0}^{t'=\infty} e^{(im\omega - 1/\tau)t'} dt' \right|^2 = \frac{1}{m^2\omega^2 + 1/\tau^2}$$

and the matrix elements $\langle m|\hat{x}^3|0\rangle$ are found using $\hat{x} = (\hbar/2m_0\omega)^{1/2}(\hat{b}^\dagger + \hat{b})$, where m_0 is the particle mass. In our case only transitions $|0\rangle \rightarrow |1\rangle$ and $|0\rangle \rightarrow |3\rangle$ are allowed.

$$\langle m|\hat{x}^3|0\rangle = (\hbar/2m_0\omega)^{3/2}(\hat{b}^{\dagger 3} + \hat{b}\hat{b}^{\dagger 2} + \hat{b}^\dagger) = (\hbar/2m_0\omega)^{3/2}(\sqrt{6}\delta_{m=3} + 3\delta_{m=1})$$

where we used $\hat{b}^\dagger|n\rangle = (n+1)^{1/2}|n+1\rangle$, $\hat{b}|n\rangle = n^{1/2}|n-1\rangle$, $\hat{b}|0\rangle = 0$, and $\langle m|n\rangle = \delta_{mn}$.

Hence,

$$P_{01} = \frac{V_0^2}{\hbar^2} |\langle 1|\hat{x}^3|0\rangle|^2 \left| \int_{t'=0}^{t'=\infty} e^{(im\omega - 1/\tau)t'} dt' \right|^2 = \left(\frac{\hbar}{2m_0\omega}\right)^3 \left(\frac{9V_0^2}{(\hbar\omega)^2 + \hbar^2/\tau^2}\right)$$

and

$$P_{03} = \frac{V_0^2}{\hbar^2} |\langle 3|\hat{x}^3|0\rangle|^2 \left| \int_{t'=0}^{t'=\infty} e^{(im\omega - 1/\tau)t'} dt' \right|^2 = \left(\frac{\hbar}{2m_0\omega}\right)^3 \left(\frac{6V_0^2}{(3\hbar\omega)^2 + \hbar^2/\tau^2}\right)$$

So, in the long time limit, $t \rightarrow \infty$, the maximum probability of the transition taking place occurs as $\tau \rightarrow \infty$.

Solution 8.2

(a) The eigenstates of a particle in a one-dimensional rectangular potential well for which $V(x) = 0$ in the range $0 < x < L$ and $V(x) = \infty$ elsewhere are

$$|n\rangle = \sqrt{\frac{2}{L}} \sin(k_n x)$$

where $k_n = n\pi/L$, $n = 1, 2, 3, \ldots$, and eigenenergies are $E_n = \hbar^2 k_n^2/2m = \hbar\omega_n$.

The perturbation $\hat{W}(x, t) = -exE_{\max}e^{-t^2/\tau^2}$ is turned on at time $t = 0$, where τ and $E_{\max}$ is the maximum strength of the applied electric-field. The probability P_{12} that the particle will be found in the first excited state in the long time limit, $t \to \infty$ is

$$P_{12} = \frac{e^2 E_{\max}^2}{\hbar^2}|\langle 2|\hat{x}|1\rangle|^2 \left| \int_{t'=0}^{t'=\infty} e^{i\omega_{21}t' - \frac{t'^2}{\tau^2}} dt' \right|^2$$

where $\hbar\omega_{21} = E_2 - E_1$. The integral for $\langle 2|x|1\rangle$ can be found by noting $k_2 = 2\pi/L$, $k_1 = \pi/L$, and making use of the relationship $2\sin(x)\sin(y) = \cos(x-y) - \cos(x+y)$ so that

$$\langle 2|\hat{x}|1\rangle = \frac{2}{L}\int_0^L x\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{\pi x}{L}\right)dx = \frac{1}{L}\int_0^L x\left(\cos\left(\frac{\pi x}{L}\right) - \cos\left(\frac{3\pi x}{L}\right)\right)dx$$

The first term on the right-hand-side in the integral is

$$\frac{1}{L}\int_0^L x\cos\left(\frac{\pi x}{L}\right)dx = \frac{1}{\pi}\left[x\sin\left(\frac{\pi x}{L}\right)\right]_0^L - \frac{1}{\pi}\int_0^L \sin\left(\frac{\pi x}{L}\right)dx = \frac{-L}{\pi^2}\left[\cos\left(\frac{\pi x}{L}\right)\right]_0^L = \frac{-2L}{\pi^2}$$

and the second term on the right-hand-side in the integral is

$$\frac{1}{L}\int_0^L x\cos\left(\frac{3\pi x}{L}\right)dx = \frac{1}{3\pi}\left[x\sin\left(\frac{3\pi x}{L}\right)\right]_0^L - \frac{1}{\pi}\int_0^L \sin\left(\frac{3\pi x}{L}\right)dx = \frac{-L}{9\pi^2}\left[\cos\left(\frac{3\pi x}{L}\right)\right]_0^L = \frac{-2L}{9\pi^2}$$

Hence,

$$\langle 2|\hat{x}|1\rangle = \frac{2}{L}\int_0^L x\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{\pi x}{L}\right)dx = \frac{-2L}{\pi^2} + \frac{2L}{9\pi^2} = \frac{-16L}{9\pi^2}$$

Substituting the value of $|\langle 2|x|1\rangle|^2$ into our expression for the probability, we have

$$P_{12} = e^2 E_{\max}^2 \left(\frac{16L}{9\hbar\pi^2}\right)^2 \left| \int_{t'=0}^{t'=\infty} e^{i\omega_{21}t' - \frac{t'^2}{\tau^2}} dt' \right|^2$$

Let $y = \frac{t}{\tau} - i\frac{\omega_{21}\tau}{2}$ so that $i\omega_{21}t - \frac{t^2}{\tau^2} = -\frac{\omega_{21}^2}{4} - y^2$ and $dt = \tau dy$. We now can write

$$P_{12} = e^2 E_{\max}^2 \left(\frac{16L}{9\hbar\pi^2}\right)^2 \left| e^{-\omega_{21}^2\tau^2/4} \int_{t'=0}^{t'=\infty} e^{-y^2} dy \right|^2 = e^2 E_{\max}^2 \left(\frac{16L}{9\hbar\pi^2}\right)^2 e^{-\omega_{21}^2\tau^2/2}\frac{\tau^2\pi}{4}$$

where $\omega_{21} = 3\pi^2\hbar/2mL^2$ and we made use of the standard integral $\int_{t'=0}^{t'=\infty} e^{-ax^2}dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}$.

(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 $L = 10\text{ nm}$, we can calculate the value of τ for which P_{12} is a maximum.

$$0 = \frac{dP_{12,\,t\to\infty}}{d\tau} = 2\tau e^{-\omega_{21}^2\tau^2/2} - 2\tau(\omega_{21}^2\tau^2/2)e^{-\omega_{21}^2\tau^2/2}$$

$$0 = \frac{dP_{12,\, t\to\infty}}{d\tau} \to 2\tau - \omega_{21}^2\tau^3 = 0$$

so that $\tau = \sqrt{2}/\omega_{21}$. We now find E_{max} for which $P_{12} = 1$.

$$P_{12} = \frac{\pi e^2 E_{max}^2}{4}\left(\frac{16L}{9\hbar\pi^2}\right)^2 \frac{2}{\omega_{21}^2} e^{-1} = \frac{\pi e^2 E_{max}^2}{4}\left(\frac{16L}{9\hbar\pi^2}\right)^2 2\left(\frac{2mL^2}{3\pi^2\hbar}\right)^2 e^{-1} = 1$$

$$E_{max}^2 = \frac{4}{2\pi e^2}\left(\frac{9\hbar\pi^2}{16L}\frac{3\pi^2\hbar}{2mL^2}\right)^2 e^1 = \frac{2}{\pi}\left(\frac{27\hbar^2\pi^4}{32meL^3}\right)^2 e^1$$

$$E_{max} = \sqrt{\frac{2}{\pi}}\left(\frac{27\hbar^2\pi^4}{32meL^3}\right)e^{0.5} = \sqrt{\frac{2}{\pi}}\left(\frac{27\times(1.05\times10^{-34})^2\times\pi^4}{32\times0.07\times9.1\times10^{-31}\times1.6\times10^{-19}\times10^{-24}}\right)\times1.65$$

$$E_{max} = 1.17\times10^8 \text{ V m}^{-1}$$

This is a large electric field corresponding to a voltage drop of 1.17 V across the potential well of width $L = 10$ nm.