Chem. 2430, Problem Set 2, Solutions, Nov. 2009.

1) Using the defining relation between the *c*'s and *b*'s, i.e.:

$$\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \exp\left[-i(E_1+E_2)t/2\hbar\right]\begin{pmatrix} b_1(t) \\ b_2(t) \end{pmatrix}$$

the first row of Eq. [1] transforms to:

$$i\hbar\left\{\frac{-i\left(E_1+E_2\right)}{2\hbar}\dot{c}_1+\exp\left[-i(E_1+E_2)t/2\hbar\right]\dot{b}_1\right\}=E_1c_1+\Delta c_2$$

which is equivalent to:

$$i\hbar\dot{b}_1=\frac{(E_1-E_2)}{2}b_1+\Delta b_2 \qquad \text{[A1a]}$$

The second row of Eq. [1] can be transformed similarly:

$$i\hbar\left\{\frac{-i\left(E_1+E_2\right)}{2\hbar}\dot{c}_2+\exp\left[-i(E_1+E_2)t/2\hbar\right]\dot{b}_2\right\}=\Delta c_1+E_2c_2$$

or equivalently:

$$i\hbar\dot{b}_2=\Delta b_1-\frac{(E_1-E_2)}{2}b_2 \qquad \text{[A1b]}$$

Eqs. [A1a,b] together constitute matrix Eq. [2].

b) Let us write out the component equations of Eq. [2] (essentially as given in Eqs. [A1a,b] above:

$$i\hbar\dot{b}_1=\varepsilon b_1+\Delta b_2 \qquad \text{(i)}$$

$$i\hbar\dot{b}_2=\Delta b_1-\varepsilon b_2 \qquad \text{(ii)}$$

The objective is to convert Eqs. (i), (ii) into a single 2nd order linear ordinary differential equation for one of the components, say b_1. We start by taking another time derivative of both sides of Eq. (i), and then substitute as appropriate:

$$
\begin{aligned}
i\hbar\ddot{b}_1 &= \varepsilon\dot{b}_1 + \Delta\dot{b}_2 \\
&= \varepsilon\dot{b}_1 + \Delta\left(\Delta b_1 - \varepsilon b_2\right)/\,i\hbar \\
&= \varepsilon\dot{b}_1 + \Delta\left(\Delta b_1 - \varepsilon[i\hbar\dot{b}_1 - \varepsilon b_1]/\,\Delta\right)/\,i\hbar \\
&= (\Delta^2 + \varepsilon^2)b_1\,/\,i\hbar
\end{aligned}
$$

That is:

$$
\ddot{b}(t)_1 = -\omega_0^2 b_1(t) \quad ; \quad \omega_0 = \sqrt{\Delta^2 + \varepsilon^2}\,/\,\hbar \qquad \text{[A2]}
$$

The solution to the elementary differential equation [A2] is:

$$
b_1(t) = A\cos\omega_0 t + B\sin\omega_0 t \qquad \text{[A3]}
$$

where the constants of integration A,B are determined by initial conditions. We are given that $c_1(0) = 1$ and hence $b_1(0) = 1$. Similarly, we are given that $c_2(0) = 0$; hence , $b_2(0) = 0$, and thus, from equation (i) above, $\dot{b}_1(0) = -i\varepsilon/\hbar$. The solution of Eq. [A2], given initial conditions $b_1(0) = 1$, $\dot{b}_1(0) = -i\varepsilon/\hbar$ is thus seen to be:

$$
b_1(t) = \cos\omega_0 t - i\frac{\varepsilon}{\hbar\omega_0}\sin\omega_0 t = \cos\omega_0 t - i\frac{\varepsilon}{\sqrt{\Delta^2 + \varepsilon^2}}\sin\omega_0 t
$$

Finally, we want to compute the probability that the system will be found in state 1 at time t, which is given by:

$$
\begin{aligned}
|c_1(t)|^2 = |b_1(t)|^2 &= \cos^2\omega_0 t + \frac{\varepsilon^2}{\Delta^2 + \varepsilon^2}\sin^2\omega_0 t \\
&= (1 - \sin^2\omega_0 t) + \frac{\varepsilon^2}{\Delta^2 + \varepsilon^2}\sin^2\omega_0 t \\
&= 1 - \frac{\Delta^2}{\Delta^2 + \varepsilon^2}\sin^2\omega_0 t
\end{aligned}
$$

2) As discussed in class, within the RWA we map this problem to the problem of a "standard" two-level system (no time-dependent driving term), which was also featured in problem 1 above. The mapping of the off-diagonal coupling term in the two-level system (TLS) Hamiltonian was shown in class to be $\mu_0\mathcal{E}_0/2 \to \Delta$. Thus, for a symmetric TLS ($\varepsilon = 0$) the time evolution of the probability for the system to be found in state 1 is given by $P_1(t) = |c_1(t)|^2 = \cos^2(\mu_0\mathcal{E}_0 t/2\hbar)$. Furthermore, $P_2(t) = 1 - P_1(t)$. The first time, t_0, at which $P_1(t) = 0$ (i.e., there is unit probability that the system will be found in state 2) is when: $\mu_0\mathcal{E}_0 t_0/2\hbar = \pi/2$, i.e.: $t_0 = \pi\hbar/\mu_0\mathcal{E}_0$.

3) Recall the standard harmonic oscillator energy eigenfunctions:

$$\phi_0(x) = \left[\frac{m\omega}{\pi\hbar}\right]^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \qquad ;$$

$$\phi_1(x) = \frac{1}{\sqrt{2}}\left[\frac{m\omega}{\pi\hbar}\right]^{1/4} H_1\left(\sqrt{\frac{m\omega}{\hbar}}x\right)\exp\left(-\frac{m\omega}{2\hbar}x^2\right)$$
$$= \sqrt{2}\sqrt{\frac{m\omega}{\hbar}}\left[\frac{m\omega}{\pi\hbar}\right]^{1/4} x\exp\left(-\frac{m\omega}{2\hbar}x^2\right)$$

Here $\omega = \sqrt{\kappa / m}$, and H_1 is the 1st Hermite polynomial.

a) Consider the integral:

$$I_{00} = \int_{-\infty}^{\infty} dx\phi_0(x)x\phi_0(x) \propto \int_{-\infty}^{\infty} dx\exp(-\frac{m\omega}{\hbar}x^2)x \;= 0$$

The important point is that this integral vanishes by symmetry (the overall integrand is antisymmetric about x=0), so all multiplicative constants are irrelevant.

Hence: $\int_{-\infty}^{\infty} dx\phi_0(x)\hat{\mu}\phi_0(x) = q_0\int_{-\infty}^{\infty} dx\phi_0(x)x\phi_0(x) = 0$.

b) Now consider the integral:

$$I_{01} = \int_{-\infty}^{\infty} dx\phi_0(x)x\,\phi_1(x)$$

$$= \left[\frac{2m\omega}{\hbar}\right]^{1/2}\cdot\left[\frac{m\omega}{\pi\hbar}\right]^{1/2}\int_{-\infty}^{\infty} dx\,x^2\exp\left(-\frac{m\omega}{\hbar}x^2\right) = \sqrt{\frac{\hbar}{2m\omega}}$$

Here the Gaussian integral identity $\frac{1}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{\infty} dx\,x^2\exp\left(-\frac{x^2}{2\sigma^2}\right) = \sigma^2$ proves useful. An important point is that this integral does *not* vanish by symmetry, and therefore has to be worked out carefully, including keeping track of all multiplicative constants.

Finally, we obtain: $\int_{-\infty}^{\infty} dx\phi_0(x)\hat{\mu}\phi_1(x) = q_0 I_{01} = q_0\sqrt{\frac{\hbar}{2m\omega}}$.