

1. The Hamiltonian for a two-level system is represented by the matrix  $H = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ .

a. Find the energy eigenvalues and eigenvectors.

$$(\hat{H} - E)\psi = 0$$

$$\begin{vmatrix} -E & 1 \\ 1 & -E \end{vmatrix} = 0$$

$$E^2 - 1 = 0$$

$$E = \pm 1 \quad (1)$$

$$E_1 = 1:$$

$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Rightarrow |\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad (1)$$

$$E_2 = -1:$$

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Rightarrow |\psi_2\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad (1)$$

 b. If the system starts out in a state  $|S(0)\rangle = A \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ , what is  $A$  (assuming it is real-valued) and what is  $|S(t)\rangle$ , the ket as a function of time  $t > 0$ ?

$$A = \frac{1}{\sqrt{2}} \text{ s.t. } \langle S|S \rangle = 1 \quad (1)$$

$$\text{Since } |S\rangle = |\psi_1\rangle, \quad |S(t)\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} e^{-i \frac{E_1}{\hbar} t} \quad (1)$$

 c. If the system starts out in a state  $|S(0)\rangle = B \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ , what is  $B$  (assuming it is real-valued) and what is  $|S(t)\rangle$ ?

~~What is the expectation value of the (hermitian) operator  $G = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$  as a function of time?~~

$$B = 1 \text{ s.t. } \langle S|S \rangle = 1 \quad (1)$$

$$|S(0)\rangle = \frac{1}{\sqrt{2}} (|\psi_1\rangle - |\psi_2\rangle) \quad (1) \text{ so}$$

$$|S(t)\rangle = \frac{1}{2} \begin{bmatrix} 1 \\ 1 \end{bmatrix} e^{-i E_1 / \hbar t} - \frac{1}{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix} e^{-i E_2 / \hbar t} = \begin{bmatrix} -i \sin \omega t \\ \cos \omega t \end{bmatrix} \quad (\omega \equiv E_1 / \hbar) \quad (1)$$

(Since  $E_2 = -E_1$ )

d. Calculate the four matrix elements of  $H$  in the basis  $|1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} i \\ 1 \end{bmatrix}$ ,  $|2\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} i \\ -1 \end{bmatrix}$

$$\langle 1|H|1\rangle = \frac{1}{2} \begin{bmatrix} -i & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} i \\ 1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} -i & 1 \end{bmatrix} \begin{bmatrix} 1 \\ i \end{bmatrix} = 0$$

$$\langle 2|H|2\rangle = \frac{1}{2} \begin{bmatrix} -i & -1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} i \\ -1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} -i & -1 \end{bmatrix} \begin{bmatrix} -1 \\ i \end{bmatrix} = 0$$

$$\langle 1|H|2\rangle = \frac{1}{2} \begin{bmatrix} -i & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} i \\ -1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} -i & 1 \end{bmatrix} \begin{bmatrix} -1 \\ i \end{bmatrix} = i$$

$$\langle 2|H|1\rangle = -i \quad \text{by symmetry}$$

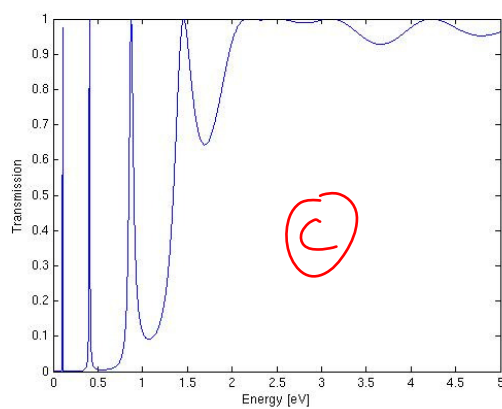
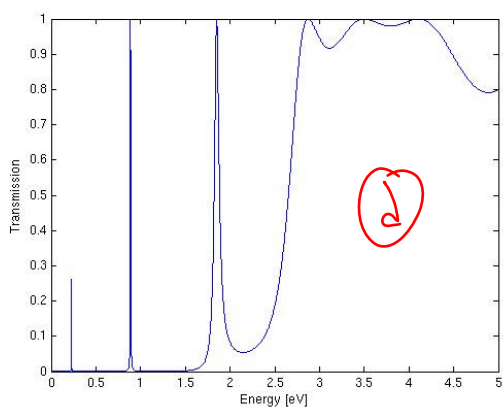
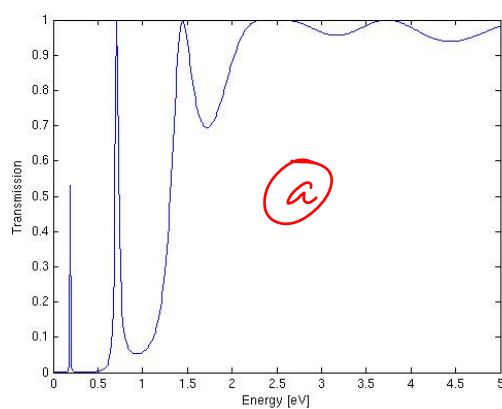
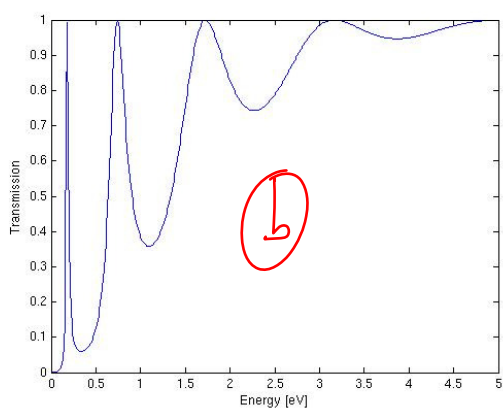
So

$$H \text{ in this basis is } \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix} \quad \textcircled{2}$$

2. The following are transmission functions calculated for scattering through double barrier potentials. The sets of parameters used to define the potentials are

	Barrier width [nm]	Well width [nm]	Barrier height [eV]
<b>a</b>	0.5	1	1
<b>b</b>	0.25	1	1
<b>c</b>	0.5	1.5	1
<b>d</b>	0.5	1	2

By considering the effects on *resonance* features, match the parameter sets (a,b,c, or d) to the appropriate result below.



1 each

3. An electron is incident from  $x < 0$  on a step-function scattering potential  $V(x) = V_0 \Theta(x)$ .

a) Write down the propagating solutions of the 1-d time-independent Schrodinger Eq

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi + V\Psi = E\Psi$$

for both  $x < 0$  and  $x > 0$ . Assume only a forward-propagating solution for  $x > 0$ .

$$x < 0: \psi_- = e^{ik_1 x} + r e^{-ik_1 x}$$

$$(k_1 = \sqrt{\frac{2mE}{\hbar^2}}) \quad (1)$$

$$x > 0: \psi_+ = t e^{ik_2 x}$$

$$(k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}) \quad (1)$$

b) What are the boundary conditions at  $x=0$ ?

$$\psi_-(0) = \psi_+(0) \quad (1)$$

$$\psi'_-(0) = \psi'_+(0) \quad (1)$$

c) Apply these boundary conditions and determine the amplitude of the transmitted wavefunction.

$$1 + r = t \rightarrow r = t - 1 \quad (1)$$

$$ik_1 - ik_1 r = ik_2 t \quad (1)$$

$$k_1 (1 - (t - 1)) = k_2 t$$

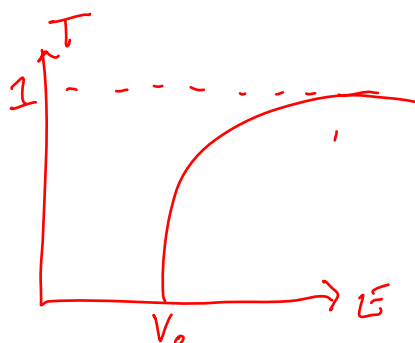
$$2k_1 = (k_1 + k_2)t \rightarrow t = \frac{2k_1}{k_1 + k_2} \quad (1)$$

d) What is the transmission coefficient  $T$  (the ratio of transmitted probability current to incident probability current)? [hint: probability current is the product of wavefunction group velocity and particle density] Plot  $T(E)$ , and label axes and important values.

$$T = \frac{J_{trans}}{J_{inc}} = \frac{\frac{\hbar k_2}{m} \cdot |t|^2}{\frac{\hbar k_1}{m} \cdot 1} = \frac{k_2}{k_1} \frac{4k_1^2}{(k_1 + k_2)^2} = \frac{4k_1 k_2}{(k_1 + k_2)^2} \quad (1)$$

• As  $E \rightarrow \infty$ ,  $k_2 \rightarrow k_1$   
so  $T \rightarrow 1$

• For  $E = V_0$ ,  $k_2 = 0$  so  $T = 0$



4. An electron is bound in a 3-dimensional isotropic harmonic oscillator potential  $V(\vec{r}) = \frac{1}{2} m \omega^2 |\vec{r}|^2$ , where  $\vec{r} = \sqrt{x^2 + y^2 + z^2}$ .

- a. Write down the corresponding time-independent Schrodinger equation in Cartesian (x,y,z) coordinates.

$$\left[ \frac{-\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{1}{2} m \omega^2 (x^2 + y^2 + z^2) \right] \psi = E \psi \quad (1)$$

- b. Use separation of variables to convert this partial differential equation into three ordinary differential equations.

$$\psi = \psi_{xy} \psi_z$$

$$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial z^2} \psi_z + \frac{1}{2} m \omega^2 z^2 \psi_z - E \psi_z = \frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi_{xy} + \frac{1}{2} m \omega^2 (x^2 + y^2) \psi_{xy} \quad \psi_{xy} = -E_{xy} \psi_{xy}$$

$$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial z^2} \psi_z + \frac{1}{2} m \omega^2 z^2 \psi_z = (E - E_{xy}) \psi_z \quad (1) \Rightarrow E - E_{xy} = E_z = \hbar \omega \left( n_z + \frac{1}{2} \right)$$

$$\psi_{xy} = \psi_x \psi_y \quad n_z = 0, 1, 2, \dots$$

$$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_x + \frac{1}{2} m \omega^2 x^2 \psi_x - E_{xy} \psi_x = \frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} \psi_y - \frac{1}{2} m \omega^2 y^2 \psi_y = -E_y \psi_y$$

$$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_x + \frac{1}{2} m \omega^2 x^2 \psi_x = (E_{xy} - E_y) \psi_x \quad (1) \Rightarrow E_{xy} - E_y = E_x = \hbar \omega \left( n_x + \frac{1}{2} \right)$$

$$n_x = 0, 1, 2, \dots$$

$$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial y^2} \psi_y + \frac{1}{2} m \omega^2 y^2 \psi_y = E_y \psi_y \quad (1) \Rightarrow E_y = \hbar \omega \left( n_y + \frac{1}{2} \right)$$

$$n_y = 0, 1, 2, \dots$$

Note That  $(E - E_{xy}) + (E_{xy} - E_y) + E_y = E_z + E_x + E_y = E! \quad (1)$

- c. What are the possible total energy eigenvalues? What are the degeneracies of the first three energy levels?

$$E = E_x + E_y + E_z = \hbar\omega \left[ \left(n_x + \frac{1}{2}\right) + \left(n_y + \frac{1}{2}\right) + \left(n_z + \frac{1}{2}\right) \right] = \hbar\omega \left( n_x + n_y + n_z + \frac{3}{2} \right)$$

$$n_x, n_y, n_z = 0, 1, 2, \dots \quad (1)$$

$E_{n_x n_y n_z}$	degeneracy
$E_{000} \rightarrow$	1
$E_{100} \rightarrow$	3
$E_{110/200} \rightarrow$	6

(2)

- d. What shape do the constant electron density surfaces form in the ground state?

$$\psi_{000}^* \psi_{000} \sim e^{-\frac{x^2}{2\alpha^2}} e^{-\frac{y^2}{2\alpha^2}} e^{-\frac{z^2}{2\alpha^2}}$$

Since the potential is isotropic,  $\Delta x = \Delta y = \Delta z$   
and

$$\psi^* \psi \sim e^{-\frac{(x^2 + y^2 + z^2)}{2\alpha^2}} = e^{-\frac{r^2}{2\alpha^2}} \quad (1)$$

This is constant at fixed radius  $\rightarrow$  sphere