QUANTUM MECHANICS III

PHYS 518

Problem Set # 4

Distributed: Oct.26, 2011

Due: Nov. 4, 2011

There are 5 problems. Do any 4.

1. Analytic Expressions for Transfer Matrix: Show that the matrix elements $m_{ij}(E,x)$ $(1 \leq i,j \leq 2)$ satisfy differential equations of the form

$$\frac{d}{dx}\left[\begin{array}{cc} m_{11}(E,x) & m_{12}(E,x) \\ m_{21}(E,x) & m_{22}(E,x) \end{array}\right] = \text{something}$$

where "something" depends on the potential $V(x)$ and the incident energy E through $(E - V(x))$.

a. Construct these equations.

b. Show that each matrix element obeys an equation equivalent to the time-independent Schrödinger equation.

c. What are the initial conditions for each matrix element?

d. Explain (in words) how you would go about integrating the equations for these matrix elements.

2. Bands and Gaps: The potential in a single unit cell of width $2L$ in a one-dimensional lattice is $V(x) = V_0 e^{-(2x/L)^2}$, $-L \leq x \leq +L$. Choose $V_0 = -10.0$ eV and $L = 2.5$. Compute the energy ranges of the allowed energy bands and the intermediate band gaps.

3. The Sine Transformation: Determine the allowed eigenvalues λ for the the potential $V(x) \simeq |x|^p$ by solving the equation

$$\frac{d^2y(x)}{dx^2} + (\lambda - V(x))y(x) = 0$$

using the sine transformation. Solve in the range $0 < \lambda < 50$. Choose some value of p in the range $1.0 \leq p \leq 4.0$. Provide a plot of the phase change

ϕ/π vs. λ and identify the eigenvalues. (Recommendation: shake your code out using $p = 2$ (harmonic oscillator)).

4. Wavefunction Metamorphosis: Inside a potential well of width $L = 8$ the potential is 0 eV. Outside the potential is V eV (c.f., Fig. 25.1, pg. 106). Describe quantitatively how the wavefunction at the fourth transmission resonance ($E_4 = \frac{\hbar^2}{2m}\left(\frac{4\pi}{L}\right)^2$) transforms itself from a scattering state for $V = E_4 - \epsilon$ to a bound state for $V = E_4 + \epsilon$.

5. Density of Scattering States: Two barriers of height 5eV and width D (Ang) are separated by a distance $L = 8$ (A). The potential outside the barriers is 0 eV. The two barriers form a "metastable potential well". $D = 2, 3, 4$ A.

a. Determine the energy of the lowest transmission resonance.

b. Determine the width of this transmission resonance.

c. Compute the probability density outside the metastable potential well.

d. Compute the probability density inside the resonance well.

e. Compute the ratio of these densities: $PD_{\text{outside}}/PD_{\text{inside}}$.

f. Plot this ratio as a function of the well width D for $D = 2, 3, 4$.

g. Extrapolate for larger D: make some intuitive statements about the behavior of the wavefunction as the width of the "confining barriers" increase.