Quantum Mechanics A
Fall 2010
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Problem Set 6

Problem 1

A particle of mass m is under the influence of a 1D potential shown in Fig. 1, i.e., of the form

$$V(x) = \left\{ \begin{array}{cc} -V\delta(x) & 0 \leq |x| < a \\ \infty, & |x| \geq a \end{array} \right\} \tag{1}$$

where $V > 0$. More simply the particle is in an infinite square well with a delta function at the center of the well.

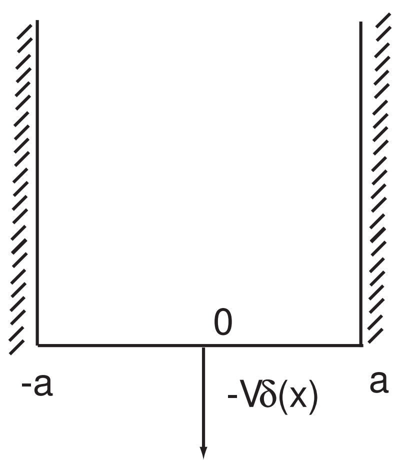

Figure 1:

a) Find the equation that determines the negative energy eigenvalues.

b) Provide a graphical solution for the energy eigenvalues.

c) In the large a limit, i.e., when $\epsilon = \hbar^2/(mVa) << 1$ show that the ground state energy is given by

$$E = -\frac{\hbar^2 k_0^2}{2m}, \tag{2}$$

where k_0 to first order in ϵ can be approximated by

$$k_0 \simeq \frac{1}{a\epsilon}, \tag{3}$$

Namely,

$$E = -\frac{mV^2}{2\hbar^2}. \tag{4}$$

Problem 2

Now consider the potential shown in Fig. 2, i.e.,

$$V(x) = \left\{ \begin{array}{cc} -V & 0 \leq |x| < b \\ 0 & b \leq |x| < a \\ \infty, & |x| \geq a \end{array} \right\} \tag{5}$$

where $V > 0$.

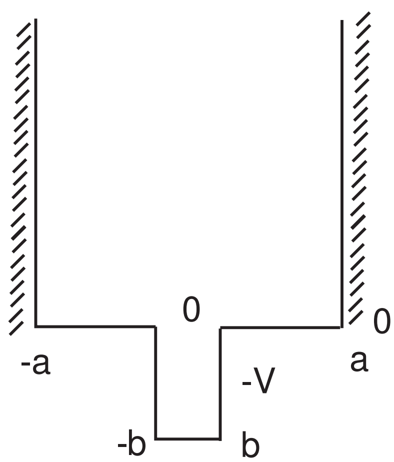

Figure 2:

a) Find the equation that determines the negative energy eigenvalues.

b) Provide a graphical solution for the energy eigenvalues.

c) Take the appropriate limit of this square well potential to obtain exactly the same δ function potential as in the previous problem. Show that in this limit, the equation that determines the energy eigenvalues is the same as the previous problem.

Problem 3

The effective mass m^* of an electron in a solid with energy dispersion $E(k)$ is defined in 1D by

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E(k)}{dk^2}. \tag{6}$$

Verify that this formula in the case of a simple quadratic energy dispersion $E(k) = \hbar^2k^2/(2m)$ gives the bare mass, i.e., $m^* = m$ for this case. Therefore, this formula can be generalized such that the coefficient of the k^2 term of the Taylor expansion of $E(k)$ near $k = 0$ gives the inverse effective mass.

Calculate m^*, in the Kronig-Penney model with delta functions, at the bottom and at the top of the lowest energy band. Explain the physical significance of the results.

Problem 4

Consider the "necklace" shown in Fig. 3, where there are N cites forming the chain and each cite is at a distance a from its nearest neighbor cite. Imagine that each cite n has an attractive potential to bind a particle, thus, forming a bound state $|n\rangle$ with energy ϵ_0.

However, because these cites are close enough together, the particle is not entirely "committed" to a particular cite as it can lower its energy by "hopping" from one potential minimum to a nearest neighboring potential minimum. Consider, therefore, the states formed from all the N localized bound state wave-functions $|n\rangle$, $n = 1, 2, ..., N$ as a basis set of functions to carry out an approximate calculation.

The states $|n\rangle$ are normalized, however, they are not orthogonal to each other. Namely,

$$\langle n|n\rangle = 1, \tag{7}$$

$$\langle n|n+1\rangle = \langle n-1|n\rangle = \gamma. \tag{8}$$

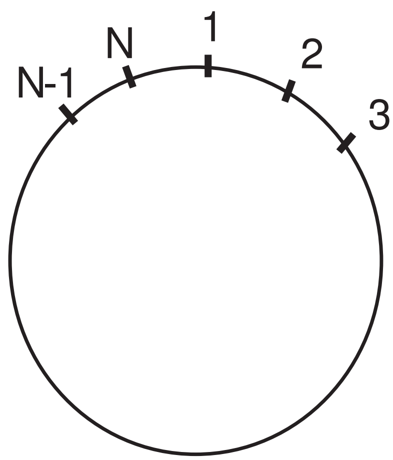

Figure 3:

and $\langle n|m\rangle = 0$ if the cites m and n are not nearest neighbors. In the above notation, when $n = N$, then $n + 1 \rightarrow 1$ and where $n = 1$, then $n - 1 \rightarrow N$ due to the cyclical boundary conditions.

In this basis, only the following matrix elements of the Hamiltonian are significantly different from zero for any cite n:

$$\langle n|\hat{H}|n\rangle = \epsilon_0, \tag{9}$$

$$\langle n|\hat{H}|n+1\rangle = -\beta, \tag{10}$$

$$\langle n-1|\hat{H}|n\rangle = -\beta, \tag{11}$$

and also, here, when $n = N$, then $n+1 \rightarrow 1$ and where $n = 1$, then $n-1 \rightarrow N$ due to the cyclical boundary conditions. Therefore, the particle when it is in any given cite n it can "hop" to only to its two nearest neighboring cites.

Now, we wish to diagonalize the Hamiltonian matrix in this basis. The problem, however, is that the Hamiltonian is an $N \times N$ matrix. Let us utilize the symmetry of the problem, namely, that the Hamiltonian commutes with the operator $\hat{T}_a$ which translates by one cite (i.e., by spacing a), i.e.,

$$\hat{T}_a|n\rangle = |n+1\rangle. \tag{12}$$

a) Show that the following state

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikn}|n\rangle, \tag{13}$$

when $k = 2\pi/Nm$ where m is an integer is an eigenstate of the this translation operator. What is the corresponding eigenvalue?

b) Consider a given state $|\psi\rangle$ and let us suppose that we know this state and, therefore, we can compute the overlap integrals with the also known basis states $|n\rangle$:

$$\lambda_i = \langle n|\psi\rangle. \tag{14}$$

Now, we wish to write $|\psi\rangle$ as a linear combination of the basis states $|n\rangle$ as follows:

$$|\psi\rangle = \sum_{n=1}^{N} c_n |n\rangle, \tag{15}$$

and, thus, we need to determine the coefficients c_n. Show that these N coefficients satisfy the following N algebraic equations:

$$c_n + \gamma(c_{n+1} + c_{n-1}) = \lambda_n, \tag{16}$$

and as already discussed $c_{N+1} = c_1$ and $c_0 = c_N$. In order to approximately solve the system of the N equations above we will assume that $\gamma << 1$, because γ is the overlap integral between two normalized wave-functions which are displaced by distance a. Clearly, when we take $\gamma = 0$ the solution to these equations is trivial: $c_n = \lambda_n$. Now, write $c_n = \lambda_n + \delta_n$ and determine the small correction δ_n to first order in γ.

c) Now, we are ready to apply the previous findings to our problem. To first order in γ show that the state given by Eq. 13 is an eigenstate of the Hamiltonian. Find the corresponding eigenvalue. To do that you may proceed as follows: Apply the Hamiltonian operator explicitly on the state given by Eq. 13. This will yield a state $|\psi\rangle$. Then, expand this known state $|\psi\rangle = \hat{H}|k\rangle$ in the basis $|n\rangle$ and find the approximate coefficients c_n as described in the previous step b). Then, use these results to show that

$$|\psi\rangle = \hat{H}|k\rangle = E(k)|k\rangle. \tag{17}$$

d) Plot the function $E(k)$ in the first Brillouin Zone, i.e., for $\pi/a < k \leq \pi/a$, using $\epsilon_0 = 1$, $\gamma = 0.1$ and $\beta = 0.2$.