Problem 1

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

$$V(x) = \begin{cases} \ -V\delta(x) & 0 \leq |x| < a \\ \ -\infty, & |x| \geq a \end{cases}$$

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](image-url)

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

$$E = -\frac{\hbar^2 k_0^2}{2m},$$
where \( k_0 \) to first order in \( \epsilon \) can be approximated by

\[
k_0 \simeq \frac{1}{a\epsilon},
\]

(3)

Namely,

\[
E = -\frac{mV^2}{2\hbar^2}.
\]

(4)

**Problem 2**

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

\[
V(x) = \begin{cases} 
-V & 0 \leq |x| < b \\
0 & b \leq |x| < a \\
\infty & |x| \geq a
\end{cases}
\]

(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 $\delta$ 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

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

Verify that this formula in the case of a simple quadratic energy dispersion $E(k) = \hbar^2 k^2/(2m)$ 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 $\epsilon_0$.

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,

$$\langle n|n\rangle = 1, \quad (7)$$

$$\langle n|n + 1\rangle = \langle n - 1|n\rangle = \gamma. \quad (8)$$
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 \( n \):

\[
\langle n|\hat{H}|n \rangle = \epsilon_0, \quad (9)
\]
\[
\langle n|\hat{H}|n + 1 \rangle = -\beta, \quad (10)
\]
\[
\langle n - 1|\hat{H}|n \rangle = -\beta, \quad (11)
\]

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.,

\[
\hat{T}_a|n \rangle = |n + 1 \rangle. \quad (12)
\]

a) Show that the following state

\[
|k \rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikn}|n \rangle, \quad (13)
\]
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 \( |n\rangle \):

\[
\lambda_n = \langle n|\psi\rangle. \tag{14}
\]

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 \( \gamma \ll 1 \), because \( \gamma \) 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 \( \delta_n \) to first order in \( \gamma \).

c) Now, we are ready to apply the previous findings to our problem. To first order in \( \gamma \) 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 \( \beta = 0.2 \).