J15Q.3 (solution by Jim Wu)

(a) Consider the Hamiltonian for a general time-independent, one-dimensional potential $V(x)$,

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

Show that for an arbitrary continuous function $\phi(x)$, the value of

$$E = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle}$$

gives an upper bound on the ground state energy for the potential $V(x)$

(b) For a particle moving in a triangular potential well

$$V(x) = \begin{cases} 
\infty & \text{if } x < 0 \\
V_0 x / L & \text{if } x > 0 
\end{cases}$$

the energy levels take the form

$$E_n = \alpha_n V_0 \left( \frac{\hbar^2 q}{m L^2 V_0} \right)$$

where $\alpha_n$ and $q$ are numerical constants. Determine the value of the exponent $q$.

(c) Using the approach in part (a), find an estimate for the constant $\alpha_0$ corresponding to the ground state in the triangular potential well. (The estimate needs not be optimal, but should be based on a reasonable variational calculation.)

Solution:

(a) Let $|\psi_n\rangle$ be the energy eigenstates of the Hamiltonian with eigenvalues of $E_n$. Then, we know that

$$E_n = \frac{\langle \psi_n | H | \psi_n \rangle}{\langle \psi_n | \psi_n \rangle} = \langle \psi_n | H | \psi_n \rangle$$

if the eigenstates are normalized. Now let $|\phi\rangle$ be any arbitrary continuous wave function and note that it can be expressed in the basis of energy eigenstates:

$$|\phi\rangle = \sum_n c_n |\psi_n\rangle$$
The expectation value of the energy for this state is

$$\tilde{E} = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle} = \frac{1}{\langle \phi | \phi \rangle} \sum_n |c_n|^2 \langle \psi_n | H | \psi_n \rangle$$

$$= \frac{1}{\sum_n |c_n|^2 \langle \psi_n | \psi_n \rangle} \sum_n |c_n|^2 \langle \psi_n | \psi_n \rangle E_n$$

$$\geq E_0 \left( \sum_n |c_n|^2 \langle \psi_n | \psi_n \rangle \right)$$

$$= E_0 \sum_n |c_n|^2 \langle \psi_n | \psi_n \rangle E$$

Hence, $E$ gives an upper bound on the ground state energy $E_0$ for the potential $V(x)$.

(b) In the region $x > 0$, the Schrödinger’s equation is given by

$$\left( -\frac{\hbar^2 d^2}{2m d^2} + \frac{V_0 x}{L} \right) \phi(x) = E \phi(x)$$

Letting $y = ax$, where $a$ is a constant, and multiplying through by $\frac{La}{V_0}$, we have

$$\left( -\frac{\hbar^2 a^3 d^2}{2m V_0 dy^2} + y \right) \phi(y) = E \frac{La}{V_0} \phi(y)$$

Choosing $a = \left( \frac{\hbar^2 L}{2m V_0} \right)^{-1/3}$, we eliminate the constants in front of the second derivative, leaving us with

$$\left( -\frac{d^2}{dy^2} + y \right) \phi(y) = E \frac{\hbar^2}{V_0} \left( \frac{\hbar^2}{2m L^2 V_0} \right)^{-1/3} \phi(y)$$

We have a completely dimensionless expression on the left, and so the expression on the right must be as well. If we let the coefficient of $\phi(y)$ on the right be equal to $\alpha_n$, then we have

$$E = \alpha_n V_0 \left( \frac{\hbar^2}{2m L^2 V_0} \right)^{1/3}$$

and so $q = 1/3$. Furthermore, we have reduced the Schrödinger equation to

$$\left( -\frac{d^2}{dy^2} + y \right) \phi(y) = \alpha_n \phi(y)$$

(c) Since $V(x)$ is infinite for $x < 0$, then we require $\phi(y) = 0$ for $y \leq 0$. Furthermore, since we have a linear function for $x > 0$, then let’s suppose a trial wave function

$$\phi(y) = ye^{-by/2}$$

where $b$ is some parameter. The first and second derivatives of the trial wave function are

$$\phi'(y) = e^{-by/2} - \frac{by}{2} e^{-by/2}$$

$$\phi''(y) = -be^{-by/2} + \frac{1}{4} b^2 ye^{-by/2}$$
and so,
\[
\langle \phi | H | \phi \rangle = \int_0^\infty y e^{-by/2} \left( b e^{-by/2} - \frac{1}{4} b^2 y e^{-by/2} + \frac{1}{4} b^2 y e^{-by/2} + y^2 e^{-by/2} \right) dy
\]
\[
= \int_0^\infty \left( by - \frac{1}{4} b^2 y^2 + y^3 \right) e^{-by} dy
\]
\[
= \int_0^\infty \left( b \left( \frac{1}{b} \right)^2 u - \frac{1}{4} b^2 \left( \frac{1}{b} \right)^3 u^2 + \left( \frac{1}{b} \right)^4 u^3 \right) e^{-u} \, du
\]
\[
= \frac{1}{b} (1!) - \frac{1}{4b} (2!) + \frac{1}{b^4} (3!)
\]
\[
= \frac{b^3 + 12}{2b^4}
\]
Furthermore,
\[
\langle \phi | \phi \rangle = \int_0^\infty y^2 e^{-by} = \left( \frac{1}{b^3} \right) (2!) = \frac{2}{b^3}
\]
and the value of \( \alpha_0 \) is
\[
\alpha_0 = \frac{\langle \phi | H | \phi \rangle}{\langle \phi | \phi \rangle} = \frac{b^3 + 12}{4b}
\]
Now, we must minimize the value of \( \alpha_0 \) with respect to \( b \) by taking a first derivative with respect to \( b \) and setting it equal to zero:
\[
0 = \frac{d\alpha_0}{db} = \frac{4b(3b^2) - (b^3 + 12)(4)}{16b^2} = \frac{b^3 - 6}{2b^2}
\]
which means that \( b = 6^{1/3} \). Substituting this back into \( \alpha_0 \), we have \( \alpha_0 = \frac{9}{2 \cdot 6^{1/3}} \) and the ground state energy of the potential is approximately
\[
E_0 \approx \frac{9}{2 \cdot 6^{1/3}} V_0 \left( \frac{\hbar^2}{2mL^2V_0} \right)^{1/3}
\]