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

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

where α_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 α_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

$$\begin{aligned}\tilde{E} = \frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle} &= \frac{1}{\langle\phi|\phi\rangle}\sum_n |c_n|^2\langle\psi_n|H|\psi_n\rangle \\ &= \frac{1}{\sum_n |c_n|^2\langle\psi_n|\psi_n\rangle}\sum_n |c_n|^2\langle\psi_n|\psi_n\rangle E_n \\ &\geq E_0\left(\frac{\sum_n |c_n|^2\langle\psi_n|\psi_n\rangle}{\sum_n |c_n|^2\langle\psi_n|\psi_n\rangle}\right) \\ &= E_0\end{aligned}$$

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

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

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

$$\left(-\frac{\hbar^2 La^3}{2mV_0}\frac{d^2}{dy^2} + y\right)\phi(y) = E\frac{La}{V_0}\phi(y)$$

Choosing $a = \left(\frac{\hbar^2 L}{2mV_0}\right)^{-1/3}$, we eliminate the constants in front of the second derivative, leaving us with

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

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 α_n, then we have

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

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

$$\begin{aligned}\phi'(y) &= e^{-by/2} - \frac{by}{2}e^{-by/2} \\ \phi''(y) &= -be^{-by/2} + \frac{1}{4}b^2ye^{-by/2}\end{aligned}$$

and so,

$$\begin{aligned}
\langle\phi|H|\phi\rangle &= \int_0^\infty ye^{-by/2}\left(be^{-by/2} - \frac{1}{4}b^2ye^{-by/2} + y^2e^{-by/2}\right)\,dy \\
&= \int_0^\infty \left(by - \frac{1}{4}b^2y^2 + y^3\right)e^{-by}\,dy \\
&= \int_0^\infty \left(b\left(\frac{1}{b}\right)^2 u - \frac{1}{4}b^2\left(\frac{1}{b}\right)^3 u^2 + \left(\frac{1}{b}\right)^4 u^3\right)e^{-u}\,du \\
&= \frac{1}{b}(1!) - \frac{1}{4b}(2!) + \frac{1}{b^4}(3!) \\
&= \frac{b^3+12}{2b^4}
\end{aligned}$$

Furthermore,

$$\langle\phi|\phi\rangle = \int_0^\infty y^2e^{-by} = \left(\frac{1}{b^3}\right)(2!) = \frac{2}{b^3}$$

and the value of α_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 α_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 α_0, we have $\alpha_0 = \frac{9}{2\cdot 6^{1/3}}$ and the ground state energy of the potential is approximately

$$\boxed{E_0 \approx \frac{9}{2\cdot 6^{1/3}}V_0\left(\frac{\hbar^2}{2mL^2V_0}\right)^{1/3}}$$

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