VARIATIONAL PRINCIPLE AND THE DELTA FUNCTION WELL

Here’s another example of the variational principle, this time applied to the delta function well. We use a normalized function \( \psi \) as a test function for the hamiltonian \( H \) and get an upper bound on the ground state energy \( E_0 \):

\[
E_0 \leq \langle \psi | H | \psi \rangle \equiv \langle H \rangle
\]  

(1)

In this case, the potential is given by

\[
V(x) = -\alpha \delta(x)
\]

(2)

and we’ll take as the test function

\[
\psi = \begin{cases} 
0 & x < -a \\
A(x+a) & -a \leq x < 0 \\
A(-x+a) & 0 \leq x < a \\
0 & x \geq a 
\end{cases}
\]

(3)

where \( A \) and \( a \) are parameters.

We can find \( A \) from normalization:

\[
|A|^2 \left[ \int_{-a}^{0} (x+a)^2 \, dx + \int_{0}^{a} (-x+a)^2 \, dx \right] = 1
\]

(4)

\[
\frac{2}{3} |A|^2 a^3 = 1
\]

(5)

\[
A = \frac{\sqrt{6}}{2a^{3/2}}
\]

(6)

To calculate \( \langle H \rangle \), we need the second derivative of \( \psi \), so we have
\begin{equation}
\frac{d\psi}{dx} = \begin{cases} 
0 & x < -a \\
A & -a \leq x < 0 \\
-A & 0 \leq x < a \\
0 & x \geq a 
\end{cases}
\end{equation}

For the second derivative, we need the derivative of the step function, which is a delta function, so we get

\begin{equation}
\frac{d^2\psi}{dx^2} = A\delta(x+a) - 2A\delta(x) + A\delta(x-a)
\end{equation}

Following the usual procedure and using (2), we get:

\begin{equation}
\langle H \rangle = -\frac{\hbar^2 A}{2m} \int_{-a}^{a} [\delta(x+a) - 2\delta(x) + \delta(x-a)] \psi(x) \, dx - \alpha (Aa)^2
\end{equation}

\begin{equation}
= -\frac{\hbar^2 A^2}{m} a - \alpha (Aa)^2
\end{equation}

\begin{equation}
= \frac{3}{2a^3} \left( \frac{\hbar^2 a}{m} - \alpha a^2 \right)
\end{equation}

The first and third delta functions in (9) contribute nothing since \( \psi(-a) = \psi(a) = 0 \), and we substitute (6) into (10) to get (11).

The free parameter here is \( a \), so taking the derivative with respect to \( a \) and setting to zero, we get

\begin{equation}
a_{\text{min}} = \frac{2\hbar^2}{\alpha m}
\end{equation}

\begin{equation}
E_0 \leq -\frac{3\alpha^2 m}{8\hbar^2}
\end{equation}

The exact bound state energy is \( E_0 = -\frac{\alpha^2 m}{2\hbar^2} \), so this upper limit is higher by \( \frac{\alpha^2 m}{8\hbar^2} \).