

VARIATIONAL PRINCIPLE AND THE DELTA FUNCTION WELL

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 7.3.

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

$$(0.1) \quad E_0 \leq \langle \psi | H | \psi \rangle \equiv \langle H \rangle$$

In this case, the potential is given by

$$(0.2) \quad V(x) = -\alpha \delta(x)$$

and we'll take as the test function

$$(0.3) \quad \psi = \begin{cases} 0 & x < -a \\ A(x+a) & -a \leq x < 0 \\ A(-x+a) & 0 \leq x < a \\ 0 & x \geq a \end{cases}$$

where A and a are parameters.

We can find A from normalization:

$$(0.4) \quad |A|^2 \left[\int_{-a}^0 (x+a)^2 dx + \int_0^a (-x+a)^2 dx \right] = 1$$

$$(0.5) \quad \frac{2}{3} |A|^2 a^3 = 1$$

$$(0.6) \quad A = \frac{\sqrt{6}}{2a^{3/2}}$$

To calculate $\langle H \rangle$, we need the second derivative of ψ , so we have

$$(0.7) \quad \frac{d\psi}{dx} = \begin{cases} 0 & x < -a \\ A & -a \leq x < 0 \\ -A & 0 \leq x < a \\ 0 & x \geq a \end{cases}$$

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

$$(0.8) \quad \frac{d^2\psi}{dx^2} = A\delta(x+a) - 2A\delta(x) + A\delta(x-a)$$

Following the usual procedure and using 0.2, we get:

$$(0.9) \quad \langle H \rangle = -\frac{\hbar^2 A}{2m} \int_{-a}^a [\delta(x+a) - 2\delta(x) + \delta(x-a)] \psi(x) dx - \alpha(Aa)^2$$

$$(0.10) \quad = \frac{\hbar^2 A^2}{m} a - \alpha(Aa)^2$$

$$(0.11) \quad = \frac{3}{2a^3} \left(\frac{\hbar^2 a}{m} - \alpha a^2 \right)$$

The first and third delta functions in 0.9 contribute nothing since $\psi(-a) = \psi(a) = 0$, and we substitute 0.6 into 0.10 to get 0.11.

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

$$(0.12) \quad a_{min} = \frac{2\hbar^2}{\alpha m}$$

$$(0.13) \quad E_0 \leq -\frac{3}{8} \frac{\alpha^2 m}{\hbar^2}$$

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