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 ψas a test function for the hamiltonian H and get an upper bound on the ground state energy E_0:

$$E_0 \le \langle\psi|H|\psi\rangle \equiv \langle H\rangle \tag{1}$$

In this case, the potential is given by

$$V(x) = -\alpha\delta(x) \tag{2}$$

and we'll take as the test function

$$\psi = \begin{cases} 0 & x < -a \\ A(x+a) & -a \le x < 0 \\ A(-x+a) & 0 \le x < a \\ 0 & x \ge a \end{cases} \tag{3}$$

where A and a are parameters.

We can find A from normalization:

$$|A|^2 \left[\int_{-a}^{0} (x+a)^2 dx + \int_0^a (-x+a)^2 dx\right] = 1 \tag{4}$$

$$\frac{2}{3}|A|^2 a^3 = 1 \tag{5}$$

$$A = \frac{\sqrt{6}}{2a^{3/2}} \tag{6}$$

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

$$\frac{d\psi}{dx} = \begin{cases} 0 & x < -a \\ A & -a \le x < 0 \\ -A & 0 \le x < a \\ 0 & x \ge a \end{cases} \tag{7}$$

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

$$\frac{d^2\psi}{dx^2} = A\delta(x+a) - 2A\delta(x) + A\delta(x-a) \tag{8}$$

Following the usual procedure and using 2, we get:

$$\langle H\rangle = -\frac{\hbar^2 A}{2m}\int_{-a}^{a}\left[\delta(x+a) - 2\delta(x) + \delta(x-a)\right]\psi(x)\,dx - \alpha(Aa)^2 \tag{9}$$

$$= \frac{\hbar^2 A^2}{m}a - \alpha(Aa)^2 \tag{10}$$

$$= \frac{3}{2a^3}\left(\frac{\hbar^2 a}{m} - \alpha a^2\right) \tag{11}$$

The first and third delta functions in 9 contribute nothing since $\psi(-a) = \psi(a) = 0$, and we substitue 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

$$a_{min} = \frac{2\hbar^2}{\alpha m} \tag{12}$$

$$E_0 \le -\frac{3}{8}\frac{\alpha^2 m}{\hbar^2} \tag{13}$$

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