VARIATIONAL PRINCIPLE AND THE DELTA FUNCTION WELL

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 16.1; Exercise 16.1.3.

Here we'll apply the variational principle to the delta function well, with potential

$$V=-aV_0\delta(x) \tag{1}$$

where a and V_0 are positive constants. As we've seen earlier, there is a single bound state with energy

$$E=-\frac{ma^2V_0^2}{2\hbar^2} \tag{2}$$

[In the earlier treatment, based on Griffiths's book, $V=-\alpha\delta(x)$ for a positive constant α.] The exact wave function has a discontinuous derivatve at $x=0$, and decays exponentially on both sides of $x=0$. To apply the variational principle, we'll use a Gaussian as a trial function, so that

$$\psi(x)=Ae^{-bx^2} \tag{3}$$

for some constants A and b. From normalization, we can find A:

$$\int_{-\infty}^{\infty}\psi^2dx=A^2\int_{-\infty}^{\infty}e^{-2bx^2}dx=1 \tag{4}$$

Evaluating the Gaussian integral we have

$$\int_{-\infty}^{\infty}e^{-2bx^2}dx=\sqrt{\frac{\pi}{2b}} \tag{5}$$

This gives

$$A=\left(\frac{2b}{\pi}\right)^{1/4} \tag{6}$$

To apply the variational principle, we need to work out the integral

$$\langle\psi|H|\psi\rangle=\sqrt{\frac{2b}{\pi}}\int_{-\infty}^{\infty}e^{-bx^2}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}-aV_0\delta(x)\right)e^{-bx^2}dx \tag{7}$$

We calculate the derivative:

$$\frac{d^2}{dx^2}e^{-bx^2} = 2b\left(2bx^2-1\right)e^{-bx^2} \tag{8}$$

We therefore have (using Maple to integrate the first term; the delta function integral is easy)

$$\langle H\rangle = \langle\psi|H|\psi\rangle = \frac{\hbar^2}{2m}b - a\sqrt{\frac{2b}{\pi}}V_0 \tag{9}$$

We now want the value of b that minimizes the energy, so we take the derivative

$$\frac{d\langle H\rangle}{db} = \frac{\hbar^2}{2m} - \frac{aV_0}{\sqrt{2\pi}}b^{-1/2} = 0 \tag{10}$$

$$b_0 = \frac{2a^2V_0^2m^2}{\pi\hbar^4} \tag{11}$$

Substituting $b = b_0$ into 9 we get

$$E_0 = -\frac{ma^2V_0^2}{\pi\hbar^2} \tag{12}$$

Comparing this with 2 we see that the variational estimate is

$$E = \frac{\pi}{2}E_0 \approx 1.57E_0 \tag{13}$$

Note that E_0 still provides an *upper* bound on E since the energy is negative. In this case, the Gaussian estimate isn't that good.