

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

$$V = -aV_0\delta(x) \quad (1)$$

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

$$E = -\frac{ma^2V_0^2}{2\hbar^2} \quad (2)$$

[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 derivative 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

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

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

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

Evaluating the Gaussian integral we have

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

This gives

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

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

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

We calculate the derivative:

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

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

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

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

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

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

Substituting $b = b_0$ into 9 we get

$$E_0 = -\frac{ma^2 V_0^2}{\pi \hbar^2} \quad (12)$$

Comparing this with 2 we see that the variational estimate is

$$E = \frac{\pi}{2} E_0 \approx 1.57 E_0 \quad (13)$$

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.