

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

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

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

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

[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

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

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

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

Evaluating the Gaussian integral we have

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

This gives

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

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

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

We calculate the derivative:

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

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

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

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

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

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

Substituting $b = b_0$ into 9 we get

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

Comparing this with 2 we see that the variational estimate is

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

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.