VARIATIONAL PRINCIPLE AND THE INFINITE SQUARE WELL

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 16.1; Exercise 16.1.2.

Although we're looking at the variational principle, the example in this post isn't technically an application of this, as there isn't anything to vary. However, the idea behind the variational principle is that if we take *any* wave function ψ then, for a given Hamiltonian H, the ground state energy E_0 is bounded by

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

Given this, then we don't need to vary a parameter in the wave function in order to get an upper bound on the ground state energy. As an example, suppose we look at the infinite square well. The exercise in Shankar uses the square well centred on the origin, so that

$$V(x) = \begin{cases} 0 & -a < x < a \\ \infty & \text{otherwise} \end{cases} \tag{2}$$

We know that the exact normalized ground state wave function is

$$\psi_1(x) = \frac{1}{\sqrt{a}}\cos\left(\frac{\pi x}{2a}\right) \tag{3}$$

and the corresponding ground state energy is

$$E_1 = \frac{\pi^2\hbar^2}{8ma^2} \tag{4}$$

Suppose we didn't know this, but guessed that the wave function was peaked at $x = 0$ and went to 0 at $x = \pm a$. We might then try a parabolic function such as

$$\psi = (x+a)(x-a) = x^2 - a^2 \tag{5}$$

Although ψ actually has a minimum at $x=0$, we could convert it into a function with a maximum at $x=0$ by taking the negative, which amounts to multiplying by a phase factor of $e^{i\pi}$, so has no effect on physical measurements.

In this case, 1 gives us

$$\langle\psi|\psi\rangle = \int_{-a}^{a}\left(x^2-a^2\right)^2 dx \tag{6}$$

$$= \frac{16}{15}a^5 \tag{7}$$

$$\langle\psi|H|\psi\rangle = -\frac{\hbar^2}{2m}\int_{-a}^{a}\left(x^2-a^2\right)\frac{d^2}{dx^2}\left(x^2-a^2\right)dx \tag{8}$$

$$= -\frac{\hbar^2}{m}\int_{-a}^{a}\left(x^2-a^2\right)dx \tag{9}$$

$$= \frac{4\hbar^2 a^3}{3m} \tag{10}$$

The ground state energy estimate is then

$$E_{1,est} \le \frac{5\hbar^2}{4ma^2} \tag{11}$$

Comparing with the exact answer 4 we see that

$$\frac{E_{1,est}}{E_1} = \frac{10}{\pi^2} \approx 1.013 \tag{12}$$

Thus the estimate of E_1 using this parabolic wave function is actually not too bad.

The fact that $\frac{d^2\psi}{dx^2}$ is discontinuous at the boundaries $x=\pm a$ doesn't affect the energy since $\psi=0$ at the boundaries, so the particle is never found there.