THE VARIATIONAL PRINCIPLE IN QUANTUM MECHANICS

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 7.1.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.2, Exercise 5.2.2a.

We've used the calculus of variations to derive the geodesic equation in general relativity, but a similar approach can be used in quantum mechanics to get an upper bound on the ground state energy for a given hamiltonian. The technique rests on the following theorem:

Theorem. *If ψ is any normalized function and H is a hamiltonian, then the ground state energy E_0 of this hamiltonian has an upper bound given by*

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

Although we don't know the eigenfunctions or eigenvalues of H, we do know that the eigenfunctions satisfy $H\psi_n = E_n\psi_n$ and form a complete orthonormal set, so we can expand ψ in terms of them:

$$\psi = \sum_n c_n\psi_n \tag{2}$$

Therefore

$$\langle\psi|H|\psi\rangle = \sum_{n,m} c_m^* c_n \langle\psi_m|H|\psi_n\rangle \tag{3}$$

$$= \sum_{n,m} c_m^* c_n E_n \langle\psi_m|\psi_n\rangle \tag{4}$$

$$= \sum_n |c_n|^2 E_n \tag{5}$$

Since $E_n \ge E_0$ for all n, we get

$$\langle\psi|H|\psi\rangle \ge E_0 \sum_n |c_n|^2 = E_0 \tag{6}$$

This theorem is usually applied by choosing the function ψ such that it depends on one or more parameters which can then be varied to find the minimum value for $\langle H\rangle$.

Example 1. We'll use a Gaussian trial function to get an upper bound on the ground state energy for the potential

$$V(x) = \alpha|x| \tag{7}$$

The trial function is

$$\psi = Ae^{-bx^2} \tag{8}$$

The parameter A is determined by normalization:

$$|A|^2 \int_{-\infty}^{\infty} e^{-2bx^2} dx = 1 \tag{9}$$

$$A = \left(\frac{2b}{\pi}\right)^{1/4} \tag{10}$$

We get

$$\langle H \rangle = \sqrt{\frac{2b}{\pi}} \int_{-\infty}^{\infty} \left[-\frac{\hbar^2}{2m} e^{-bx^2} \frac{d^2}{dx^2} \left(e^{-bx^2}\right) + e^{-2bx^2} \alpha |x| \right] dx \tag{11}$$

The integrand is an even function of x, so this is equivalent to

$$\langle H \rangle = 2\sqrt{\frac{2b}{\pi}} \int_{0}^{\infty} \left[-\frac{\hbar^2}{2m} e^{-bx^2} \frac{d^2}{dx^2} \left(e^{-bx^2}\right) + e^{-2bx^2} \alpha x \right] dx \tag{12}$$

$$= \frac{1}{2\sqrt{2\pi} m} \left(\hbar^2 b \sqrt{2\pi} + \frac{2\alpha m}{\sqrt{b}} \right) \tag{13}$$

where we did the integral using Maple.

We want to vary the parameter b to find the minimum of this expression, so we take the derivative and set it to zero:

$$\frac{d\langle H \rangle}{db} = \frac{1}{2\sqrt{2\pi} m} \left(\hbar^2 \sqrt{2\pi} - \frac{\alpha m}{b^{3/2}} \right) = 0 \tag{14}$$

$$b = \frac{(\alpha m)^{2/3}}{(2\pi)^{1/3} \hbar^{4/3}} \tag{15}$$

This gives the upper bound on E_0 as

$$\boxed{E_0 \le \frac{3(2\alpha\hbar)^{2/3}}{4(\pi m)^{1/3}}} \tag{16}$$

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Example 2. Now we'll use the potential

$$V(x) = \alpha x^4 \tag{17}$$

Doing the calculations yields (since the potential is again an even function):

$$\langle H\rangle = 2\sqrt{\frac{2b}{\pi}}\int_0^\infty \left[-\frac{\hbar^2}{2m}e^{-bx^2}\frac{d^2}{dx^2}\left(e^{-bx^2}\right)+e^{-2bx^2}\alpha x^4\right]dx \tag{18}$$

$$= \frac{1}{16}\frac{8\hbar^2 b^3+3\alpha m}{b^2 m} \tag{19}$$

$$= \frac{\hbar^2 b}{2m}+\frac{3\alpha}{16b^2} \tag{20}$$

Finding the parameter value that minimizes $\langle H\rangle$ we get

$$\frac{d\langle H\rangle}{db} = \frac{\hbar^2}{2m}-\frac{3\alpha}{8b^3}=0 \tag{21}$$

$$b = \frac{(6\alpha m)^{1/3}}{2\hbar^{2/3}} \tag{22}$$

$$E_0 \le \frac{3}{8}\left(\frac{6\hbar^4\alpha}{m^2}\right)^{1/3} \tag{23}$$

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