

VARIATIONAL PRINCIPLE IN QUANTUM MECHANICS

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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 1. *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*

$$E_0 \leq \langle \psi | H | \psi \rangle \equiv \langle H \rangle \quad (1)$$

Proof. 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:

$$\psi = \sum_n c_n \psi_n \quad (2)$$

Therefore

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

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

$$= \sum_n |c_n|^2 E_n \quad (5)$$

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

$$\langle \psi | H | \psi \rangle \geq E_0 \sum_n |c_n|^2 = E_0 \quad (6)$$

□

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

$$V(x) = \alpha|x| \quad (7)$$

The trial function is

$$\psi = Ae^{-bx^2} \quad (8)$$

The parameter A is determined by normalization:

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

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

We get

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

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

$$\langle H \rangle = 2\sqrt{\frac{2b}{\pi}} \int_0^{\infty} \left[-\frac{\hbar^2}{2m} e^{-bx^2} \frac{d^2}{dx^2} (e^{-bx^2}) + e^{-2bx^2} \alpha x \right] dx \quad (12)$$

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

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:

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

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

This gives the upper bound on E_0 as

$$E_0 \leq \frac{3(2\alpha\hbar)^{2/3}}{4(\pi m)^{1/3}} \quad (16)$$

Example 2. Now we'll use the potential

$$V(x) = \alpha x^4 \quad (17)$$

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

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

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

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

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

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

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

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

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