Γ XNH

PROBLEM 6: Variational approach

A particle with mass, m, moving in one dimension finds itself in a potential given by,

$$V = \infty \quad \text{for} \quad x < 0$$

and

$$V = \beta x^3 \quad \text{for} \quad x > 0$$

where β is a positive constant.

a) Find an approximation to the ground state energy, using the trial wavefunction

$$\Psi = 0 \quad \text{for} \quad x < 0$$

and

$$\Psi = Cxe^{-\alpha x} \quad \text{for} \quad x > 0.$$

where C and α are positive constants. (5 Points)

b) Would you expect the exact ground state energy to be less than your answer to part (a), or greater than it? Justify. (3 Points)

c) How would you go about finding an excited state in this system using the same approach? (2 Points)

Hint: $\int_0^\infty x^2 e^{-ax} = 2a^{-3}$, for $a > 0$.

(a)

We know that

$$E_{gs} \leq \langle \psi | H | \psi \rangle ,$$

where ψ is our normalized trial wavefunction and H is the Hamiltonian. For $x < 0$, we have

$$\psi = 0 ,$$

so the particle will not be found in this region. Thus, we focus on the region $x > 0$. The Hamiltonian is given by

$$H = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + \beta x^3 ,$$

and our trial wavefunction is

$$\psi(x) = C x e^{-\alpha x} ,$$

where α is our variational parameter. We want to normalize this wavefunction to begin our analysis. So

$$\int_0^\infty |\psi(x)|^2 \, dx = 1$$

$$C^2 \int_0^\infty x^2 e^{-2\alpha x} \, dx = 1 .$$

But, in general,

$$\int_0^\infty x^2 e^{-bx} = 2b^{-3} .$$

If we let $b = 2\alpha$, then

(a), cont'd...

$$C^2 \int_0^\infty x^2 e^{-2\alpha x}\, dx = 1$$

$$C^2 \left[2\,(2\alpha)^{-3} \right] = 1$$

$$C^2 \left[\frac{2}{8\alpha^3} \right] = 1$$

$$C^2 = 4\alpha^3$$

$$C = \sqrt{4\alpha^3}$$

and our trial wavefunction is

$$\psi(x) = \sqrt{4\alpha^3}\, x\, e^{-\alpha x}.$$

Now we want to find the expectation value of the Hamiltonian.

$$\langle \psi | H | \psi \rangle = \int_0^\infty \sqrt{4\alpha^3}\, x e^{-\alpha x} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \beta x^3 \right) \sqrt{4\alpha^3}\, x e^{-\alpha x}\, dx$$

$$= 4\alpha^3 \int_0^\infty x e^{-\alpha x} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \beta x^3 \right) x e^{-\alpha x}\, dx$$

$$= 4\alpha^3 \left[\int_0^\infty x e^{-\alpha x} \beta x^3 x e^{-\alpha x}\, dx - \frac{\hbar^2}{2m} \int_0^\infty x e^{-\alpha x} \frac{d^2}{dx^2}\left(x e^{-\alpha x} \right) dx \right]$$

$$= 4\alpha^3 \left[\beta \int_0^\infty x^5 e^{-2\alpha x}\, dx - \frac{\hbar^2}{2m} \int_0^\infty x e^{-\alpha x} \frac{d^2}{dx^2}\left(x e^{-\alpha x} \right) dx \right]$$

We know, in general, that

$$\int_0^\infty x^n e^{-bx} = \frac{n!}{b^{n+1}} \qquad (n = 0, 1, 2, \ldots)$$

(a), cont'd...

So

$$\int_0^\infty x^5 e^{-2\alpha x}\,dx = \frac{5!}{(2\alpha)^6} = \frac{15}{8\alpha^6},$$

and

$$\langle\psi|H|\psi\rangle = 4\alpha^3\left[\frac{15\beta}{8\alpha^6} - \frac{\hbar^2}{2m}\int_0^\infty xe^{-\alpha x}\frac{d^2}{dx^2}\left(xe^{-\alpha x}\right)dx\right].$$

We have

$$\frac{d}{dx}\left(xe^{-\alpha x}\right) = e^{-\alpha x} - \alpha x e^{-\alpha x}$$
$$= (1-\alpha x)e^{-\alpha x}$$

$$\frac{d^2}{dx^2}\left(xe^{-\alpha x}\right) = -\alpha e^{-\alpha x} - \alpha\left(e^{-\alpha x} - \alpha x e^{-\alpha x}\right)$$
$$= -2\alpha e^{-\alpha x} + \alpha^2 x e^{-\alpha x},$$

so

$$\int_0^\infty xe^{-\alpha x}\left(-2\alpha e^{-\alpha x} + \alpha^2 x e^{-\alpha x}\right)dx = \int_0^\infty\left(-2\alpha x e^{-2\alpha x} + \alpha^2 x^2 e^{-2\alpha x}\right)dx$$
$$= -2\alpha\int_0^\infty xe^{-2\alpha x}\,dx + \alpha^2\int_0^\infty x^2 e^{-2\alpha x}\,dx$$
$$= -2\alpha\left(\frac{1}{4\alpha^2}\right) + \alpha^2\left(\frac{1}{4\alpha^3}\right)$$
$$= -\frac{1}{4\alpha}$$

(a), cont'd...

Then

$$\langle\psi|H|\psi\rangle = 4\alpha^3\left[\frac{15\beta}{8\alpha^6} - \frac{\hbar^2}{2m}\left(-\frac{1}{4\alpha}\right)\right]$$
$$= \frac{15\beta}{2\alpha^3} + \frac{\hbar^2\alpha^2}{2m}.$$

Now we need to minimize this expectation value with respect to α.

$$\frac{d\langle H\rangle}{d\alpha} = 0$$

$$\frac{d}{d\alpha}\left(\frac{15\beta}{2\alpha^3} + \frac{\hbar^2\alpha^2}{2m}\right) = 0$$

$$-\frac{45\beta}{2\alpha^4} + \frac{\hbar^2\alpha}{m} = 0$$

$$\frac{\hbar^2\alpha}{m} = \frac{45\beta}{2\alpha^4}$$

$$\alpha^5 = \frac{45\beta m}{2\hbar^2}$$

$$\alpha = \left(\frac{45\beta m}{2\hbar^2}\right)^{1/5}.$$

Plugging this back in...

$$\langle H\rangle = \frac{15\beta}{2}\cdot\left(\frac{45\beta m}{2\hbar^2}\right)^{-3/5} + \frac{\hbar^2}{2m}\left(\frac{45\beta m}{2\hbar^2}\right)^{2/5}$$
$$= \frac{15\beta}{2}\left(\frac{2\hbar^2}{45\beta m}\right)^{3/5} + \frac{\hbar^2}{2m}\left(\frac{45\beta m}{2\hbar^2}\right)^{2/5}$$

and

$$\boxed{E_{gs} \leq \frac{15\beta}{2}\left(\frac{2\hbar^2}{45\beta m}\right)^{3/5} + \frac{\hbar^2}{2m}\left(\frac{45\beta m}{2\hbar^2}\right)^{2/5}}.$$

(b)

I would expect the exact ground state energy to be less than my result in (a) since the variational method yields an upper bound for E_{gs}.

We know

$$\langle H \rangle = |c_{gs}|^2 E_{gs} + \sum_{n \neq 0} |c_n|^2 E_n .$$

But the ground state has the lowest energy eigenvalue by definition, so

$$|c_{gs}|^2 E_{gs} + \sum_{n\neq 0} |c_n|^2 E_n \geq |c_{gs}|^2 E_{gs} + \sum_{n \neq 0} |c_n|^2 E_{gs} = E_{gs}$$

Thus,

$$\langle H \rangle \geq E_{gs} .$$

(c)

If we let ψ be the trial wavefunction and ψ_{gs} the ground state wavefunction, where $\langle \psi | \psi_{gs} \rangle = 0$, then

$$\langle H \rangle = \langle \psi | H | \psi \rangle \geq E_1 ,$$

where E_1 is the first excited energy. We know

$$\langle \psi | H | \psi \rangle = \left(\sum_n c_n^* \langle n | \right) H \left(\sum_m c_m | m \rangle \right)$$

$$= \sum_{n,m} c_n^* c_m \langle n | H | m \rangle$$

$$= \sum_{n,m} c_n^* c_m \langle n | E_m | m \rangle$$

(c), cont'd...

$$\langle\Psi|H|\Psi\rangle = \sum_{n,m} c_n^* c_m E_m \langle n|m\rangle$$

$$= \sum_n E_n |c_n|^2,$$

but since $\langle\Psi|\Psi_0\rangle = 0$, we have

$$\langle\Psi|H|\Psi\rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n \geq |c_1|^2 E_1 + \sum_{n\neq 1} |c_n|^2 E_1 = E_1 .$$

Thus,

$$\langle H\rangle \geq E_1 .$$