

Spring 1999 Solution 8

Andrew Collette

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1 Outline

This is a "cookbook" variational problem. We are given a Hamiltonian and a trial wave function ϕ with a parameter μ , and want to use it to estimate the energy of a state. The procedure is as follows:

- Normalize the trial wave function
- Find an expression for $E(\mu)$ (i.e. $\langle\phi(\mu)|H|\phi(\mu)\rangle$)
- Find the value of μ which corresponds to an extremum of E
- Evaluate E at the determined μ

See also Abers §7.5 and §3.2.

2 Solution

2.1 Normalization

Enforce the condition

$$1 = \langle\phi|\phi\rangle = N^2 \int_{-\infty}^{\infty} x^2 e^{-2\mu x} dx \quad (1)$$

$$\frac{1}{N^2} = \int_0^{\infty} x^2 e^{-2\mu x} = \frac{2}{(2\mu)^3} = \frac{1}{4\mu^3} \quad (2)$$

So

$$N^2 = 4\mu^3 \quad N = 2\mu^{3/2} \quad (3)$$

2.2 Finding $\langle\phi(\mu)|H|\phi(\mu)\rangle$

The wave function is identically zero for $x \leq 0$, so we'll only worry about $x > 0$. The Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \quad (4)$$

We want to find $\langle\phi|H|\phi\rangle$; to make it easier, split it up into

$$\langle\phi|H|\phi\rangle = \langle\phi|\frac{p^2}{2m}|\phi\rangle + \langle\phi|\frac{1}{2}m\omega^2 x^2|\phi\rangle \quad (5)$$

The kinetic energy term is:

$$\langle \phi | \frac{p^2}{2m} | \phi \rangle = 4\mu^3 \int_0^\infty x e^{-\mu x} \left(-\frac{1}{2m}\right) \frac{\partial^2}{\partial^2 x} (x e^{-\mu x}) dx \quad (6)$$

The derivative is

$$\frac{\partial^2}{\partial^2 x} (x e^{-\mu x}) = \frac{\partial}{\partial x} (e^{-\mu x} - \mu x e^{-\mu x}) = -(2\mu e^{-\mu x} - \mu^2 x e^{-\mu x}) \quad (7)$$

so

$$\langle \phi | \frac{p^2}{2m} | \phi \rangle = \frac{2\mu^3}{m} \int_0^\infty x e^{-\mu x} (2\mu e^{-\mu x} - \mu^2 x e^{-\mu x}) dx \quad (8)$$

$$= \frac{2\mu^4}{m} \int_0^\infty (2x e^{-2\mu x} - \mu x^2 e^{-2\mu x}) dx \quad (9)$$

$$= \frac{2\mu^4}{m} \left(2 \frac{1}{(2\mu)^2} - \mu \left(\frac{2}{(2\mu)^3} \right) \right) \quad (10)$$

$$= \frac{\mu^2}{2m} \quad (11)$$

The potential energy term is a bit simpler:

$$\langle \phi | \frac{1}{2} m \omega^2 x^2 | \phi \rangle = 4\mu^3 \int_0^\infty x e^{-\mu x} \left(\frac{1}{2} m \omega^2 x^2 \right) x e^{-\mu x} dx \quad (12)$$

$$= 2\mu^3 m \omega^2 \int_0^\infty x^4 e^{-2\mu x} dx \quad (13)$$

$$= \mu^3 m \omega^2 \left(\frac{2 \cdot 4 \cdot 3 \cdot 2 \cdot 1}{(2\mu)^5} \right) \quad (14)$$

$$= \mu^3 m \omega^2 \left(\frac{2^4 \cdot 3}{2^5 \mu^5} \right) \quad (15)$$

$$= \frac{3}{2} m \omega^2 \frac{1}{\mu^2} \quad (16)$$

2.3 Determine energy of the state

Now that we have $E(\mu)$ we can find the extrema. The total expectation value of H is:

$$\langle \phi | H | \phi \rangle = \frac{\mu^2}{2m} + \frac{3}{2} m \omega^2 \frac{1}{\mu^2} \quad (17)$$

So do

$$\frac{\partial}{\partial \mu} \left(\frac{\mu^2}{2m} + \frac{3}{2} m \omega^2 \frac{1}{\mu^2} \right) = 0 \quad (18)$$

$$\frac{\mu}{m} - \frac{3m\omega^2}{\mu^3} = 0 \quad (19)$$

$$\mu^4 = 3m^2\omega^2 \quad \mu^2 = \sqrt{3}m\omega \quad (20)$$

And the value of the energy at the specified value of μ is:

$$E = \frac{\sqrt{3}m\omega}{2m} + \frac{3m\omega^2}{2} \frac{1}{\sqrt{3}m\omega} \quad (21)$$

$$= \frac{\sqrt{3}}{2}\omega + \frac{\sqrt{3}}{2}\omega \quad (22)$$

$$= \sqrt{3}\omega \approx 1.7\omega \quad (23)$$

2.4 Exact ground-state energy

For the region $x > 0$, the problem is just the simple harmonic oscillator. The general solutions to the time-independent Schrodinger equation will be the same. Solutions go like (Abers 3.73)

$$\phi_n(x) \sim \left(x - \frac{d}{dx}\right)^n e^{-x^2} \quad (24)$$

The difference here is the boundary condition $\phi = 0$ for $x \leq 0$. The ground state of the SHO (even) has the wave function (Abers 3.70):

$$\phi_0(x) = \left(\frac{m\omega}{\pi}\right)^{1/4} e^{-\frac{m\omega x^2}{2}} \quad (25)$$

which does not satisfy the boundary conditions. The next lowest state ($\phi_1 \sim xe^{x^2}$) (odd) does work. The energy of this state is

$$E_n = \left(n + \frac{1}{2}\right)\omega \quad E_1 = \frac{3}{2}\omega = 1.5\omega \quad (26)$$

So our variational solution of $\sqrt{3}\omega$ was not that far off.