Worksheet 6B Solutions

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1. The Hamiltonian for the harmonic oscillator is:

$$\hat{H} = -\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + \frac{kx^2}{2}$$
(1)

We are asked to use the trial function

$$|\psi(x)\rangle = \frac{1}{1+\beta x^2} \tag{2}$$

to find an approximate energy:

$$E_{\phi} = \frac{\langle \phi | \hat{H} | \phi \rangle}{\langle \phi | \phi \rangle} \tag{3}$$

(a) We evaluate the denominator of the expression, $\langle \phi | \phi \rangle$ via:

$$\langle \phi | \phi \rangle = \int_{-\infty}^{\infty} \frac{dx}{(1+\beta x^2)^2} = \frac{\pi}{2\beta^{1/2}} \tag{4}$$

- (b) The function is smooth as both it and its first derivative are finite. The limits of the integral are negative to positive infinity.
- (c) The wavefunction $|\phi\rangle$ is not normalized. Normalization is inherent in the equation (1), with the denominator being the normalization constant squared.
- 2. We are required to evaluate the numerator, $\langle \phi | \hat{H} | \phi \rangle$
 - (a) This requires us to evaluate the separate terms:

$$\langle \phi | -\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + \frac{kx^2}{2} |\phi\rangle = \langle \phi | -\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} |\phi\rangle + \langle \phi | \frac{kx^2}{2} |\phi\rangle \tag{5}$$

$$\langle \phi | -\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} | \phi \rangle = -\frac{\hbar^2}{2\mu} \left(\int_{-\infty}^{\infty} \frac{2\beta dx}{(1+\beta x^2)^2} + \int_{-\infty}^{\infty} \frac{4\beta x^2 dx}{(1+\beta x^2)^4} \right)$$
(6)

$$\langle \phi | \frac{kx^2}{2} | \phi \rangle = \frac{k}{2} \int_{-\infty}^{\infty} \frac{x^2 dx}{(1+\beta x^2)} \tag{7}$$

We will make use of the following integrals:

$$\int_{-\infty}^{\infty} \frac{dx}{(1+\beta x^2)^2} = \frac{\pi}{2\beta^{1/2}}$$
(8)

$$\int_{-\infty}^{\infty} \frac{x^2 dx}{(1+\beta x^2)^2} = \frac{\pi}{2\beta^{3/2}}$$
(9)

$$\int_{-\infty}^{\infty} \frac{x^2 dx}{(1+\beta x^2)^4} = \frac{\pi}{16\beta^{3/2}}$$
(10)

Using relations (8) and (10) to simplify (6) and relation (9) to simplify (7) the numerator terms become:

$$\langle \phi | -\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + \frac{kx^2}{2} | \phi \rangle = -\frac{\hbar^2}{2\mu} \left(2\beta \left(\frac{\pi}{2\beta^{1/2}}\right) + 4\beta \left(\frac{\pi}{16\beta^{3/2}}\right) \right) + \frac{k}{2} \left(\frac{\pi}{16\beta^{3/2}}\right) \tag{11}$$

Putting together results (11) and (4), so multiplying the above terms by $\frac{2\beta^{1/2}}{\pi}$ we finally have:

$$E_{\phi} = \frac{\langle \phi | \hat{H} | \phi \rangle}{\langle \phi | \phi \rangle} = -\frac{\hbar^2}{\mu} \left(\beta + \frac{1}{8\beta} \right) + \frac{k}{32\beta} = -\frac{\hbar^2}{\mu} \beta + \left(\frac{k}{32} - \frac{\hbar^2}{8\mu} \right) \frac{1}{\beta}$$
(12)