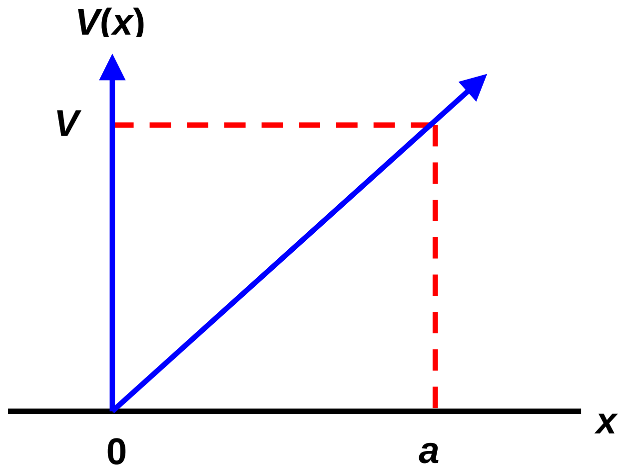
PH30030: Quantum Mechanics   Problems Sheet 5 Solutions

1. The Hamiltonian $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{V_0 x}{a}$ for $x > 0$.

So, $\hat{H}\psi = -\frac{\hbar^2}{2m}A\left(-2\lambda + \lambda^2 x\right)e^{-\lambda x} + A\frac{V_0}{a}x^2 e^{-\lambda x}$



The expectation value

$$\langle \hat{H} \rangle = \langle \hat{T} \rangle + \langle \hat{V} \rangle$$

$$= -A^2\frac{\hbar^2}{2m}\int_0^\infty \left(-2\lambda x e^{-2\lambda x} + \lambda^2 x^2 e^{-2\lambda x}\right)dx + A^2\frac{V_0}{a}\int_0^\infty x^3 e^{-2\lambda x}dx = A^2\frac{\hbar^2}{2m}\left(\frac{1}{2\lambda} - \frac{1}{4\lambda}\right) + A^2\frac{V_0}{a}\frac{3}{8\lambda^4}$$

Normalisation: $A^2\int_0^\infty x^2 e^{-2\lambda x}dx = A^2\frac{2}{(2\lambda)^3} = 1 \quad \Rightarrow \quad A^2 = 4\lambda^3$.

So, $\langle \hat{H} \rangle = \frac{\hbar^2\lambda^2}{2m} + \frac{3V_0}{2a}\frac{1}{\lambda}$. Minimising with respect to λ

$$\frac{d\langle \hat{H} \rangle}{d\lambda} = \left(\frac{\hbar^2\lambda}{m} - \frac{3V_0}{2a}\frac{1}{\lambda^2}\right) = 0 \quad \Rightarrow \quad \lambda^3 = \frac{3mV_0}{2\hbar^2 a}$$

Hence, $\langle \hat{H} \rangle_{\min} = \frac{\hbar^2}{2m}\left(\frac{3mV_0}{2\hbar^2 a}\right)^{\frac{2}{3}} + \frac{3V_0}{2a}\left(\frac{2\hbar^2 a}{3mV_0}\right)^{\frac{1}{3}} = \left(\frac{\hbar^2 V_0^2}{ma^2}\right)^{\frac{1}{3}}\left[\left(\frac{9}{8\times 4}\right)^{\frac{1}{3}} + \left(\frac{9}{4}\right)^{\frac{1}{3}}\right]$

$$= \left(\frac{\hbar^2 V_0^2}{ma^2}\right)^{\frac{1}{3}}\left(\frac{9}{4}\right)^{\frac{1}{3}}\left[\frac{1+8^{\frac{1}{3}}}{8^{\frac{1}{3}}}\right] = \frac{3}{2}\left(\frac{9}{4}\right)^{\frac{1}{3}}\left(\frac{\hbar^2 V_0^2}{ma^2}\right)^{\frac{1}{3}} = \left(\frac{243}{32}\frac{\hbar^2 V_0^2}{ma^2}\right)^{\frac{1}{3}}$$

and the ground state energy $E_{\text{ground}} \le \left(\frac{243}{32}\frac{\hbar^2 V_0^2}{ma^2}\right)^{\frac{1}{3}}$.

2. For the infinite square well, the wavefunction is zero outside the box and the boundary conditions require that $\psi(x=0)=\psi(x=a)=0$. The trial wavefunction must satisfy these boundary conditions. The ground state wavefunction is not expected to have any nodes interior to the boundary points. So the trial wavefunction should also satisfy this requirement. A simple function satisfying these properties is the parabola

$$\psi(x)=Ax(a-x) \quad \text{for} \quad 0\le x\le a \quad \text{with} \quad \psi(x)=0 \text{ outside the box.}$$

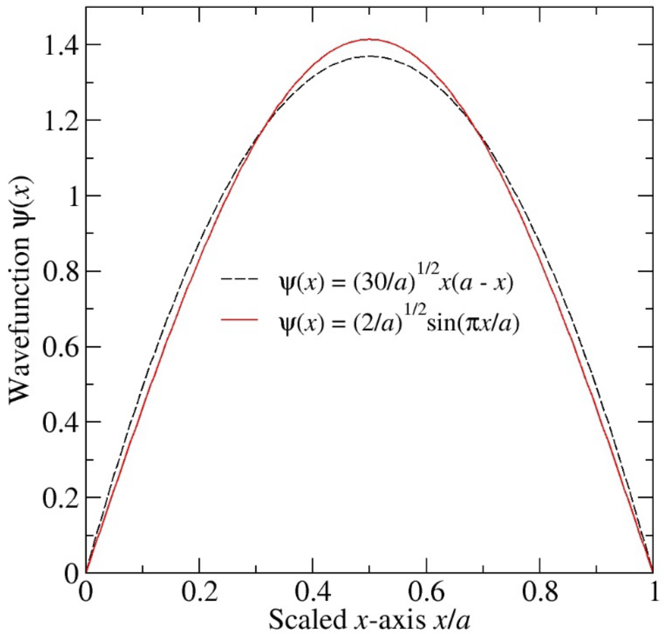
The Hamiltonian $\hat{H}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$, so $\hat{H}\psi=+\frac{\hbar^2}{m}A$. The expectation value

$$\langle\hat{H}\rangle=\int_0^a\psi^*\hat{H}\psi dx=A^2\frac{\hbar^2}{m}\int_0^a\left(ax-x^2\right)dx=A^2\frac{\hbar^2}{m}\left[\frac{ax^2}{2}-\frac{x^3}{3}\right]_0^a=A^2\frac{\hbar^2a^3}{6m}$$

which has no adjustable parameters.

Normalisation: $A^2\int_0^a x^2(a-x)^2dx=A^2\left[\frac{a^2x^3}{3}-\frac{ax^4}{2}+\frac{x^5}{5}\right]_0^a=A^2\frac{a^5}{30}=1 \quad\Rightarrow\quad A^2=\frac{30}{a^5}$

So the ground state energy $E_{\text{ground}}\le\frac{5\hbar^2}{ma^2}$. From the full solution of the TISE for the 1D infinite square well we know that $E_{\text{ground}}=\frac{\hbar^2\pi^2}{2ma^2}$, i.e., the discrepancy in the estimated ground state energy is $\frac{5-\left(\pi^2/2\right)}{5}=0.013$ or 1.3%. The normalised trial wavefunction $\psi(x)=\left(\frac{30}{a}\right)^{\frac{1}{2}}x(a-x)$ closely resembles the actual ground state wavefunction: -



3. Normalisation: $A^2\int_{-\infty}^{\infty} e^{-2bx^2}dx = A^2\left(\frac{\pi}{2b}\right)^{\frac{1}{2}} = 1 \quad \Rightarrow \quad A = \left(\frac{2b}{\pi}\right)^{\frac{1}{4}}$

The expectation value $\langle \hat{H} \rangle = \langle \hat{T} \rangle + \langle \hat{V} \rangle$. Now

$$\langle \hat{T} \rangle = -\frac{\hbar^2}{2m}A^2\int_{-\infty}^{\infty} e^{-bx^2}\frac{d^2}{dx^2}\left(e^{-bx^2}\right)dx = -\frac{\hbar^2}{2m}A^2\int_{-\infty}^{\infty}\left(-2be^{-2bx^2} + 4b^2x^2e^{-2bx^2}\right) = \frac{\hbar^2 b}{2m}$$

and

$$\langle \hat{V} \rangle = \frac{1}{2}m\omega^2 A^2\int_{-\infty}^{\infty} e^{-2bx^2}x^2dx = \frac{m\omega^2}{8b}$$

so

$$\langle \hat{H} \rangle = \frac{\hbar^2 b}{2m} + \frac{m\omega^2}{8b}$$

Minimising with respect to b: $\frac{d\langle \hat{H} \rangle}{db} = \frac{\hbar^2}{2m} - \frac{m\omega^2}{8b^2} = 0 \quad \Rightarrow \quad b = \frac{m\omega}{2\hbar}$

So the ground state energy $E_{\text{ground}} \le \langle \hat{H} \rangle_{\min} = \frac{1}{2}\hbar\omega$. In this case, the variational method delivers the actual ground state energy because the trial wavefunction $\psi(x) = Ae^{-bx^2} = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}\exp\left(-\frac{m\omega x^2}{2\hbar}\right)$ is exact. The Gaussian is easy to work with, so it is a popular trial wavefunction, even when it bears little resemblance to the ground state.

4. The Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \alpha\delta(x).$$

The normalisation constant of the Gaussian trial wavefunction follows from question 3, i.e., $A = \left(\frac{2b}{\pi}\right)^{\frac{1}{4}}$, and the expectation value of the kinetic energy was also calculated in question 3, i.e., $\langle \hat{T} \rangle = \frac{\hbar^2 b}{2m}$. The expectation value for the potential energy

$$\langle \hat{V} \rangle = -\alpha A^2\int_{-\infty}^{\infty} e^{-2bx^2}\delta(x)dx = -\alpha A^2 = -\alpha\left(\frac{2b}{\pi}\right)^{\frac{1}{2}}.$$

So the expectation value of the Hamiltonian $\langle \hat{H} \rangle = \langle \hat{T} \rangle + \langle \hat{V} \rangle = \frac{\hbar^2 b}{2m} - \alpha\left(\frac{2b}{\pi}\right)^{\frac{1}{2}}$. Minimising with respect to b gives

$$\frac{d\left\langle \hat{H}\right\rangle}{db} = \frac{\hbar^2}{2m} - \frac{\alpha}{\pi}\left(\frac{2b}{\pi}\right)^{-\frac{1}{2}} = 0 \quad \Rightarrow \quad b = \frac{2m^2\alpha^2}{\pi\hbar^4}$$ such that $\left\langle \hat{H}\right\rangle_{\min} = -\frac{m\alpha^2}{\pi\hbar^2}$ where the negative sign indicates a bound state. Hence the ground state energy $E_{\text{ground}} \le \left\langle \hat{H}\right\rangle_{\min} = -\frac{m\alpha^2}{\pi\hbar^2}$.

The full solution of the TISE (e.g. Griffiths and Schroeter 2018) shows that there is only one bound state described by the wavefunction $\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2}$ with energy eigenvalue $E = -\frac{m\alpha^2}{2\hbar^2}$. The use of a trial Gaussian wavefunction overestimates the ground state energy because $\pi > 2$, i.e., it is less negative.

5. The Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \alpha x^4 .$$

The normalisation constant of the Gaussian trial wavefunction follows from question 3, i.e., $A = \left(\frac{2b}{\pi}\right)^{\frac{1}{4}}$, and the expectation value of the kinetic energy was also calculated in question 3, i.e., $\left\langle \hat{T}\right\rangle = \frac{\hbar^2 b}{2m}$. The expectation value for the potential energy

$$\left\langle \hat{V}\right\rangle = \alpha A^2 \int_{-\infty}^{\infty} x^4 e^{-2bx^2} dx = \alpha A^2 \frac{3}{4}\left[\frac{\pi}{(2b)^5}\right]^{\frac{1}{2}} = \frac{3\alpha}{16}\frac{1}{b^2} .$$

So the expectation value of the Hamiltonian $\left\langle \hat{H}\right\rangle = \left\langle \hat{T}\right\rangle + \left\langle \hat{V}\right\rangle = \frac{\hbar^2 b}{2m} + \frac{3\alpha}{16}\frac{1}{b^2}$. Minimising with respect to *b* gives

$$\frac{d\left\langle \hat{H}\right\rangle}{db} = \frac{\hbar^2}{2m} - \frac{3\alpha}{8}\frac{1}{b^3} = 0 \quad \Rightarrow \quad b = \left(\frac{3\alpha m}{4\hbar^2}\right)^{\frac{1}{3}}$$ such that

$$\left\langle \hat{H}\right\rangle_{\min} = \frac{\hbar^2}{2m}\left(\frac{3\alpha m}{4\hbar^2}\right)^{\frac{1}{3}} + \frac{3\alpha}{16}\left(\frac{4\hbar^2}{3\alpha m}\right)^{\frac{2}{3}} = \left(\frac{\hbar^6}{8m^3}\frac{3\alpha m}{4\hbar^2}\right)^{\frac{1}{3}} + \left(\frac{3^3\alpha^3}{16^3}\frac{16\hbar^4}{3^2\alpha^2 m^2}\right)^{\frac{1}{3}}$$

$$= \left(\frac{3\hbar^4\alpha}{32m^2}\right)^{\frac{1}{3}}\left[1 + \left(\frac{1}{8}\right)^{\frac{1}{3}}\right] = \frac{3}{2}\left(\frac{3\hbar^4\alpha}{32m^2}\right)^{\frac{1}{3}} = \frac{3}{4}\left(\frac{3\hbar^4\alpha}{4m^2}\right)^{\frac{1}{3}}$$

Hence the ground state energy $E_{\text{ground}} \le \left\langle \hat{H}\right\rangle_{\min} = \frac{3}{4}\left(\frac{3\hbar^4\alpha}{4m^2}\right)^{\frac{1}{3}}$.