NTNU – Trondheim
Norwegian University of
Science and Technology

NTNU, Department of Physics

FY2045 Solutions Problem set 11 fall 2023

Professor Jens O. Andersen, updated by Henning G. Hugdal

November 10, 2023

Problem 1

a) The normalization constant is determined by

$$1 = \int d\mathbf{r}\ |\psi(r)|^2 = 4\pi|A|^2 \int_0^\infty dr\ r^3 e^{-2\alpha r}, \tag{1}$$

where the angular integration gives only a factor 4π since ψ is a function of r only. We calculate the integral using derivation under the integral sign,

$$1 = 4\pi|A|^2 \left(-\frac{1}{2}\frac{\partial}{\partial\alpha}\right)^3 \int_0^\infty e^{-2\alpha r} = 4\pi|A|^2 \left(-\frac{1}{2}\frac{\partial}{\partial\alpha}\right)^3 \frac{1}{2\alpha} = 4\pi|A|^2 \frac{3}{8\alpha^4}. \tag{2}$$

Choosing A real and positive, we get

$$A = \sqrt{\frac{2}{3\pi}}\alpha^2. \tag{3}$$

b) The expectation value of the kinetic energy can be expressed as the integral

$$\langle T\rangle = -\frac{\hbar^2}{2m}\int d\mathbf{r}\ \psi^*\nabla^2\psi. \tag{4}$$

For a spherically symmetric function $\psi(r)$, the Laplace operator reduces to

$$\begin{aligned}
\nabla^2\psi = \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) &= \frac{A}{2r^2}\frac{d}{dr}\left(1-2\alpha r\right)r^{3/2}e^{-\alpha r} \\
&= \frac{A}{2r^2}\left[-2\alpha r^{3/2}+\frac{3}{2}r^{1/2}-3\alpha r^{3/2}-\alpha r^{3/2}+2\alpha^2 r^{5/2}\right]e^{-\alpha r} \\
&= \frac{A}{4r^2}\left[3\sqrt{r}-12\alpha r^{3/2}+4\alpha^2 r^{5/2}\right]e^{-\alpha r}.
\end{aligned} \tag{5}$$

Inserted into the equation for $\langle T\rangle$, we get

$$\begin{aligned}
\langle T\rangle &= -\frac{4\pi\hbar^2 A^2}{2m}\int_0^\infty dr\ r^2\sqrt{r}e^{-\alpha r}\frac{1}{4r^2}\left[3\sqrt{r}-12\alpha r^{3/2}+4\alpha^2 r^{5/2}\right]e^{-\alpha r} \\
&= -\frac{\pi\hbar^2 A^2}{2m}\int_0^\infty dr\ \left[3r-12\alpha r^2+4\alpha^2 r^3\right]e^{-2\alpha r}.
\end{aligned} \tag{6}$$

Using the same integration trick as above, we get

$$\langle T\rangle = -\frac{\pi\hbar^2}{2m}\frac{2\alpha^4}{3\pi}\cdot\left(-\frac{3}{4\alpha^2}\right) = \frac{\hbar^2\alpha^2}{4m^2}. \tag{7}$$

c) The expectation value of the potential energy is

$$\langle V\rangle = -k\int d\mathbf{r}\ \frac{|\psi|^2}{r} = -4\pi k A^2\int_0^\infty dr\ r^2 e^{-2\alpha r}. \tag{8}$$

Again, using the same integration trick, we get

$$\langle V\rangle - 4\pi k\frac{2\alpha^4}{3\pi}\frac{1}{4\alpha^3} = -\frac{2k\alpha}{3} = -\frac{4}{3}\frac{\hbar^2}{2m}\frac{\alpha}{a_0}, \tag{9}$$

where we have used $k = \frac{e^2}{4\pi\epsilon_0} = \frac{\hbar^2}{ma_0}$.

d) The expectation value for the total energy is

$$\langle E\rangle = \langle T\rangle + \langle V\rangle = \frac{\hbar^2}{2m}\left[\frac{\alpha^2}{2}-\frac{4\alpha}{3a_0}\right]. \tag{10}$$

We minimize the expectation value with respect to α,

$$0 = \frac{d}{d\alpha}\langle E\rangle \propto \alpha - \frac{4}{3a_0} \qquad \Rightarrow \underline{\alpha_{\text{min}} = \frac{4}{3a_0}}. \tag{11}$$

Inserted back into the expectation value for the energy, we find

$$\underline{\langle E\rangle_{\text{min}} = -\frac{8}{9}\frac{\hbar^2}{2ma_0^2} = \frac{8}{9}E_0^{\text{exact}}} > E_0^{\text{exact}}, \tag{12}$$

which is slightly higher than the true value.

Problem 2

a) The condition $V(x) = \infty$ for $x \leq 0$ requires that $\psi(0) = 0$. This means that for $x > 0$, the wavefunctions are simply described by those of the 1D harmonics oscillator *and* $\psi(0) = 0$. Hence, the eigenfunctions are the "odd" ($n = 1, 3, 5, \dots$) eigenfunctions of the 1D harmonics oscillator and the ground state ($n = 1$) gives

$$E_0 = \hbar\omega \left(n + \frac{1}{2}\right)\bigg|_{n=1} = \frac{3}{2}\hbar\omega. \tag{13}$$

b) The expectation value of the energy is given by

$$\langle H \rangle = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}. \tag{14}$$

In what follows, the constant C will cancel out. We find

$$\langle H \rangle = \frac{\int_0^\infty dx\ xe^{-\alpha x} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2\right) xe^{-\alpha x}}{\int_0^\infty dx\ x^2 e^{-2\alpha x}}. \tag{15}$$

In the first integral, we need to compute

$$\frac{d^2}{dx^2}(xe^{-\alpha x}) = (-2\alpha + \alpha^2 x)e^{-\alpha x}. \tag{16}$$

Hence, we have

$$\langle H \rangle = \frac{\int_0^\infty dx\ \left[\frac{\hbar^2}{2m}(2\alpha x - \alpha^2 x^2) + \frac{1}{2}m\omega^2 x^4\right) e^{-2\alpha x}}{\int_0^\infty dx\ x^2 e^{-2\alpha x}}. \tag{17}$$

All the integrals are of the type

$$\int_0^\infty dx\ x^n e^{-2\alpha x}, \tag{18}$$

which can be solve using the same trick as in Problem 1, using integration by parts, or looked up in a formula collection. The result is

$$\langle H \rangle = \frac{\hbar^2}{2m}\alpha^2 + \frac{3}{2}m\omega^2 \frac{1}{\alpha^2}. \tag{19}$$

To find the minimum, we differentiate:

$$0 = \frac{d}{d\alpha}\langle H \rangle = \frac{\hbar^2}{m}\alpha - 3m\omega^2 \frac{1}{\alpha^3} \quad \Rightarrow \alpha_{\text{min}}^4 = \frac{3m^2\omega^2}{\hbar^2}. \tag{20}$$

Inserted into the expression for $\langle H \rangle$, we get

$$\langle H \rangle_{\text{min}} = \sqrt{3}\hbar\omega \approx 1.732\hbar\omega > 1.5\hbar\omega. \tag{21}$$

Hence, the approximation is reasonable, but not especially good.