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Assignment #2

3.13

$$\left(-\frac{\hbar^2}{2m_0}\nabla^2 + V\right)\psi = i\hbar\frac{\partial}{\partial t}\psi \quad (\text{T.D.S.E.})$$

where $\alpha = \dfrac{4\hbar\pi^2}{2m_0L_z^2}$ & $\beta = \dfrac{2\pi}{L_z}$

ii) $e^{i\left(\frac{4\hbar\pi^2}{2m_0L_z^2}\right)t}\sin\left(\frac{2\pi}{L_z}z\right) = \psi(z,t) = e^{i\alpha t}\sin(\beta z)$

Sign on time component is wrong. $\rightarrow$ Because of this, it will not be a solution.

$$\frac{\partial\psi}{\partial t} = i\alpha e^{i\alpha t}\sin(\beta z) \qquad \nabla\psi = e^{i\alpha t}\beta\cos(\beta z) \rightarrow \nabla^2\psi = e^{i\alpha t}(-\beta^2\sin(\beta z))$$
$$= -e^{i\alpha t}\beta^2\sin(\beta z)$$

$$-\frac{\hbar^2}{2m_0}\left(-e^{-i\alpha t}\sin(\beta z)\beta^2\right) + Ve^{i\alpha t}\sin(\beta z) = i\hbar\left(i\alpha e^{i\alpha t}\sin(\beta z)\right)$$

$$\frac{\hbar^2}{2m_0}\beta^2\cancel{e^{i\alpha t}}\cancel{\sin(\beta z)} + V\cancel{e^{i\alpha t}}\cancel{\sin(\beta z)} = -\hbar\alpha\cancel{e^{i\alpha t}}\cancel{\sin(\beta z)}$$

$$\frac{\hbar^2}{2m_0}\left(\frac{2\pi}{L_z}\right)^2 + V = -\frac{4\hbar^2\pi^2}{2m_0L_z^2}$$

– when $V=0$ –

$$\frac{4\hbar^2\pi^2}{2m_0L_z^2} = -\frac{4\hbar^2\pi^2}{2m_0L_z^2}$$

$1 = -1$ Not a solution

iv)

$$\Psi(z,t) = 2e^{-i\left(\frac{\hbar\pi^2}{2m_0L_z^2}\right)t}\sin\left(\frac{\pi}{L_z}z\right) - ie^{-i\left(\frac{9\hbar\pi^2}{2m_0L_z^2}\right)t}\sin\left(\frac{3\pi}{L_z}z\right)$$

Linear combination of two solutions, so also a solution.

$$\alpha = \frac{\hbar\pi^2}{2m_0L_z^2}, \quad \beta = \frac{\pi}{L_z}$$

$$\Psi(z,t) = 2e^{-i\alpha t}\sin(\beta z) - ie^{-i9\alpha t}\sin(3\beta z)$$

$$\frac{\partial\Psi}{\partial t} = -2i\alpha e^{-i\alpha t}\sin(\beta z) - 9\alpha e^{-i9\alpha t}\sin(3\beta z)$$

$$\nabla\Psi = 2e^{-i\alpha t}\beta\cos(\beta z) - ie^{-i9\alpha t}3\beta\cos(3\beta z)$$

$$\nabla^2\Psi = -2e^{-i\alpha t}\beta^2\sin(\beta z) + ie^{-i9\alpha t}3^2\beta^2\sin(3\beta z)$$

$$-\frac{\hbar^2}{2m_0}\left(-2e^{-i\alpha t}\beta^2\sin(\beta z) + i9e^{-i9\alpha t}\beta^2\sin(3\beta z)\right) + V\left(-2e^{-i\alpha t}\beta^2\sin(\beta z) + i9e^{-i9\alpha t}\beta^2\sin(3\beta z)\right)$$

$$= i\hbar\left(-2i\alpha e^{-i\alpha t}\sin(\beta z) - 9\alpha e^{-i9\alpha t}\sin(3\beta z)\right)$$

$$\frac{\hbar}{2m_0}\beta^2\left(\cancel{2e^{-i\alpha t}\sin(\beta z) - i9e^{-i9\alpha t}\sin(3\beta z)}\right) - V\beta^2\left(\cancel{2e^{-i\alpha t}\sin(\beta z) - i9e^{-i9\alpha t}\sin(3\beta z)}\right)$$

$$= \hbar\alpha\left(\cancel{2e^{-i\alpha t}\sin(\beta z) - i9e^{-i9\alpha t}\sin(3\beta z)}\right)$$

$$\frac{\hbar^2}{2m_0}\beta^2 - V\beta^2 = \hbar\alpha$$

$$- V = 0 -$$

$$\frac{\hbar^2}{2m_0}\left(\frac{\pi}{L_z}\right)^2 = \hbar\left(\frac{\hbar\pi^2}{2m_0L_z^2}\right)$$

$$\frac{\hbar^2\pi^2}{2m_0L_z^2} = \frac{\hbar^2\pi^2}{2m_0L_z^2}$$ is a solution

$$1 = 1$$

3.6.1

From page 62:

"... if we make a linear superposition of two energy eigenstates with energies E_a & E_b, the resulting probability distribution will oscillate at the frequency $\omega_{ab} = |E_a - E_b|/\hbar$."

From page 52:

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L_z}\right)^2, \quad n = 1, 2, \ldots$$

radians per second

Units

$$\left\{\frac{J \cdot s}{kg \cdot m^2}\right\} \equiv \left\{\frac{kg \cdot m^2}{s^2}\,\frac{s}{kg \cdot m^2}\right\} = \left\{\frac{1}{s}\right\}$$

$$L_z = 4\,\mathring{A} = 4 \times 10^{-10}\,m$$

$n_a = 1$

$n_b = 3$

$|1 - 9| = 8$

$$\omega_{13} = \frac{|E_a - E_b|}{\hbar} = \frac{\hbar^2\pi^2}{2mL_z^2}\left|n_a^2 - n_b^2\right|\left(\frac{1}{\hbar}\right) = \frac{\hbar\pi^2}{2mL_z^2}\left|n_a^2 - n_b^2\right|$$

$$= \frac{8\hbar\pi^2}{2mL_z^2} = \frac{4\hbar\pi^2}{mL_z^2} = \frac{4(1.055\times10^{-34})(3.142)^2}{(9.109\times10^{-31})(4\times10^{-10})^2}$$

$$\omega_{13} = 2.858 \times 10^{16}\ s^{-1}$$ in radians per sec

3.6.3

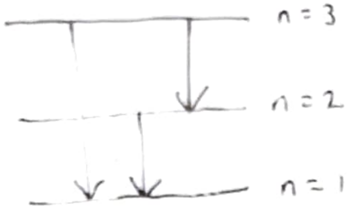
$L_z = 1\,nm = 10^{-9}\,m$

$$\psi = c_1 e^{-iE_1 t/\hbar} \sin\left(\frac{\pi}{L_z} z\right) + c_2 e^{-iE_2 t/\hbar} \sin\left(\frac{2\pi}{L_z} z\right) + c_3 e^{-iE_3 t/\hbar} \sin\left(\frac{3\pi}{L_z} z\right)$$

$$E_n = \frac{\hbar^2}{2m}\left(\frac{\pi n}{L_z}\right)^2 = \frac{\hbar^2 \pi^2 n^2}{2mL_z^2}$$

$\hbar = 1.055 \times 10^{-34}\ J\cdot s$

$m_e = 9.11 \times 10^{-31}\ kg$



$3 \to 1$
$3 \to 2$
$2 \to 1$

$\Delta E_{31} = \hbar(\omega_3 - \omega_1)$

$\Delta E_{32} = \hbar(\omega_3 - \omega_2)$

$\Delta E_{21} = \hbar(\omega_2 - \omega_1)$

$$\omega_{31} = \frac{\Delta E_{31}}{\hbar} = \omega_3 - \omega_1 = \frac{\hbar\pi^2}{2mL_z^2}(3^2 - 1^2) = 8\frac{\hbar\pi^2}{2mL_z^2}$$

$$\omega_{32} = \frac{\Delta E_{32}}{\hbar} = \omega_3 - \omega_2 = \frac{\hbar\pi^2}{2mL_z^2}(3^2 - \overset{2^2}{4}) = 5\frac{\hbar\pi^2}{2mL_z^2}$$

$$\omega_{21} = \frac{\Delta E_{21}}{\hbar} = \omega_2 - \omega_1 = \frac{\hbar\pi^2}{2mL_z^2}(2^2 - 1^2) = 3\frac{\hbar\pi^2}{2mL_z^2}$$

$$\frac{\hbar\pi^2}{2mL_z^2} = 5.71 \times 10^{14}\ rads/s \cdot \frac{1}{2\pi}$$

$$= 9.10 \times 10^{13}\ Hz$$

$\omega_{31} = 8(9.10 \times 10^{13}\ Hz) = 7.28 \times 10^{14}\ Hz$

$\omega_{32} = 5(9.10 \times 10^{13}\ Hz) = 4.55 \times 10^{14}\ Hz$

$\omega_{21} = 3(9.10 \times 10^{13}\ Hz) = 2.73 \times 10^{14}\ Hz$

3.12.1

Page 62 & 52

i)

$$\omega_{21} = \frac{E_2 - E_1}{\hbar} = \frac{1}{\hbar}\left(\frac{\hbar^2 \pi^2 n_a^2}{2mL_z^2} - \frac{\hbar^2 \pi^2 n_b^2}{2mL_z^2}\right) = \frac{\hbar \pi^2}{2mL_z^2}\left(n_a^2 - n_b^2\right)$$

$$2^2 - 1^2 = 3$$

$n_a = 2$
$n_b = 1$

$$\omega_{21} = 3\frac{\hbar \pi^2}{2mL_z^2}$$

ii)

$$\hat{p} = -i\hbar\nabla$$

Page 52

$$\psi_n(z) = \sqrt{\frac{2}{L_z}}\sin\left(\frac{n\pi z}{L_z}\right)$$

$$\langle \hat{p} \rangle = \int_0^{L_z} \psi^* (-i\hbar\nabla)\psi \, dz$$

Page 60

$$\Psi_{12} = c_1 e^{-iE_1 t/\hbar}\psi_1(r) + c_2 e^{-iE_2 t/\hbar}\psi_2(r)$$

Page 61

$$= \frac{1}{\sqrt{L_z}}\left(e^{-iE_1 t/\hbar}\sin\left(\frac{\pi}{L_z}z\right) + e^{-iE_2 t/\hbar}\sin\left(\frac{2\pi}{L_z}z\right)\right)$$

$$-i\hbar\nabla\psi = -i\hbar\frac{1}{\sqrt{L_z}}\nabla\left(e^{-iE_1 t/\hbar}\sin\left(\frac{\pi}{L_z}z\right) + e^{-iE_2 t/\hbar}\sin\left(\frac{2\pi}{L_z}z\right)\right)$$

$$= \frac{-i\hbar}{\sqrt{L_z}}\left(\frac{\pi}{L_z}e^{-iE_1 t/\hbar}\cos\left(\frac{\pi}{L_z}z\right) + \frac{2\pi}{L_z}e^{-iE_2 t/\hbar}\cos\left(\frac{2\pi}{L_z}z\right)\right)$$

$$= -\frac{i\hbar\pi}{L_z^{3/2}}\left(e^{-iE_1 t/\hbar}\cos\left(\frac{\pi}{L_z}z\right) + 2e^{-iE_2 t/\hbar}\cos\left(\frac{2\pi}{L_z}z\right)\right)$$

$$\psi^*(-i\hbar\nabla\psi) = \left[\frac{1}{\sqrt{L_z}}\left(e^{iE_1 t/\hbar}\sin\left(\frac{\pi}{L_z}z\right) + e^{iE_2 t/\hbar}\sin\left(\frac{2\pi}{L_z}z\right)\right)\right]$$
$$\times\left[-\frac{i\hbar\pi}{L_z^{3/2}}\left(e^{-iE_1 t/\hbar}\cos\left(\frac{\pi}{L_z}z\right) + 2e^{-iE_2 t/\hbar}\cos\left(\frac{2\pi}{L_z}z\right)\right)\right]$$

$$= -\frac{i\hbar\pi}{L_z}\left(\sin\left(\frac{\pi}{L_z}z\right)\cos\left(\frac{\pi}{L_z}z\right) + 2\sin\left(\frac{\pi}{L_z}z\right)\cos\left(\frac{2\pi}{L_z}z\right)e^{i(E_1 - E_2)t/\hbar}\right.$$
$$\left. + \sin\left(\frac{2\pi}{L_z}z\right)\cos\left(\frac{\pi}{L_z}z\right)e^{i(E_2 - E_1)t/\hbar} + 2\sin\left(\frac{2\pi}{L_z}z\right)\cos\left(\frac{2\pi}{L_z}z\right)\right)$$

$$\langle \hat{p} \rangle = -\frac{i\hbar\pi}{L_z}\int_0^{L_z} \overset{0}{\sin\left(\frac{\pi}{L_z}z\right)\cos\left(\frac{\pi}{L_z}z\right)}\, dz - \frac{i\hbar\pi}{L_z}\int_0^{L_z} \overset{2\left(-\frac{2L}{3\pi}\right)}{2\sin\left(\frac{\pi}{L_z}z\right)\cos\left(\frac{2\pi}{L_z}z\right)} e^{i(E_1-E_2)t/\hbar}\, dz$$

$$-\frac{i\hbar\pi}{L_z}\int_0^{L_z} \underbrace{\overset{\frac{4L_z}{3\pi}}{\sin\left(\frac{2\pi}{L_z}z\right)\cos\left(\frac{\pi}{L_z}z\right)}}_{\frac{4}{3}\frac{L_z}{\pi}} e^{i(E_2-E_1)t/\hbar}\, dz - \frac{i\hbar\pi}{L_z}\int_0^{L_z} \overset{0}{2\sin\left(\frac{2\pi}{L_z}z\right)\cos\left(\frac{2\pi}{L_z}z\right)}\, dz$$

$$= -\frac{i\hbar\pi}{L_z}\int_0^{L_z} 2\sin\left(\frac{\pi}{L_z}z\right)\cos\left(\frac{2\pi}{L_z}z\right) e^{i(E_1-E_2)t/\hbar}\, dz$$

$$\int_0^{L_z} \sin\left(\left(\frac{\pi}{L_z}+\frac{2\pi}{L_z}\right)z\right) + \sin\left(\left(\frac{\pi}{L_z}-\frac{2\pi}{L_z}\right)z\right) dz$$

$$\int_0^{L_z} \sin\left(\frac{3\pi}{L_z}z\right) - \sin\left(\frac{\pi}{L_z}z\right) dz = -\frac{L_z}{3\pi}\cos\left(\frac{3\pi}{L_z}z\right) + \frac{L_z}{\pi}\cos\left(\frac{\pi}{L_z}z\right)\Bigg|_0^{L_z}$$

$$= -\frac{L_z}{3\pi}\overset{-1}{\cos(3\pi)} + \frac{L_z}{\pi}\overset{-1}{\cos(\pi)} + \frac{L_z}{3\pi}\overset{1}{\cos(0)} - \frac{L_z}{\pi}\overset{1}{\cos(0)}$$

$$= \frac{L_z}{3\pi} + -\frac{L_z}{\pi} + \frac{L_z}{3\pi} - \frac{L_z}{\pi} = \frac{2L_z}{3\pi} - \frac{2L_z}{\pi}$$

$$= \frac{2L_z}{3\pi} - \frac{6L_z}{3\pi}$$

$$= -\frac{4L_z}{3\pi}$$

$$-\frac{i\hbar\pi}{L_z}\int_0^{L_z} \sin\left(\frac{2\pi}{L_z}z\right)\cos\left(\frac{\pi}{L_z}z\right) e^{\frac{i(E_2-E_1)t}{\hbar}}\, dz$$

$$\int_0^{L_z} \frac{1}{2}\left(\sin\left(\left(\frac{2\pi}{L_z}+\frac{\pi}{L_z}\right)z\right) + \sin\left(\left(\frac{2\pi}{L_z}-\frac{\pi}{L_z}\right)z\right)\right) dz$$

$$\int_0^{L_z} \frac{1}{2}\left(\sin\left(\frac{3\pi}{L_z}z\right) + \sin\left(\frac{\pi}{L_z}\right)\right) dz = \frac{1}{2}\left(-\frac{L_z}{3\pi}\cos\left(\frac{3\pi}{L_z}z\right) - \frac{L_z}{\pi}\cos\left(\frac{\pi}{L_z}z\right)\right)\Bigg|_0^{L_z}$$

$$= \frac{1}{2}\left(-\frac{L_z}{3\pi}\overset{-1}{\cos(3\pi)} - \frac{L_z}{\pi}\overset{-1}{\cos(\pi)} + \frac{L_z}{3\pi}\overset{1}{\cos(0)} + \frac{L_z}{\pi}\overset{1}{\cos(0)}\right)$$

$$= \frac{1}{2}\left(\frac{L_z}{3\pi} + \frac{L_z}{\pi} + \frac{L_z}{3\pi} + \frac{L_z}{\pi}\right) = \frac{1}{2}\left(\frac{2L_z}{3\pi} + \frac{2L_z}{\pi}\right) = \frac{1}{2}\left(\frac{2L_z}{3\pi} + \frac{6L_z}{3\pi}\right)$$

$$= \frac{1}{2}\left(\frac{8L_z}{3\pi}\right) = \frac{4L_z}{3\pi}$$

$$\cancel{\langle \hat{p} \rangle = -\frac{i\hbar\pi}{L_z}\left(-\frac{4}{3}\frac{L_z}{\pi} + \frac{4}{3}\frac{L_z}{\pi}\right)}$$

$$\cancel{\langle \hat{p} \rangle = -\frac{i\hbar\pi}{L_z}\left(\frac{4L_z}{3\pi} e^{i(E_1+E}\right.}$$

$$\langle \hat{p} \rangle = -\frac{i\hbar\pi}{L_z}\left(-\frac{4L_z}{3\pi} e^{i(E_1-E_2)t/\hbar} + \frac{4L_z}{3\pi} e^{i(E_2-E_1)t/\hbar}\right)$$

$$= \frac{4}{3}\hbar i\left(e^{i(E_1-E_2)t/\hbar} - e^{i(E_2-E_1)t/\hbar}\right)$$

$$= \frac{4}{3}\hbar i\left(e^{i(E_1-E_2)t/\hbar} - e^{-i(E_1-E_2)t/\hbar}\right) = \frac{4}{3}\hbar i\left(2\sin\left(\frac{E_1-E_2}{\hbar}t\right)\right)$$

$$\langle \hat{p} \rangle = \frac{8\hbar}{3} i \sin\left(\frac{E_1-E_2}{\hbar}t\right)$$

iii) Yes.

$$\langle \hat{p} \rangle \propto \int_0^{L_z} \cancelto{0}{\sin\left(\frac{\pi}{L_z} z\right)\cos\left(\frac{\pi}{L_z} z\right)} dz + \int_0^{L_z} 3\sin\left(\frac{\pi}{L_z} z\right)\cos\left(\frac{3\pi}{L_z} z\right) dz$$

$$+ \int_0^{L_z} \sin\left(\frac{3\pi}{L_z} z\right)\cos\left(\frac{\pi}{L_z} z\right) dz + \int_0^{L_z} \cancelto{0}{3\sin\left(\frac{3\pi}{L_z} z\right)\cos\left(\frac{3\pi}{L_z} z\right)} dz$$

$$\propto \int_0^{L_z} 3\sin\left(\frac{\pi}{L_z} z\right)\cos\left(\frac{3\pi}{L_z} z\right) dz + \int_0^{L_z} \sin\left(\frac{3\pi}{L_z} z\right)\cos\left(\frac{\pi}{L_z} z\right) dz$$

$$= \int_0^{L_z} \frac{3}{2}\left(\sin\left(\left(\frac{\pi}{L_z} + \frac{3\pi}{L_z}\right) z\right) + \sin\left(\left(\frac{\pi}{L_z} - \frac{3\pi}{L_z}\right) z\right)\right) dz + \int_0^{L_z} \frac{1}{2}\left(\sin\left(\left(\frac{3\pi}{L_z} + \frac{\pi}{L_z}\right) z\right) + \sin\left(\left(\frac{3\pi}{L_z} - \frac{\pi}{L_z}\right) z\right)\right) dz$$

$$= \frac{3}{2}\int_0^{L_z} \sin\left(\frac{4\pi}{L_z} z\right) + \sin\left(-\frac{2\pi}{L_z} z\right) + \frac{1}{2}\int_0^{L_z} \sin\left(\frac{4\pi}{L_z} z\right) + \sin\left(\frac{2\pi}{L_z} z\right) dz$$

$$= \frac{3}{2}\left(-\frac{L_z}{4\pi}\cos\left(\frac{4\pi}{L_z} z\right) + \frac{L_z}{2\pi}\cos\left(\frac{2\pi}{L_z} z\right)\right) + \frac{1}{2}\left(-\frac{L_z}{4\pi}\cos\left(\frac{4\pi}{L_z} z\right) - \frac{L_z}{2\pi}\cos\left(\frac{2\pi}{L_z} z\right)\right)\Bigg|_0^{L_z}$$

$$= \frac{3}{2}\left(-\frac{L_z}{4\pi}\cancelto{1}{\cos(4\pi)} + \frac{L_z}{2\pi}\cancelto{1}{\cos(2\pi)}\right) + \frac{1}{2}\left(-\frac{L_z}{4\pi}\cancelto{1}{\cos(4\pi)} - \frac{L_z}{2\pi}\cancelto{1}{\cos(2\pi)}\right)$$

$$- \frac{3}{2}\left(-\frac{L_z}{4\pi}\cancelto{1}{\cos(0)} + \frac{L_z}{2\pi}\cancelto{1}{\cos(0)}\right) - \frac{1}{2}\left(-\frac{L_z}{4\pi}\cancelto{1}{\cos(0)} - \frac{L_z}{2\pi}\cancelto{1}{\cos(0)}\right)$$

$$= \cancel{-\frac{3}{2}\frac{L_z}{4\pi}} + \cancel{\frac{3}{2}\frac{L_z}{2\pi}} - \cancel{\frac{L_z}{4\pi}\frac{1}{2}} - \cancel{\frac{1}{2}\frac{L_z}{2\pi}} + \cancel{\frac{3}{2}\frac{L_z}{4\pi}} - \cancel{\frac{3}{2}\frac{L_z}{2\pi}} + \cancel{\frac{1}{2}\frac{L_z}{4\pi}} + \cancel{\frac{1}{2}\frac{L_z}{2\pi}}$$

$$= 0$$

3.10.1

Using a systm of units in which the electron mass $m = 1$ and $\hbar = 1$, an electron in a potential $V(z) = z^2/2$ has a wavefunction at a given instant in time

$$\psi(z) = \frac{1}{\sqrt{2\sqrt{\pi}}}\left(1 + \sqrt{2}z\right)e^{-z^2/2}$$

What is the expectation value of the energy for the particle in this state?

Time-independent Schrodinger equation in one-dimension

$$\left(-\frac{\hbar^2}{2m_0}\frac{\partial^2}{\partial z^2} + V\right)\psi = E\psi$$

Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m_0}\frac{\partial^2}{\partial z^2} + V$$

$$\rightarrow \hat{H}\psi = E\psi$$

Expectation value of the energy

$$\langle E\rangle = \int_{-\infty}^{\infty} \psi^* \hat{H}\psi dz$$

Approximating the expectation value of the energy

$$\langle E\rangle = \int_{-\infty}^{\infty} \psi^* \hat{H}\psi dz \rightarrow \lim_{\Delta z\rightarrow 0}\sum_{n=-\infty}^{\infty} \psi_n^* \hat{H}\psi_n \Delta z$$

$$\rightarrow \psi_n^* \hat{H}\psi_n = \psi_n^*\left(-\frac{\hbar^2}{2m_0}\frac{\partial^2}{\partial z^2} + V\right)\psi_n = -\frac{\hbar^2}{2m_0}\psi_n^*\frac{\partial^2\psi_n}{\partial z^2} + V\psi_n^*\psi_n$$

Let $\psi_{n+1} - \psi_n = \psi(z + \Delta z) - \psi(z)$

$$\frac{\partial\psi_n}{\partial z} = \lim_{\Delta z\rightarrow 0}\frac{\psi_{n+1} - \psi_n}{\Delta z} \rightarrow \frac{\Delta\psi_n}{\Delta z} = \frac{\psi_{n+1} - \psi_n}{\Delta z}$$

$$\frac{\partial^2\psi_n}{\partial z^2} = \frac{\partial}{\partial z^2}\frac{\partial\psi_n}{\partial z} \rightarrow \frac{\Delta}{\Delta z}\frac{\Delta\psi_n}{\Delta z} = \frac{(\psi_{n+2} - \psi_{n+1}) - (\psi_{n+1} - \psi_n)}{\Delta z^2} = \frac{(\psi_{n+2} - 2\psi_{n+1} + \psi_n}{\Delta z^2}$$

$$\langle E\rangle = \sum_{n=-\infty}^{\infty} -\frac{\hbar^2}{2m_0}\psi_n^*\left(\frac{\psi_{n+2} - 2\psi_{n+1} + \psi_n}{\Delta z^2}\right) + V\psi_n^*\psi_n\Delta z$$

Defining additional terms

$$\psi(z=0) = \psi_0 = \frac{1}{\sqrt{2\sqrt{\pi}}}\left(1+\sqrt{2}(0)\right)e^{-(0)^2/2} = \frac{1}{\sqrt{2\sqrt{\pi}}}(1)(1) = \frac{1}{\sqrt{2\sqrt{\pi}}}$$

$$\psi(z) = \psi_0\left(1+\sqrt{2}z\right)e^{-z^2/2}$$

$$V(z) = \frac{z^2}{2}$$

$$\psi_n^* \hat{H}\psi_n = -\frac{\hbar}{2m_0}\psi_n^*\left(\frac{\psi_{n+2} - 2\psi_{n+1} + \psi_n}{\Delta z^2}\right) + \frac{z^2}{2}\psi_n^*\psi_n$$

Since we are told to use natural units, $\hbar = m = 1$. Additionally, since the wavefunction $\psi(z)$ is purely real, $\psi^* = \psi$, we can write the following.

$$\psi_n^* \hat{H}\psi_n = -\frac{1}{2}\psi_n\left(\frac{\psi_{n+2} - 2\psi_{n+1} + \psi_n}{\Delta z^2}\right) + \frac{z^2}{2}\psi_n^2$$

In [113]:

```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

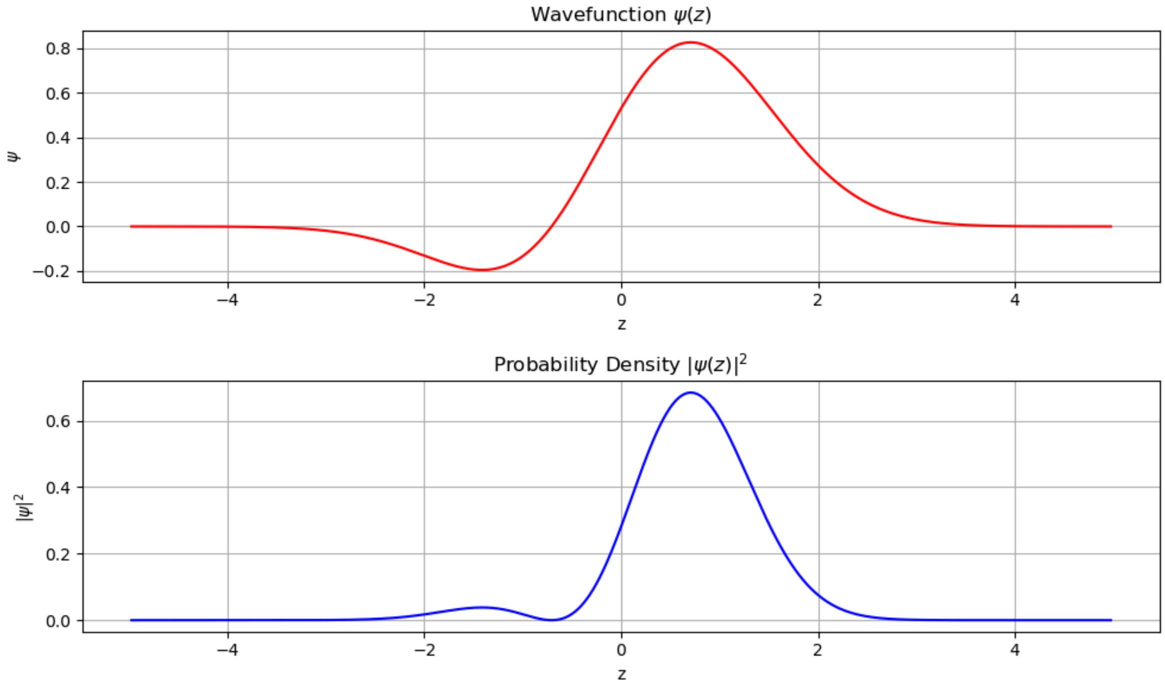
In [114]:

```
hbar = 1 # In natural units
m = 1 # We were told to use these values in the book

domain = 100 # Half the total domain. This leads to us looking at z =[-do
delta_z = 0.001 # Step size
z = np.arange(-domain, domain+delta_z, delta_z) # The domain+delta_z term
                                                # domain symmetric about

psi_0 = 1/(np.sqrt(2*np.sqrt(np.pi)))
psi = psi_0*(1+np.sqrt(2)*z)*np.e**(-z**2/2)

dpsi = np.zeros(len(psi)) # Creating empty array to store values of the w
dpsi[-1] = 0 # Defining final value as 0 because the loop below will crea
             # We will need psi and dpsi to have the same size so we can
             # which is defined below) and psi the same size in order to

for n in np.arange(len(psi)-1):
    dpsi[n] = (psi[n+1] - psi[n])/delta_z

d2psi = np.zeros(len(psi))
d2psi[-1] = 0 # Same as above. We will need d2psi to have the same size a

for n in np.arange(len(psi)-1):
    #d2psi[n] = (psi[n+2] - 2*psi[n+1] + psi[n])/delta_z**2
    # I decided against using the top because it returned substantially m
    # error than the following line.
    d2psi[n] = (dpsi[n+1] - dpsi[n])/delta_z

V = z**2/2

I = -hbar/(2*m)*psi*d2psi + V*psi**2 # The integrand we use to find the e
                                     # This is defined above as the compl
                                     # time the product of the Hamiltonia
                                     # Since our wavefunction is real, th
                                     # as multiplying the Hamilontian by

eEnergy = np.sum(I)*delta_z # expectation energy

print(f'<E> = {eEnergy} in natural units')
```

In [118]:

```
# ------- Graphing Wave Function and Probability Density -------

psi_sq = np.abs(psi)**2

zero = len(psi)/2 - 0.5 # zero is centered at one-half less than the true
num2bin = len(z)/len(np.arange(-domain, domain+1, 1)) # converts from num
interval = 5 # How far +/- from the origin you'd like to see

lowerbound = int(np.round(zero - interval*num2bin))
upperbound = int(np.round(zero + interval*num2bin))

print(f'Number of bins: {len(psi)}')
print(f'z over the interval {-100, 100}')
print(f'Ratio of bins/z = {num2bin} ')
print(f'Zero is located at bin number {int(zero)}')

zero = len(psi)/2 - 0.5 # zero is centered at the halfway point
num2bin = len(z)/len(np.arange(-domain, domain+1, 1)) # converts from num
interval = 10 # How far +/- from the original

fig, (ax1, ax2) = plt.subplots(2,1, figsize=(10,6))

ax1.plot(z[lowerbound:upperbound], psi[lowerbound:upperbound], 'r')
ax1.set_xlabel('z')
ax1.set_ylabel(r'$\psi$')
ax1.grid()
ax1.set_title(r'Wavefunction $\psi(z)$')

ax2.plot(z[lowerbound:upperbound], psi_sq[lowerbound:upperbound], 'b')
ax2.set_xlabel('z')
ax2.set_ylabel(r'$|\psi|^2$')
ax2.grid()
ax2.set_title(r'Probability Density $|\psi(z)|^2$')

plt.tight_layout()
```

```
Number of bins: 200001
z over the interval (-100, 100)
Ratio of bins/z = 995.0298507462686
Zero is located at bin number 100000
```



In [ ]:

```

```