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 [1]:

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

In [3]:

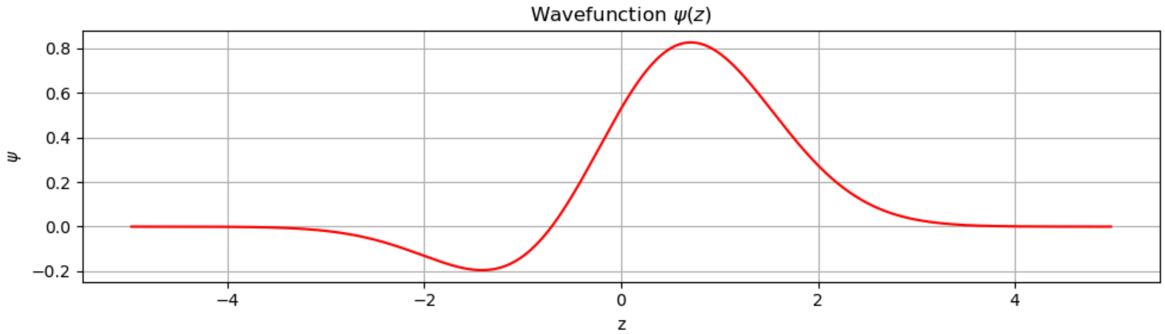
```
#%time # this is the only line I added inbetween the canvas submission an
hbar = 1 # In natural units
m = 1 # We were told to use these values in the book

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')
```

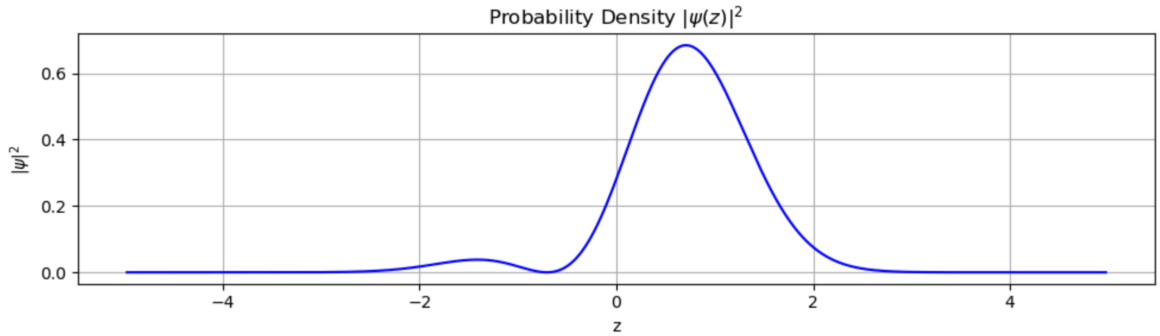
```
<E> = 0.9999993437503228 in natural units
```

In [4]:

```
# ------- 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
```


Wavefunction $\psi(z)$
0.8
0.6
0.4
0.2
0.0
−0.2
ψ
−4
−2
0
2
4
z


Probability Density $|\psi(z)|^2$
0.6
0.4
0.2
0.0
$|\psi|^2$
−4
−2
0
2
4
z

In [ ]:

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1
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