PHYS 250

Lecture 4.1

Schrodinger Equation 1

This is where it starts to get complex …

Today

Administriva
Wave Equation Review
Guessing the Schrodinger Equation (free particle case)
Schrodinger Equation and Solution Properties
Wavefunctions and Probability
Numerical Solution Examples
A Little Fourier Analysis
Heisenberg Uncertainty Principle
Including Forces in Schrodinger
Step-Potential Examples

Administrivia

WebWork 3 is due at midnight.

Worksheet 3 solutions are posted.
Practice Midterm solutions available Tuesday at 8 AM.

Midterm Exam at 5-6 PM Wednesday, in this room.

You may bring one page (both sides) of notes.
Group formula sheet is OK, but you learn more by making your own.
I don’t give you a formula sheet.

Any calculator, but no phones, tablets, laptops or anything wireless.

Today’s material on Schrodinger will <u>not</u> be on the exam.

Wednesday is more Schrodinger, Friday is tutorial worksheet.

Bohr Model Right and Wrong

Thompson “plum pudding” atom was inconsistent with Rutherford scattering.
Rutherford model of electrons orbiting a nucleus doesn’t explain uniform sizes, and the orbits are unstable and would collapse in picoseconds.

Bohr Model <u>predicts</u> the Rydberg wavelengths
by introducing Planck’s Constant to atomic structure.

It predicts all hydrogen atoms are the same size, which it predicts correctly.

It also gets a lot of stuff wrong:

- Wrong magnetic moment (angular momentum is wrong)
- Predicts that atoms are flat
- No good extension to multi-electron atoms
- Davisson-Germer experiment shows electrons are waves outside atoms

We Want a Field/Wave Equation

Photons obey Maxwell’s Equations, in particular the wave-equations derived from Maxwell (plus some quantum stuff)

Maxwell’s Equations are field equations:
partial differential equations involving space and time.

Schrodinger wanted something like that for particles like electrons, and hoped it would preserve the correct results of the Bohr Model, fix the wrong ones, and make new predictions.

Wave Equation Review

Wave Equation: $\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \cdot \frac{\partial^2 y}{\partial t^2}$ for $y(x,t)$

Second-order in both time and space. Linear. Velocity is built into the equation.

Solution: $y(x,t) = f(x \pm vt)$ for any $f(\text{one argument})$

Velocity can have either sign, but only one magnitude.

Any linear combination of above form is also a solution.

The solution doesn't <u>have</u> to be a sinusoid,

but if it <u>is</u> a sinusoid with wavelength λ and period T,

$$y(x,t) = A\sin\left[2\pi\left(\pm\frac{x}{\lambda} - \frac{t}{T}\right) + \phi\right] \text{ with } v = \frac{\lambda}{T}$$

Wave Equation Review 2

It’s convenient to write the sinusoid solutions as

$$y\left(x,t\right)=A\sin\left[\pm kx-\omega t+\phi\right] \text{ with } k=\frac{2\pi}{\lambda} \text{ and } \omega=\frac{2\pi}{T}=2\pi f$$

Putting the minus sign on ωt makes the wave direction have the same sign as k.

To satisfy the wave equation we still require $v=\dfrac{\lambda}{T}=\dfrac{2\pi/k}{2\pi/\omega}=\dfrac{\omega}{k}$

What We Want

The Davisson-Germer experiment shows that electrons can diffract like waves that obey de Broglie: $\lambda = \frac{h}{p}$.

We want a wave equation for electrons that obeys that.

But unlike light, electrons can have any velocity, including zero.
So the equation can't be the usual wave equation with a fixed velocity built-in.

We also want the equation to obey Planck: $E = hf$.

Incorporating relativity turns out to be really complicated,
so we will use the classical $E_{\text{kinetic}} = \frac{1}{2}mv^2 = \frac{1}{2}\frac{(mv)^2}{m} = \frac{p^2}{2m}$

What We Want 2

If we plug the de Broglie condition $\lambda = \frac{h}{p}$ into the convenient $k = \frac{2\pi}{\lambda}$

we get $k = \frac{2\pi}{h/p} = p \cdot \frac{2\pi}{h} = \frac{p}{h/2\pi} = \frac{p}{\hbar}$.

That implies $p = \hbar k$.

Then $E_{\text{kinetic}} = \frac{p^2}{2m}$ becomes $E_{\text{kinetic}} = \frac{(\hbar k)^2}{2m}$.

If we plug the Planck condition $E = hf$ into the convenient $\omega = \frac{2\pi}{T} = 2\pi f$

we get $\omega = 2\pi \frac{E}{h} = \frac{E}{h/2\pi} = \frac{E}{\hbar}$.

That implies $E = \hbar\omega$

Guess the Equation From the Solutions

Guess $y(x,t) = \sin\left[2\pi\left(\frac{x}{\lambda} - ft\right)\right] = \sin\left[kx - \omega t\right]$

with $k = \frac{2\pi}{\lambda}$ and $\omega = 2\pi f$. Using k and ω makes the math cleaner.

Do some derivatives:

$$\frac{\partial y}{\partial t} = \cos\left[kx - \omega t\right] \cdot (-\omega)$$

$$\frac{\partial y}{\partial x} = \cos\left[kx - \omega t\right] \cdot k \qquad \frac{\partial^2 y}{\partial x^2} = -\sin\left[kx - \omega t\right] \cdot k^2 = -k^2 \cdot y(x,t)$$

First Guess Equation

Note that $\hbar \cdot \frac{\partial y}{\partial t} = -\hbar \cdot \omega \cos\left[kx - \omega t\right] = -E\cos\left[kx - \omega t\right]$

and $\frac{\hbar^2}{2m} \cdot \frac{\partial^2 y}{\partial x^2} = -\frac{\hbar^2}{2m} \cdot k^2 \sin\left[kx - \omega t\right] = -E\sin\left[kx - \omega t\right]$

So $\hbar \frac{\partial y}{\partial t} = \frac{\hbar^2}{2m} \frac{\partial y^2}{\partial x^2}$ gives $-E\cos\left[kx - \omega t\right] = -E\sin\left[kx - \omega t\right]$

That almost works as an equation, but we have a sine vs cosine problem.

Complex Exponential Sinusoids

Complex exponential functions are also sinusoidal

$$e^{i\theta} = \exp\left(i\theta\right) = \cos\theta + i\sin\theta \qquad ie^{i\theta} = i\cos\theta - \sin\theta$$

$$\frac{d}{d\theta}e^{i\theta} = \frac{d}{d\theta}\left(\cos\theta + i\sin\theta\right) = -\sin\theta + i\cos\theta = ie^{i\theta}$$

So let's try $y\left(x,t\right) = e^{i\left(kx-\omega t\right)} = \exp\left[i\left(kx-\omega t\right)\right]$ as a solution.

The derivatives are

$$\frac{\partial y}{\partial t} = \exp\left[i\left(kx-\omega t\right)\right]\cdot\left(-i\omega\right) = -i\omega\cdot y\left(x,t\right)$$

$$\frac{\partial y}{\partial x} = \exp\left[i\left(kx-\omega t\right)\right]\cdot ik \qquad \frac{\partial^2 y}{\partial x^2} = \exp\left[i\left(kx-\omega t\right)\right]\cdot\left(ik\right)^2 = -k^2\cdot y\left(x,t\right)$$

Second Guess Equation

Note that $\hbar \cdot \frac{\partial y}{\partial t} = \hbar \cdot -i\omega y\left(x,t\right) = -iE \cdot y\left(x,t\right)$

and $\frac{\hbar^2}{2m} \cdot \frac{\partial^2 y}{\partial x^2} = \frac{\hbar^2}{2m} \cdot -k^2 y\left(x,t\right) = -E \cdot y\left(x,t\right)$

So $\hbar \frac{\partial y}{\partial t} = \frac{\hbar^2}{2m} \frac{\partial y^2}{\partial x^2}$ gives $-iE \cdot y\left(x,t\right) = -E \cdot y\left(x,t\right)$

That fixes the sine vs cosine problem, but now we have a factor of *i* problem

Schrodinger Equation

Try $i\hbar \cdot \frac{\partial y}{\partial t} = i\hbar \cdot -i\omega y(x,t) = E \cdot y(x,t)$

and $\frac{-\hbar^2}{2m} \cdot \frac{\partial^2 y}{\partial x^2} = \frac{-\hbar^2}{2m} \cdot -k^2 y(x,t) = E \cdot y(x,t)$

So $i\hbar \frac{\partial y}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial y^2}{\partial x^2}$ gives $E \cdot y(x,t) = E \cdot y(x,t)$. All problems fixed!

We have invented the Schrodinger Equation (for a free particle in 1 dimension).

It's conventional to use $\psi(x,t)$ instead of $y(x,t)$

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

Schrodinger is Linear

$$i\hbar\frac{\partial}{\partial t}\psi = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi$$

Replace ψ by $A\psi$: $i\hbar\frac{\partial}{\partial t}A\psi = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}A\psi$ then divide out A.

So if ψ is a solution, so is $A\psi$.

For solutions ψ_1 and ψ_2: $i\hbar\frac{\partial}{\partial t}A\psi_1 = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}A\psi_1$ and $i\hbar\frac{\partial}{\partial t}B\psi_2 = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}B\psi_2$

Add them and rearrange: $i\hbar\frac{\partial}{\partial t}\left(A\psi_1 + B\psi_2\right) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(A\psi_1 + B\psi_2\right)$

So $A\psi_1 + B\psi_2$ is a solution if ψ_1 and ψ_2 are solutions.

The Operator Concept

A function takes a number as input, and gives a number as output: $f\left(x\right) = y$

An operator takes a function as input, and gives a function as output.

An example of an operator is $\dfrac{d}{dx}$.

Applying $\dfrac{d}{dx}$ to $f\left(x\right)$ gives $\dfrac{d}{dx} f\left(x\right) = \left.\dfrac{df}{dx}\right|_x = f'\left(x\right)$

Momentum Operator

If we apply the operator $\frac{\partial}{\partial x}$ to $\exp\left[i\frac{px-Et}{\hbar}\right]$ we get $i\frac{p}{\hbar}\cdot\exp\left[i\frac{px-Et}{\hbar}\right]$

If we apply the operator $\frac{\hbar}{i}\frac{\partial}{\partial x}$ to $\exp\left[i\frac{px-Et}{\hbar}\right]$ we get $p\cdot\exp\left[i\frac{px-Et}{\hbar}\right]$

So we define the <u>momentum operator</u> as $p_{op}=\frac{\hbar}{i}\frac{\partial}{\partial x}$.

Apply the momentum operator twice: $p_{op}^2=\frac{\hbar}{i}\frac{\partial}{\partial x}\cdot\frac{\hbar}{i}\frac{\partial}{\partial x}=-\hbar^2\frac{\partial^2}{\partial x^2}$

So we can write Schrodinger as $i\hbar\frac{\partial\psi}{\partial t}=\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}=\frac{p_{op}^2}{2m}\psi$

Complex vs Real

The complex conjugate of $z = a + ib$

Note that $z^* \cdot z = \left(a+ib\right)\cdot\left(a-ib\right) = a^2 - iab + iba + \left(ib\right)\cdot\left(-ib\right) = a^2 + b^2$
is real and never negative.

The Schrodinger Equation $i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$ is explicitly complex.

It has no non-trivial solutions that aren't complex.

But $\psi^* \cdot \psi$ is real and positive, and that's what has a physical interpretation.

It's a bit like the *E*-field of a wave, which alternates between positive and negative. But the energy density is proportional to E^2, which is always positive.

Does $\psi^* \cdot \psi$ mean anything? Yes, it turns out to be the probability density.

Proving Probability (not on any exam)

Take $i\hbar\frac{\partial\psi}{\partial t}=\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$, and pre-multiply both sides by ψ^*:

$$\psi^*\cdot i\hbar\left[\frac{\partial\psi}{\partial t}\right]=\psi^*\cdot\frac{-\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial x^2}\right]$$

Conjugate $i\hbar\frac{\partial\psi}{\partial t}=\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$ to $-i\hbar\frac{\partial\psi^*}{\partial t}=\frac{-\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2}$ and post-multiply by ψ:

$$-i\hbar\left[\frac{\partial\psi^*}{\partial t}\right]\cdot\psi=\frac{-\hbar^2}{2m}\left[\frac{\partial^2\psi^*}{\partial x^2}\right]\cdot\psi$$

Subtract them: $i\hbar\left(\psi^*\cdot\left[\frac{\partial\psi}{\partial t}\right]+\left[\frac{\partial\psi^*}{\partial t}\right]\cdot\psi\right)=\frac{-\hbar^2}{2m}\left(\psi^*\cdot\left[\frac{\partial^2\psi}{\partial x^2}\right]-\left[\frac{\partial^2\psi^*}{\partial x^2}\right]\cdot\psi\right)$

Divide out $i\hbar$: $\left(\psi^*\cdot\left[\frac{\partial\psi}{\partial t}\right]+\left[\frac{\partial\psi^*}{\partial t}\right]\cdot\psi\right)=\frac{-\hbar}{2im}\left(\psi^*\cdot\left[\frac{\partial^2\psi}{\partial x^2}\right]-\left[\frac{\partial^2\psi^*}{\partial x^2}\right]\cdot\psi\right)$

Proving Probability 2

$$\left(\psi^*\cdot\left[\frac{\partial\psi}{\partial t}\right]+\left[\frac{\partial\psi^*}{\partial t}\right]\cdot\psi\right)=\frac{-\hbar}{2im}\left(\psi^*\cdot\left[\frac{\partial^2\psi}{\partial x^2}\right]-\left[\frac{\partial^2\psi^*}{\partial x^2}\right]\cdot\psi\right)$$

Note that $\frac{\partial}{\partial t}\left(\psi^*\cdot\psi\right)=\left(\psi^*\cdot\left[\frac{\partial\psi}{\partial t}\right]+\left[\frac{\partial\psi^*}{\partial t}\right]\cdot\psi\right)$ and that

$$\frac{\partial}{\partial x}\left(\psi^*\cdot\left[\frac{\partial\psi}{\partial x}\right]-\left[\frac{\partial\psi^*}{\partial x}\right]\cdot\psi\right)=\left(\left[\frac{\partial\psi^*}{\partial x}\right]\cdot\left[\frac{\partial\psi}{\partial x}\right]+\psi^*\cdot\left[\frac{\partial^2\psi}{\partial x^2}\right]\right)-\left(\left[\frac{\partial^2\psi^*}{\partial x^2}\right]\cdot\psi+\left[\frac{\partial\psi^*}{\partial x}\right]\cdot\left[\frac{\partial\psi}{\partial x}\right]\right)$$

$$=\left(\psi^*\cdot\left[\frac{\partial^2\psi}{\partial x^2}\right]-\left[\frac{\partial^2\psi^*}{\partial x^2}\right]\cdot\psi\right)$$

Plug those into the above, and move the right side to the left:

$$\frac{\partial}{\partial t}\left[\psi^*\cdot\psi\right]+\frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\left(\psi^*\cdot\left[\frac{\partial\psi}{\partial x}\right]-\left[\frac{\partial\psi^*}{\partial x}\right]\cdot\psi\right)\right]=0$$

Proving Probability 3

$$\frac{\partial}{\partial t}\left[\psi^{*}\cdot\psi\right]+\frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\left(\psi^{*}\cdot\left[\frac{\partial\psi}{\partial x}\right]-\left[\frac{\partial\psi^{*}}{\partial x}\right]\cdot\psi\right)\right]=0$$

Integrate from $x=-\infty$ to $x=+\infty$. The first term gives $\frac{\partial}{\partial t}\int_{-\infty}^{+\infty}\psi^{*}\psi\cdot dx$.

Integrating the second term just removes the $\frac{\partial}{\partial x}$ in front. So we have

$$\frac{\partial}{\partial t}\int_{-\infty}^{+\infty}\psi^{*}\psi\cdot dx+\left[\frac{\hbar}{2im}\left(\psi^{*}\cdot\left[\frac{\partial\psi}{\partial x}\right]-\left[\frac{\partial\psi^{*}}{\partial x}\right]\cdot\psi\right)\right]_{-\infty}^{+\infty}=0$$

Consider a wavefunction ψ that goes to zero at infinity: 

Then the square bracket term will be zero at both limits, and we have simply

$$\frac{\partial}{\partial t}\int_{-\infty}^{+\infty}\psi^{*}\psi\cdot dx=0$$

Proving Probability 4

If the wavefunction goes to zero at ± infinity, then $\frac{\partial}{\partial t}\int_{-\infty}^{+\infty}\psi^*\psi\cdot dx=0$.

That says that the area under the (real and positive) curve of $\psi^*\psi$ stays constant, even though the wavefunction ψ itself isn't constant.

We can multiply ψ by any constant and it's still a solution.

So we can require $\int_{-\infty}^{+\infty}\psi^*\psi\cdot dx=1$. This is called normalizing the wavefunction.

For a normalized wavefunction, $\psi^*\psi$ is the probability density.

Probability Current

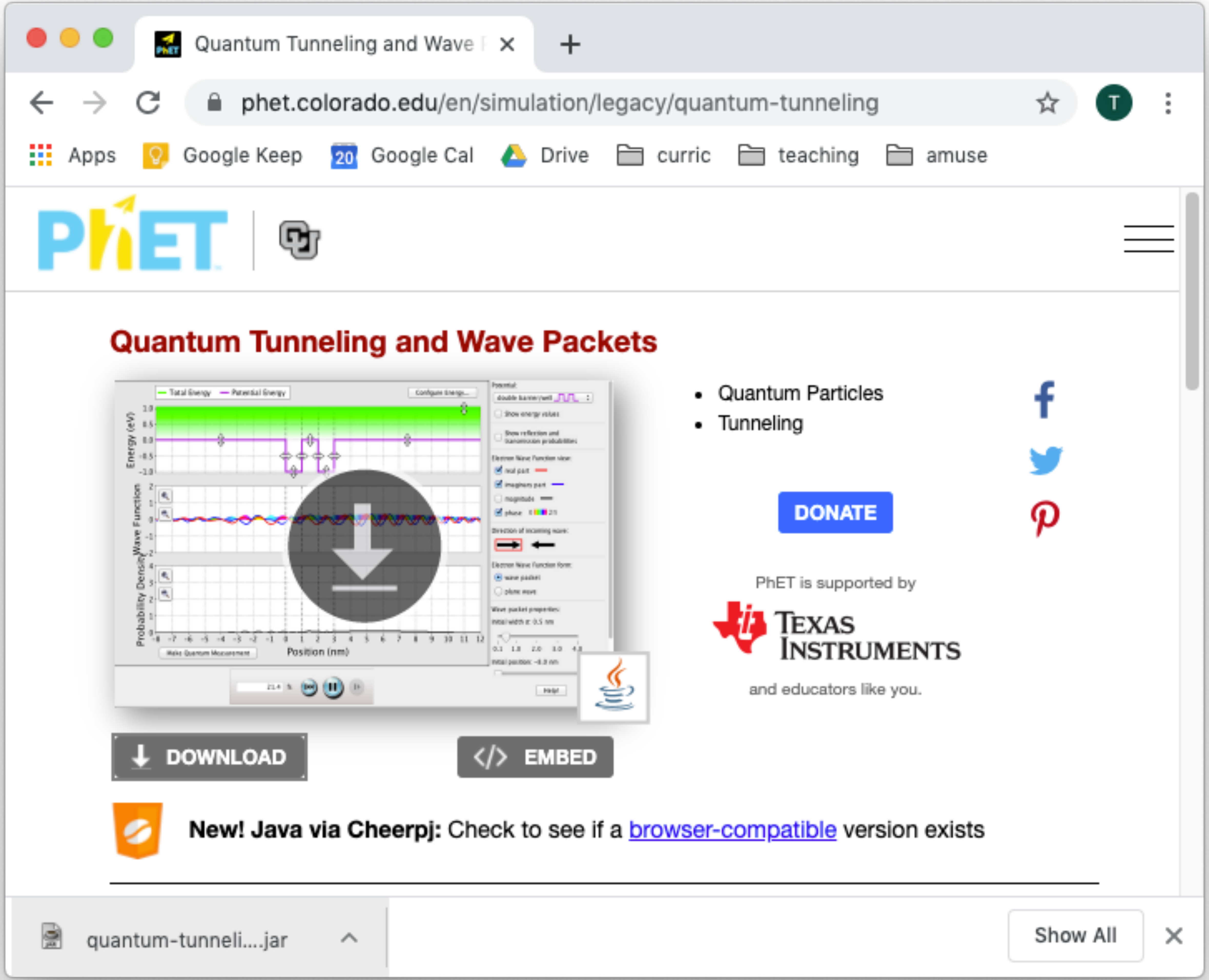
Recall the equation relating charge density ρ and current density $\vec{J}$

$$\frac{\partial}{\partial t}\rho + \vec{\nabla}\cdot\vec{J} = 0 \quad \text{or} \quad \frac{\partial}{\partial t}\rho + \left(\frac{\partial}{\partial x}J_x + \frac{\partial}{\partial y}J_y + \frac{\partial}{\partial z}J_z\right) = 0$$

We found the equation $\frac{\partial}{\partial t}\left[\psi^*\psi\right] + \frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\left(\psi^*\cdot\left[\frac{\partial\psi}{\partial x}\right] - \left[\frac{\partial\psi^*}{\partial x}\right]\cdot\psi\right)\right] = 0$

We decided that $\psi^*\psi$ was the probability density.

So $\frac{\hbar}{2im}\left(\psi^*\cdot\left[\frac{\partial\psi}{\partial x}\right] - \left[\frac{\partial\psi^*}{\partial x}\right]\cdot\psi\right)$ acts like the *x*-component of current density.



Quantum Tunneling and Wave Packets

- Quantum Particles
- Tunneling

PhET is supported by Texas Instruments and educators like you.

New! Java via Cheerpj: Check to see if a browser-compatible version exists

Examples

Wave Solution with $E = 1$ eV

Wave Solution with $E = 0.25$ eV

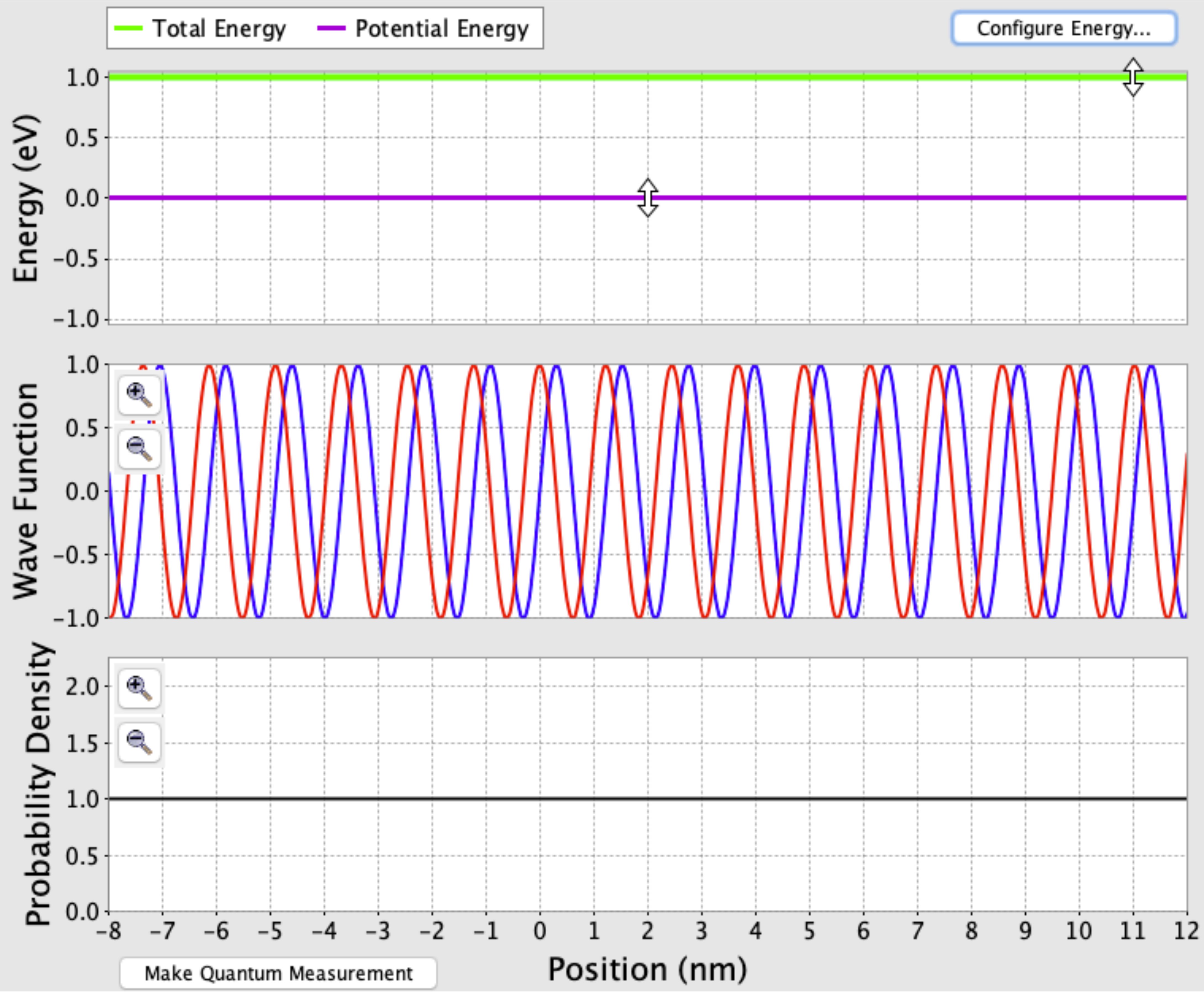
Gaussian with $E = 0$

Narrower Gaussian with $E = 0$

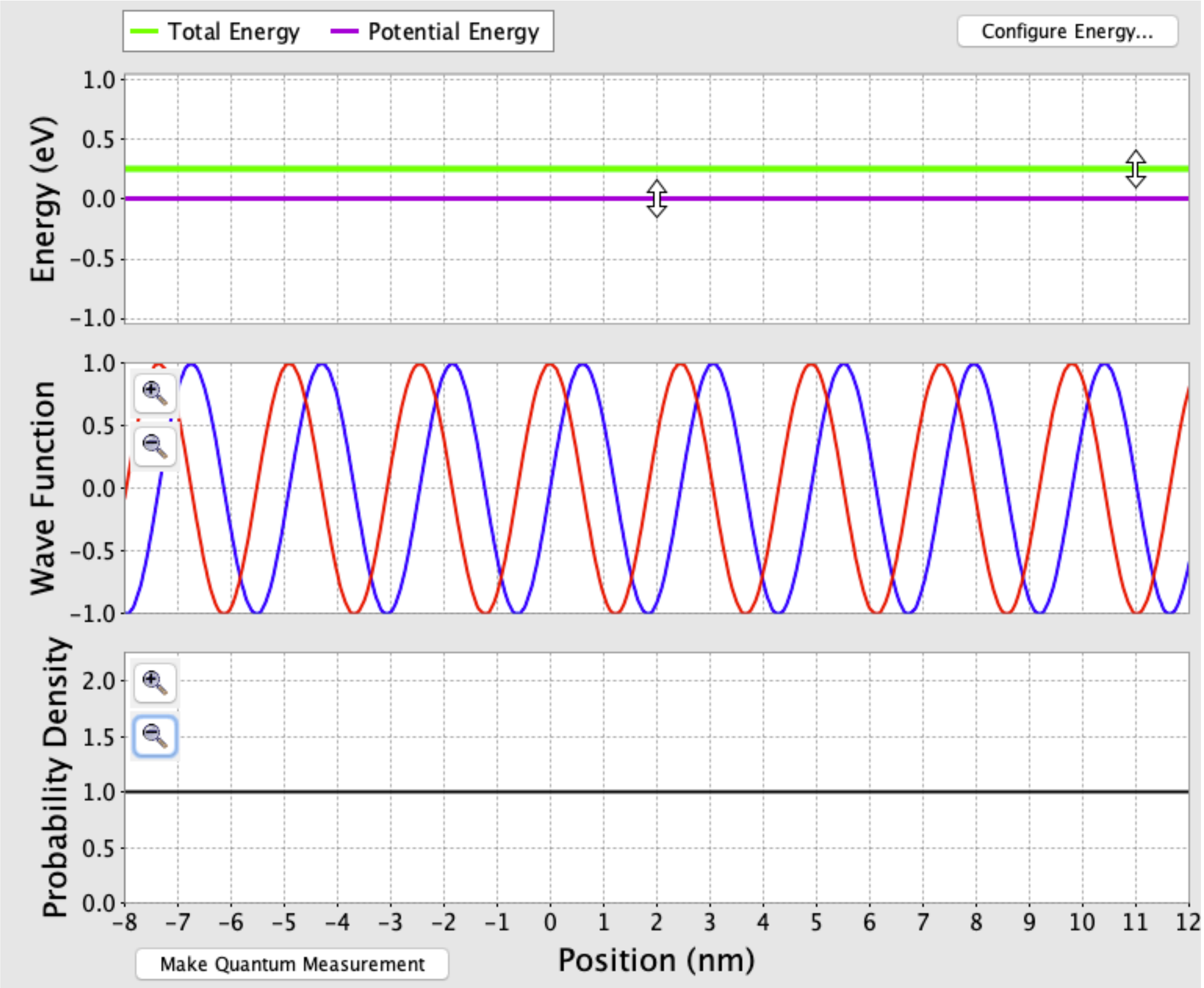
Gaussian with $E = 0.25$ eV

Narrower Gaussian with $E = 0.25$ eV

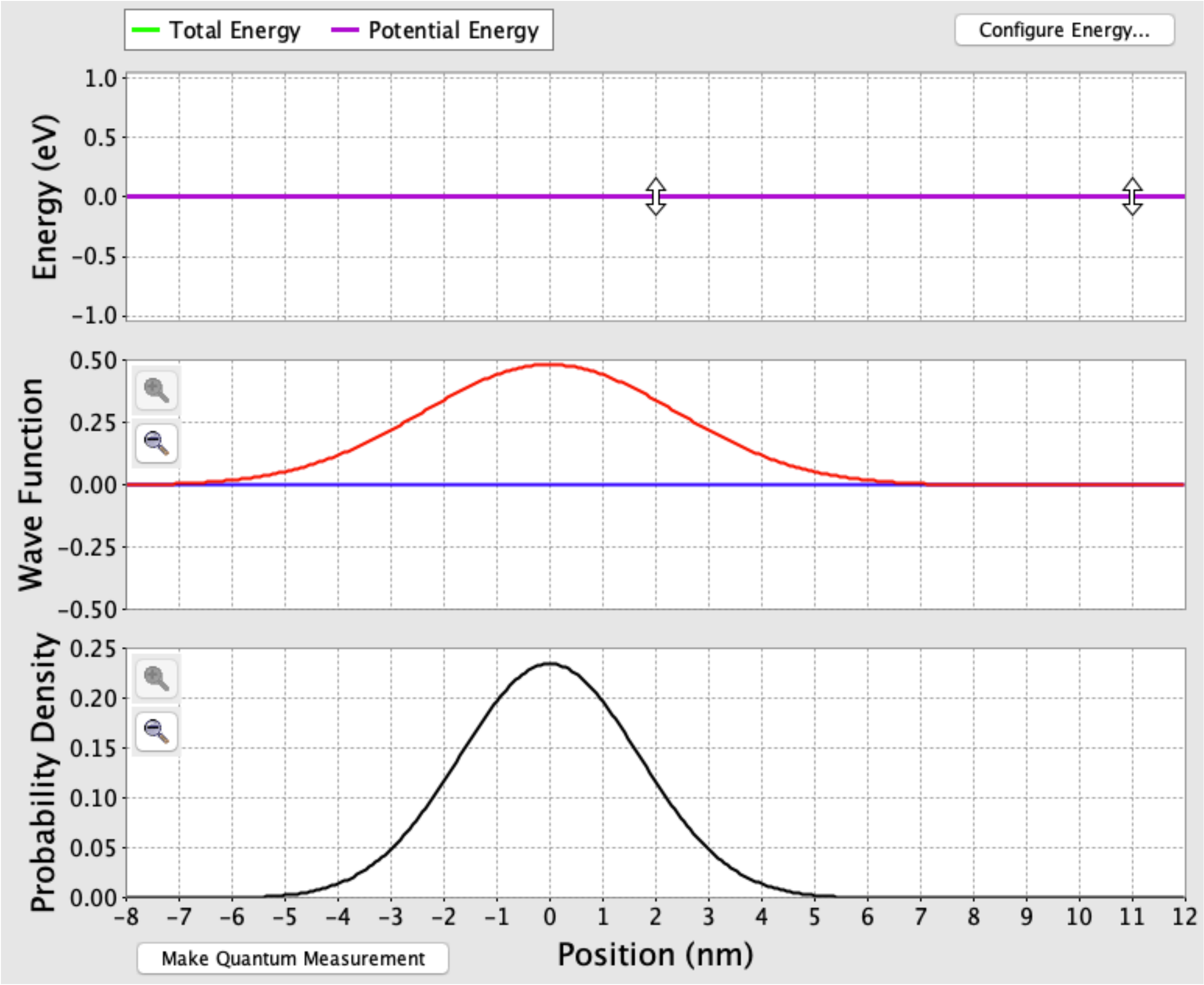
Wave Solution with $E = 1$ eV

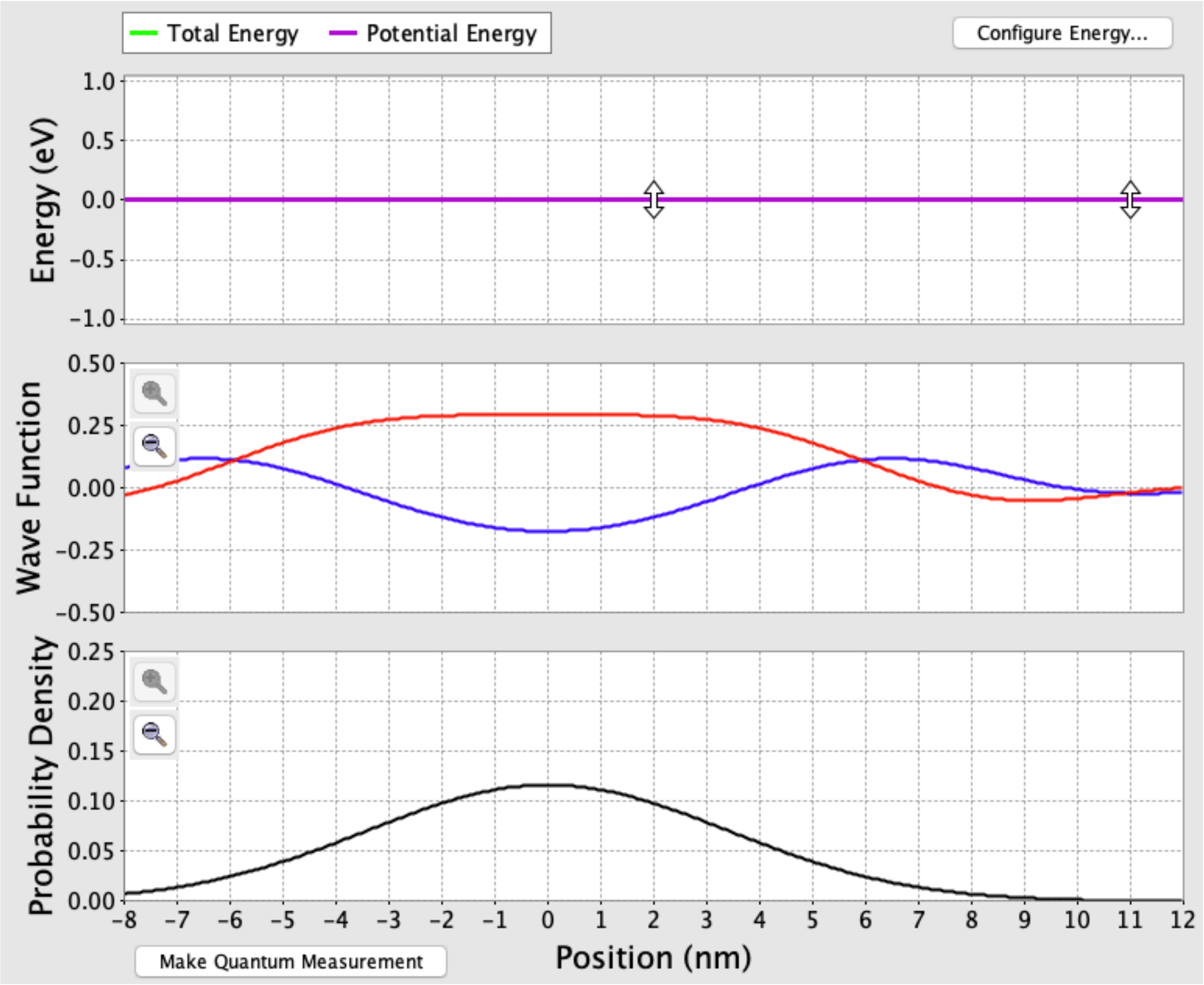


Wave Solution with $E = 0.25$ eV

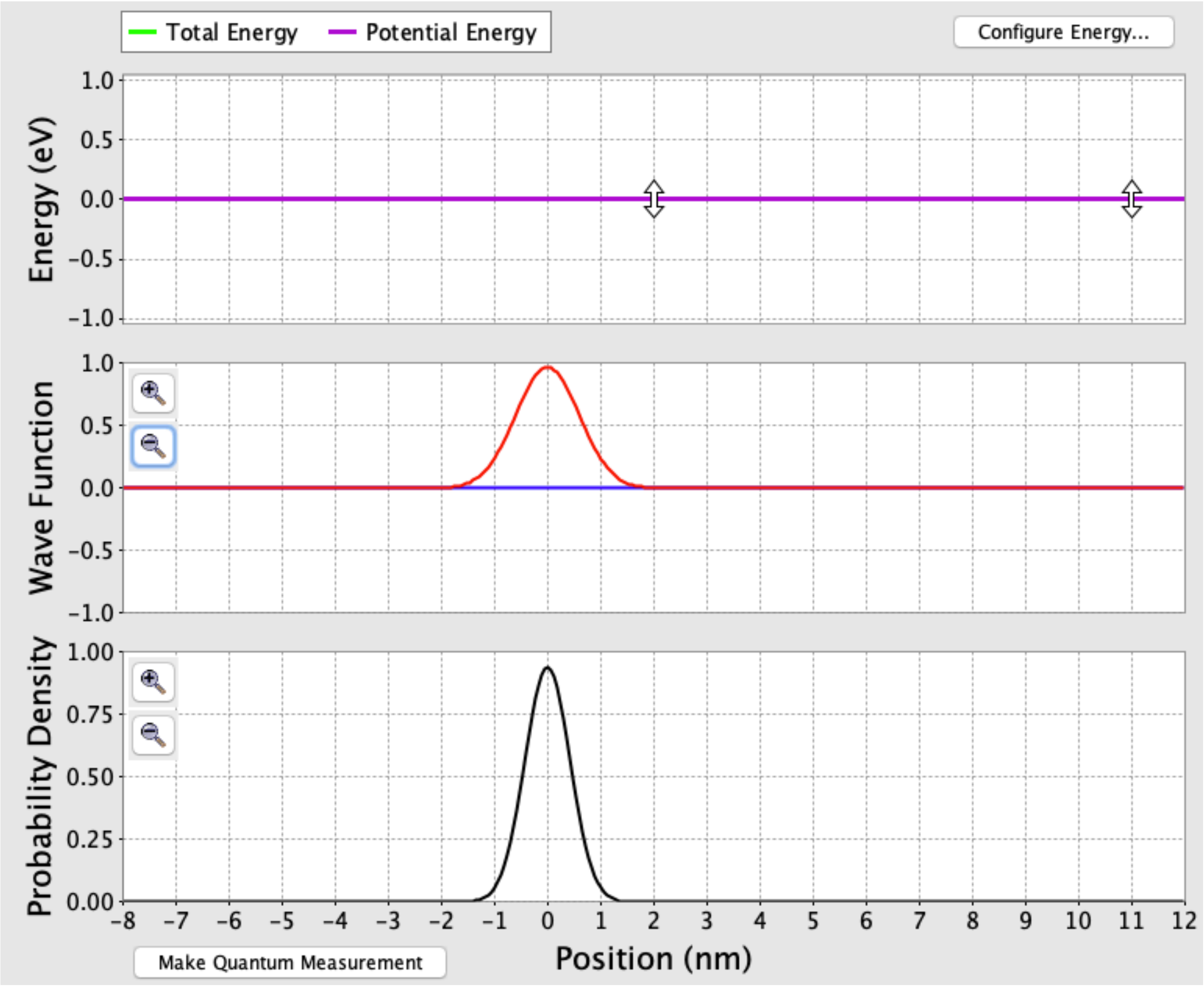


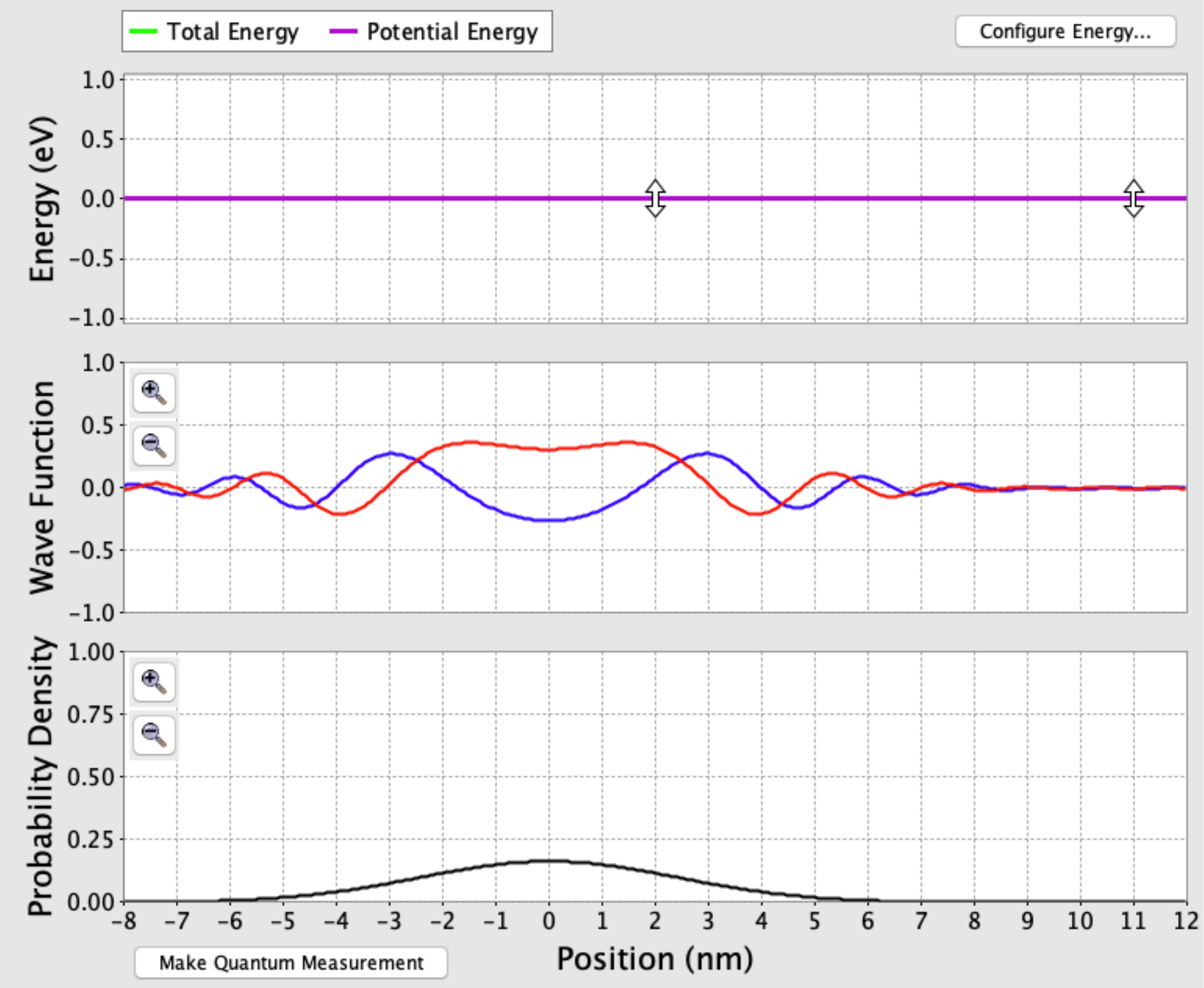
Gaussian with $E = 0$



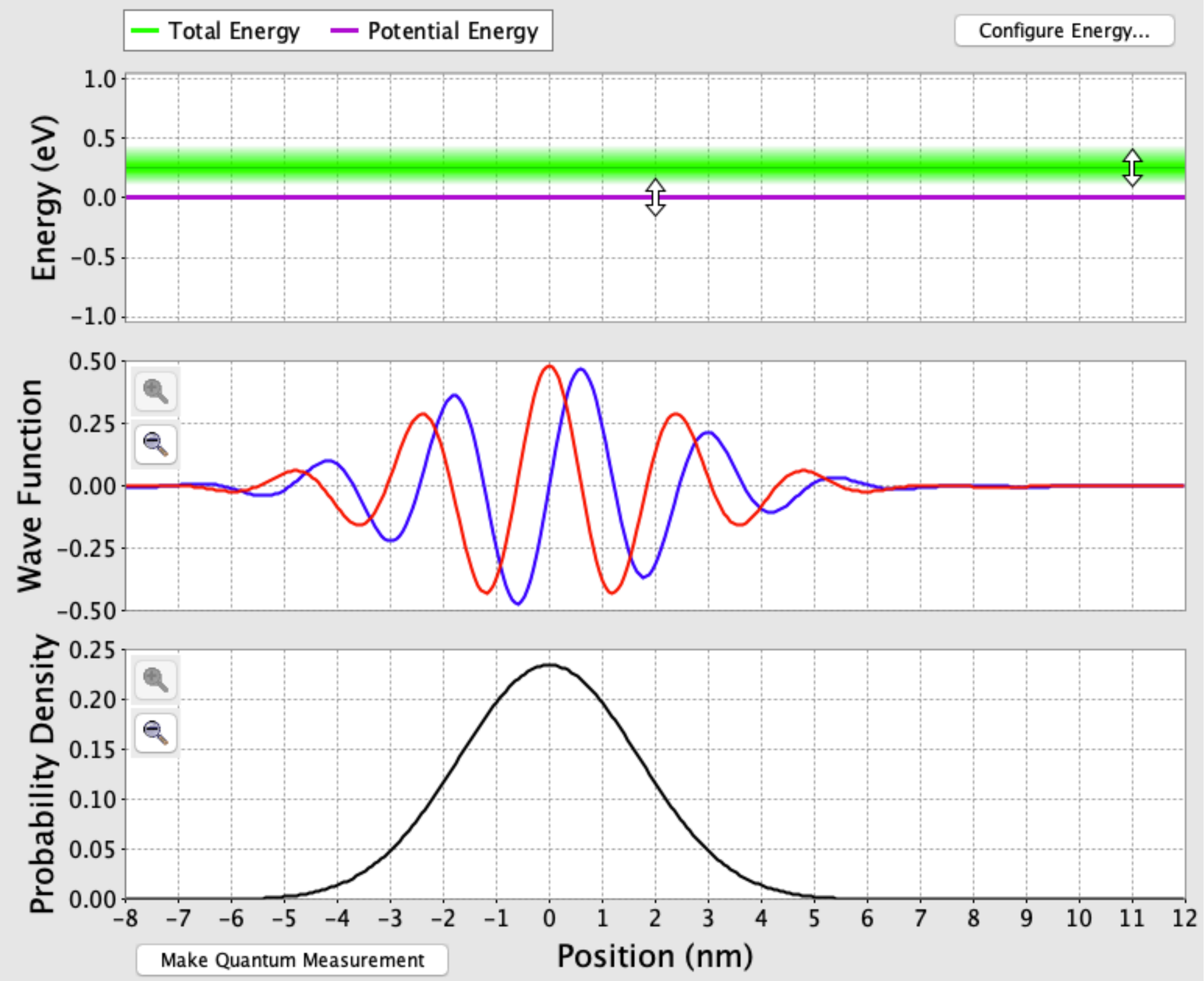


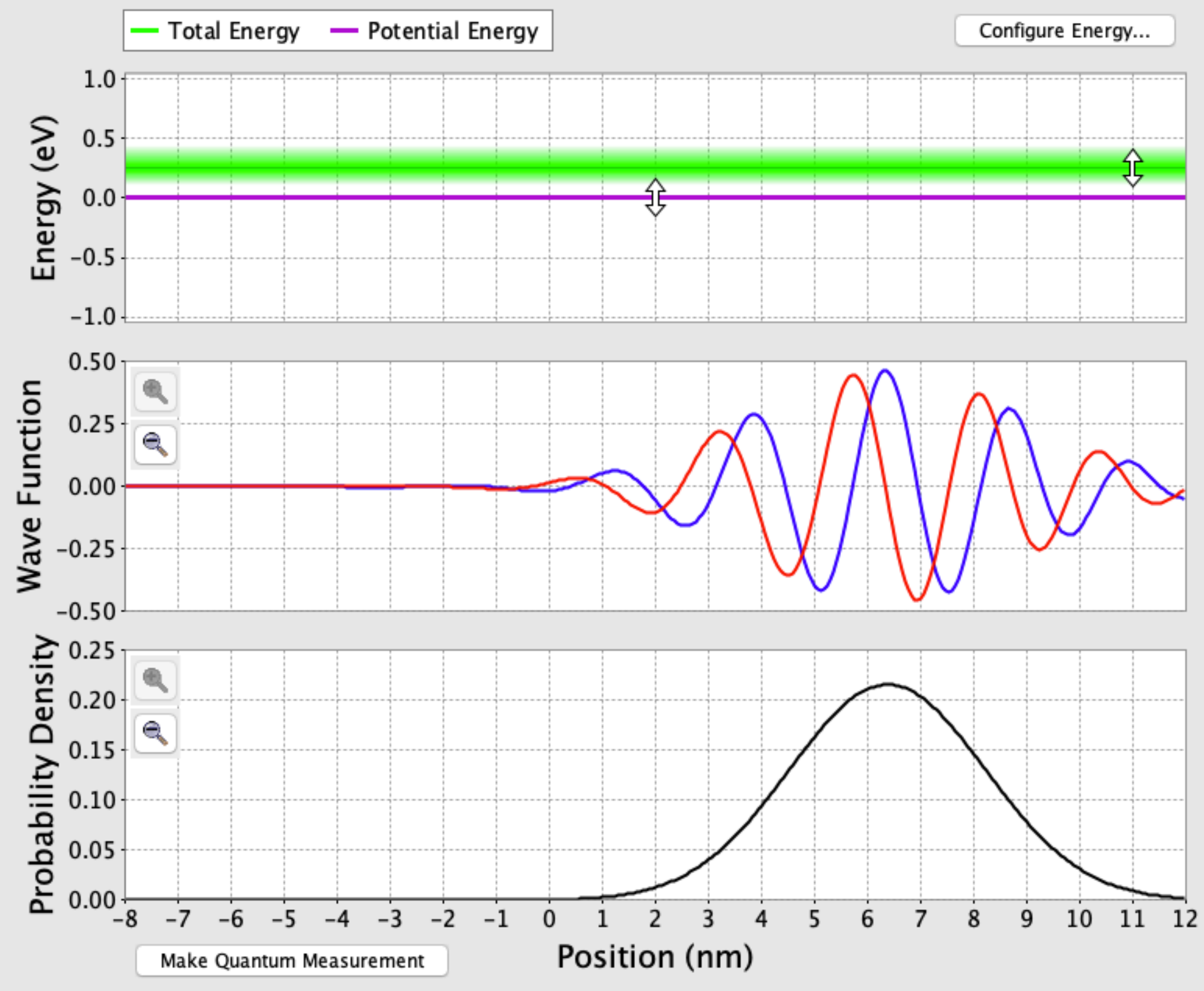
Narrower Gaussian with $E = 0$



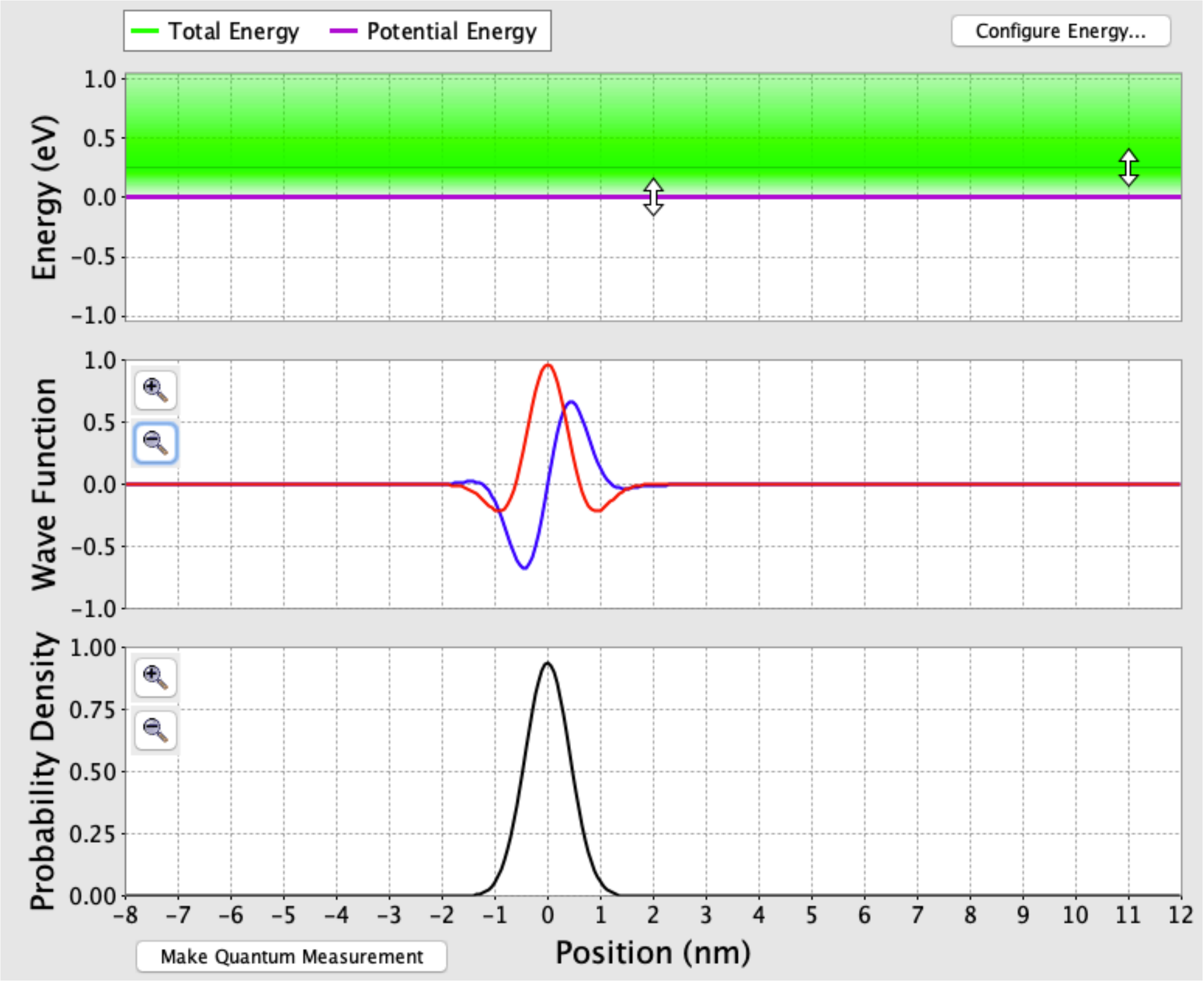


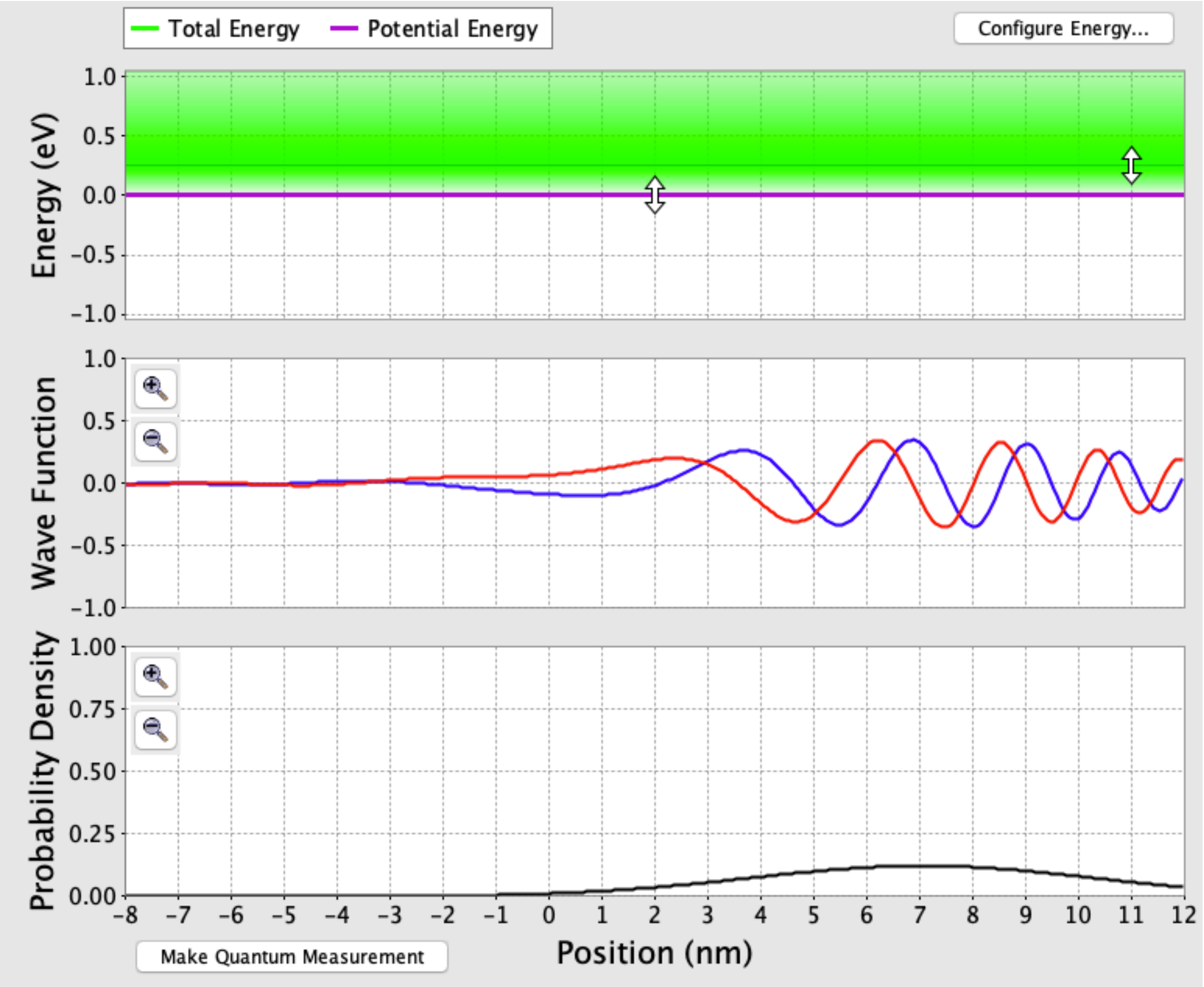
Gaussian with $E = 0.25$ eV





Narrower Gaussian with $E = 0.25$ eV





Summary

Wave Solution with $E = 1$ eV

Real and imaginary parts out of phase, everywhere, for either direction.

Wave Solution with $E = 0.25$ eV

Twice the wavelength, half the velocity.

Gaussian with $E = 0$

Starts real, gets imaginary part, probability density stays Gaussian.

Narrower Gaussian

Spreads into wider Gaussian, area under probability density looks constant.

Gaussian with $E = 0.25$ eV: Gaussian can move while spreading out.

Fourier Analysis

Fourier Analysis means decomposing a data set or function into a sum or integral of sinusoidal functions.

For N discrete data samples x_j, the transform X_k is

$$X_k = \sum_{j=0}^{N-1} x_j \exp\left[-2\pi i \frac{jk}{N}\right] \quad j \text{ and } k \text{ are indices, } i = \sqrt{-1}$$

Even if the x_j are real, the transform X_k is complex

The inverse transform is

$$x_j = \sum_{k=0}^{N-1} X_k \exp\left[+2\pi i \frac{jk}{N}\right]$$

Fourier Analysis 2

The continuous equivalent, in the signal-processing convention

$$S(f) = \int_{-\infty}^{+\infty} dt\ \ s(t) \exp\left[-2\pi i f t\right]$$

$$s(t) = \int_{-\infty}^{+\infty} df\ S(f) \exp\left[+2\pi i f t\right]$$

In the quantum mechanics convention, it looks like

$$y(x) = \int_{-\infty}^{+\infty} dk\ a(k) \exp(ikx)$$

$$a(k') = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dx\ y(x) \exp(-ik'x)$$

Fourier Transform of a Gaussian (not on exam)

Take a Gaussian with width σ_x at $t=0: y(x, t=0) = \exp\left(\frac{-x^2}{2\sigma_x^2}\right)$

Decompose it into spatial frequencies *a*(*k*):

$$a(k) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dx\ y(x)\exp(-ikx) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dx\exp\left(\frac{-x^2}{2\sigma_x^2}\right)\exp(-ikx)$$

$$= \frac{1}{2\pi}\int_{-\infty}^{+\infty} dx\exp\left(\frac{-x^2-2i\sigma_x^2 kx}{2\sigma_x^2}\right) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dx\exp\left(-\frac{x^2+2ik\sigma_x^2 x}{2\sigma_x^2}\right)$$

Notice that $\left(x+ik\sigma_x^2\right)^2 = x^2+2ik\sigma_x^2 x - k^2\sigma_x^4$

So $\frac{x^2+2ik\sigma_x^2 x}{2\sigma_x^2} = \frac{x^2+2ik\sigma_x^2 x - k^2\sigma_x^4 + k^2\sigma_x^4}{2\sigma_x^2} = \frac{\left(x+ik\sigma_x^2\right)^2}{2\sigma_x^2} + \frac{k^2\sigma_x^2}{2}$

Fourier Transform of a Gaussian 2

So $\int_{-\infty}^{+\infty} dx \exp\left(-\frac{x^2 + 2ik\sigma_x^2 x}{2\sigma_x^2}\right) = \int_{-\infty}^{+\infty} dx \exp\left(-\frac{\left(x + ik\sigma_x^2\right)^2}{2\sigma_x^2} - \frac{k^2\sigma_x^2}{2}\right)$

$$= \int_{-\infty}^{+\infty} dx \exp\left(-\frac{\left(x + ik\sigma_x^2\right)^2}{2\sigma_x^2}\right) \cdot \exp\left(-\frac{k^2\sigma_x^2}{2}\right)$$

$$= \exp\left(-\frac{k^2\sigma_x^2}{2}\right) \cdot \int_{-\infty}^{+\infty} dx \exp\left(-\frac{\left(x + ik\sigma_x^2\right)^2}{2\sigma_x^2}\right)$$

Change integration variable to $u = x + ik\sigma_x^2$

$$= \exp\left(-\frac{k^2\sigma_x^2}{2}\right) \cdot \int_{-\infty}^{+\infty} du \exp\left(-\frac{u^2}{2\sigma_x^2}\right)$$

and the integral is a number independent of k

So $a(k) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dx \; y(x) \exp(-ikx) = \exp\left(-\frac{k^2\sigma_x^2}{2}\right) \cdot \text{number}$

Fourier Transform of a Gaussian 3

Define $\sigma_k = \frac{1}{\sigma_x}$

$$a(k) = \exp\left(-\frac{k^2\sigma_x^2}{2}\right) = \exp\left(-\frac{k^2}{2\sigma_k^2}\right)$$

This is a Gaussian in k, with width $\sigma_k = \frac{1}{\sigma_x}$

So a Gaussian in x of width σ_x Fourier-transforms into

a Gaussian in k of width $\sigma_k = \frac{1}{\sigma_x}$

Note that $\sigma_x \cdot \sigma_k = \sigma_x \cdot \frac{1}{\sigma_x} = 1$

I've been sloppy about normalizations, but they don't matter for the above

And they all do work out.

Heisenberg Uncertainty Principle

Consider $a(k) = \frac{1}{\sqrt{2\pi}\,\sigma_k} \exp\left[\frac{-k^2}{2\sigma_k^2}\right]$

This is a Gaussian in *k*-space, centered on $k = 0$, and width $\sigma_k = 1/\sigma_x$

So a Gaussian envelope in *x*-space of width σ_x gives a Gaussian in *k*-space of width $\sigma_k = 1/\sigma_x$, which implies that $\sigma_x \sigma_k = 1$

Since $p = \hbar k$, the width in momentum space is $\sigma_p = \hbar \sigma_k$

Then $\sigma_x \sigma_p = \sigma_x \hbar \sigma_k = \hbar$. That's looking Heisenberg-ish.

Heisenberg Uncertainty Principle 2

Heisenberg says $\sigma_x \sigma_p \geq \frac{\hbar}{2}$. Why are we off by a factor of 2?

Heisenberg is a statement about <u>probabilities</u>, and we have been calculating with <u>wavefunctions</u>. We have to conjugate-square our wave functions.

$$\left[\exp\left(\frac{-x^2}{2\sigma^2}\right)\right]^2 = \exp\left(\frac{-2x^2}{2\sigma^2}\right) = \exp\left(\frac{-x^2}{\sigma^2}\right) = \exp\left(\frac{-x^2}{2\left(\sigma/\sqrt{2}\right)^2}\right)$$

When you square a Gaussian, the width goes down by $\sqrt{2}$.

That happens in both σ_x and σ_p. So we get $\sigma_x \sigma_p \geq \frac{\hbar}{2}$

Heisenberg Uncertainty Principle 3

Heisenberg says $\sigma_x \sigma_p \geq \frac{\hbar}{2}$. Why greater than or equal?

Gaussian wave functions are "minimum uncertainty" and give you the lower limit. You can prove formally that absolutely any other wavefunction is worse.

In fact, remember that the wave packet spreads in *x*-space, but it stays the same width in *k*-space. It doesn't get narrower in *k*-space. So we only get the minimum product at $t = 0$.

Amusingly, you can step Schrodinger backwards in time as well as forward.
The wave packet spreads in negative time as well as positive time.
That means that it is getting narrower at negative time approaches zero.

So it's not true that a wave packet always spreads out. If you construct it carefully, you can make a wave packet that gets narrower. But only for a while. It will eventually hit a minimum width, then start to get wider again.

Introducing Forces

The 1-D free-particle Schrodinger Equation is $i\hbar\frac{\partial y}{\partial t}=\frac{-\hbar^2}{2m}\frac{\partial^2 y}{dx^2}$

"Free-particle" means it doesn't include any forces.

Both sides have dimensions of energy (times the wavefunction).

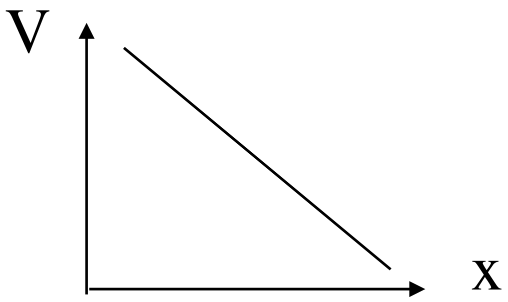
We include forces by adding a potential energy function, $V(x)$, also times the wavefunction:

$$i\hbar\frac{\partial}{\partial t}y(x,t)=\frac{-\hbar^2}{2m}\frac{\partial^2}{dx^2}y(x,t)+V(x)\cdot y(x,t)$$

Potential Types

The potential is (minus) the integral of force over distance.

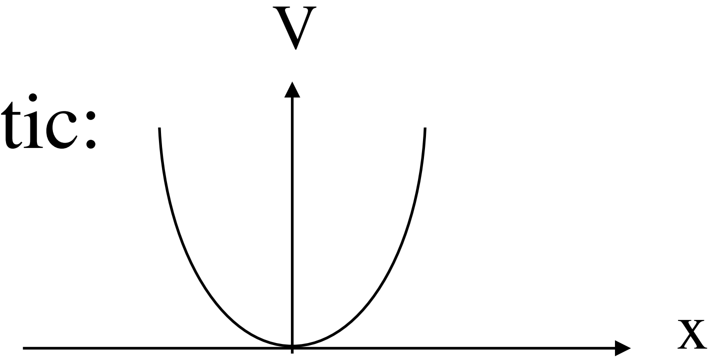
A constant force gives a linear potential:



$$F\left(x\right)=F_{\text{constant}}\rightarrow V\left(x\right)=-F_{\text{constant}}\cdot x$$

The Schrodinger solutions for that turn out to be something called the Airy function. You probably haven't seen it, but it's not hard to work with.

A (restoring) force proportional to distance gives a quadratic:

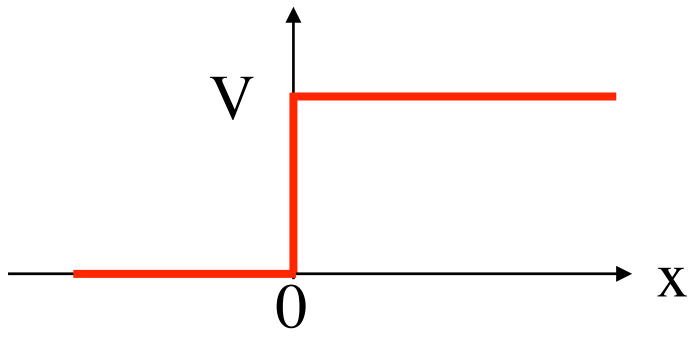


$$F\left(x\right)=-kx\rightarrow V\left(x\right)=+\frac{1}{2}kx^{2}$$

This is the potential for a harmonic oscillator.
The solutions turn out to be a Gaussian times polynomials in *x*.

Step Potential

The simplest cases are when the potential is zero at $x < 0$, and steps to a different value for $x > 0$, then maybe steps back.



Classically, if a particle comes in from the left with energy E, and $V > E$, the particle will bounce back.

If $V < E$, the particle will continue to positive x, but at a reduced velocity.

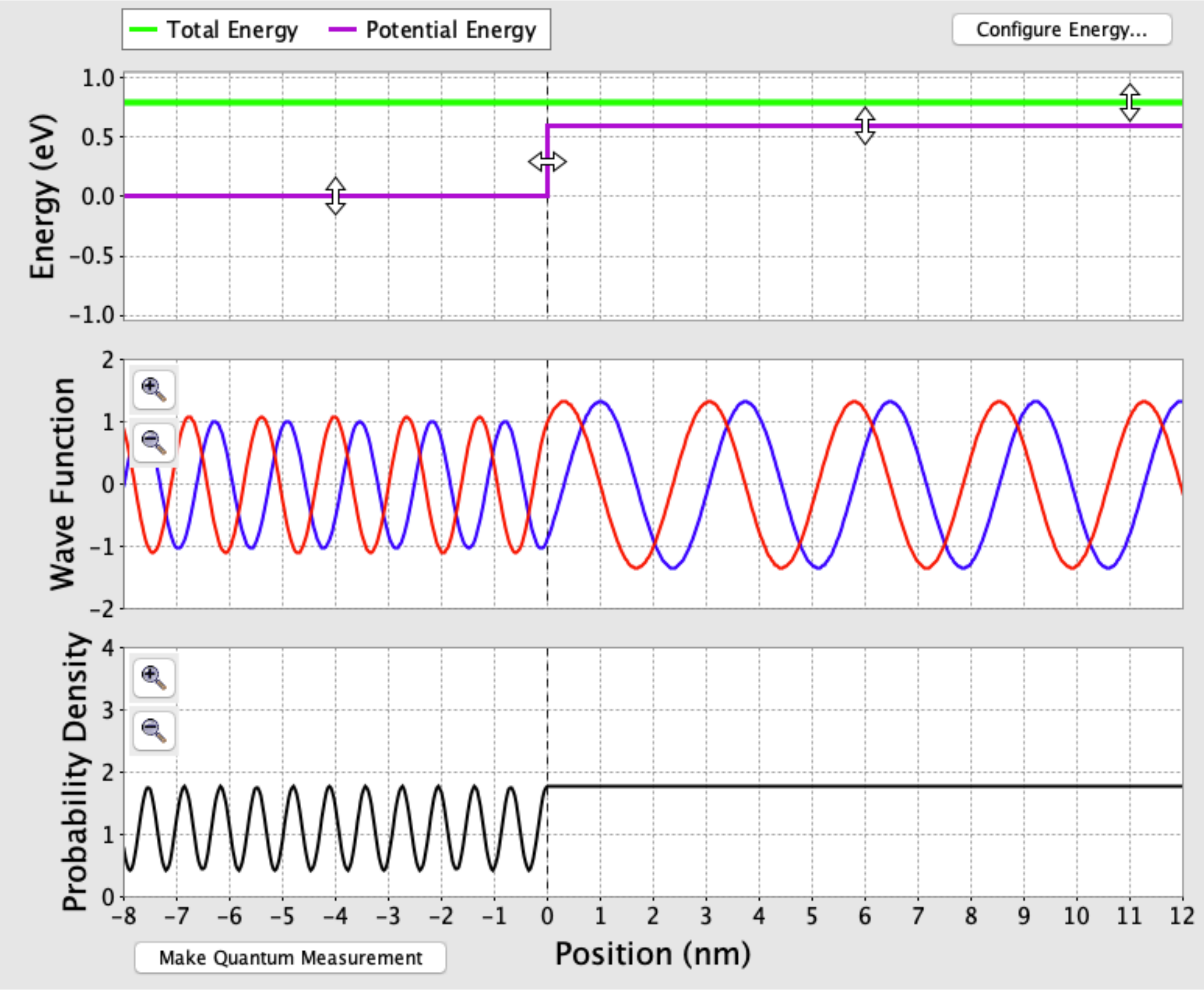
Examples with E = 0.8 eV

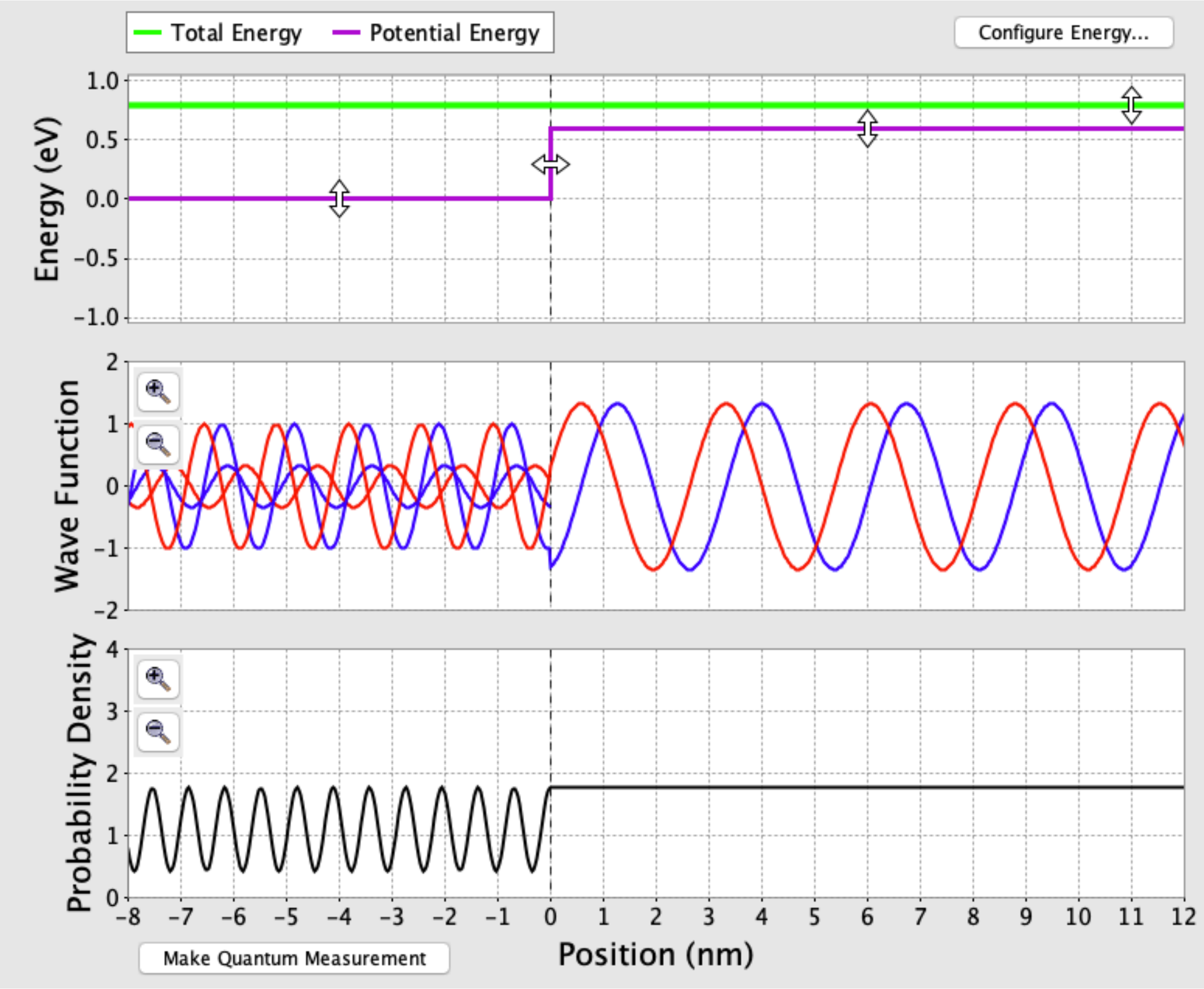
V = 0.6 eV

V = 1.0 eV

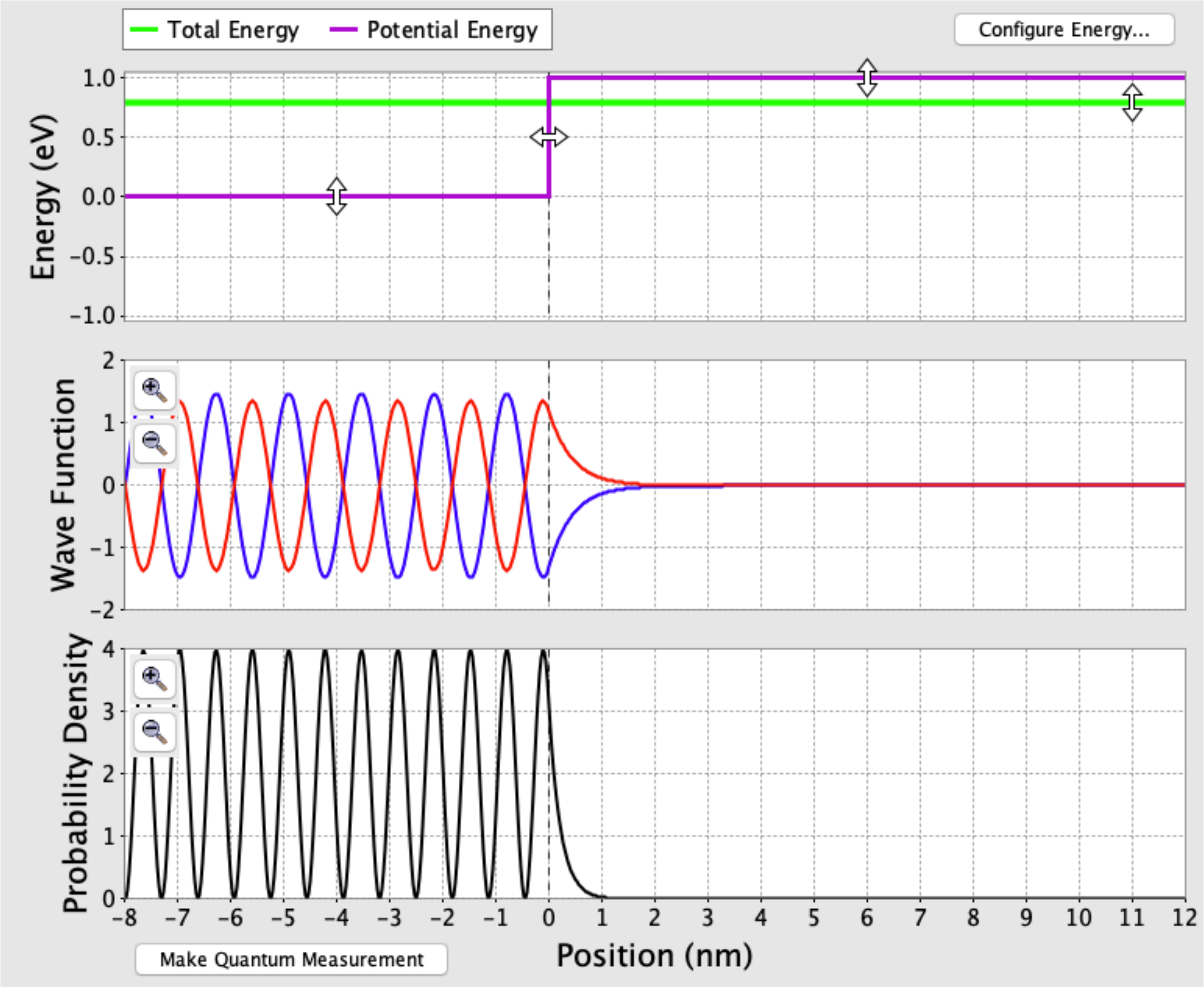
V = 1.0 eV, then back to V = 0

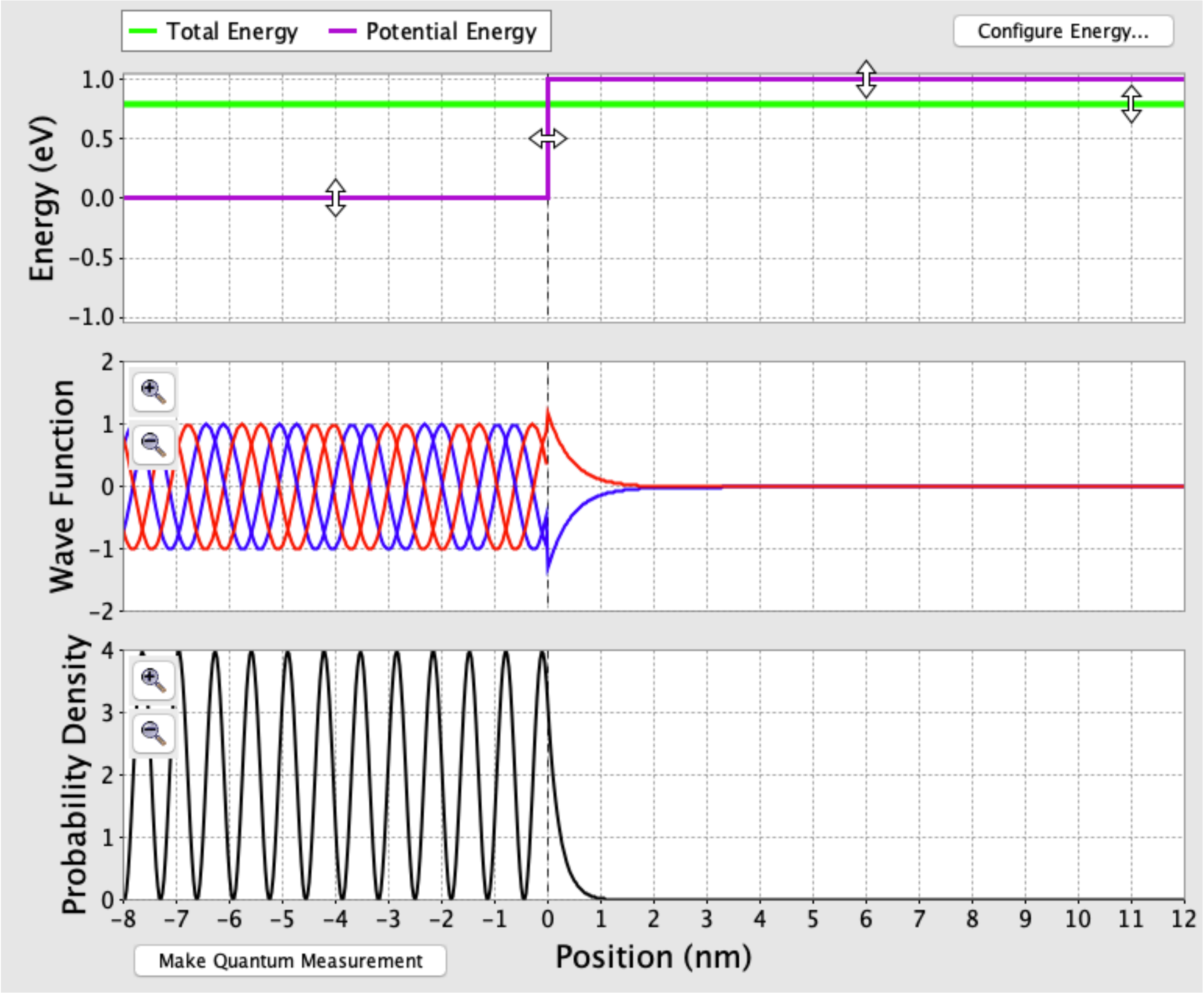
Step of 0.6 eV, $E = 0.8$ eV



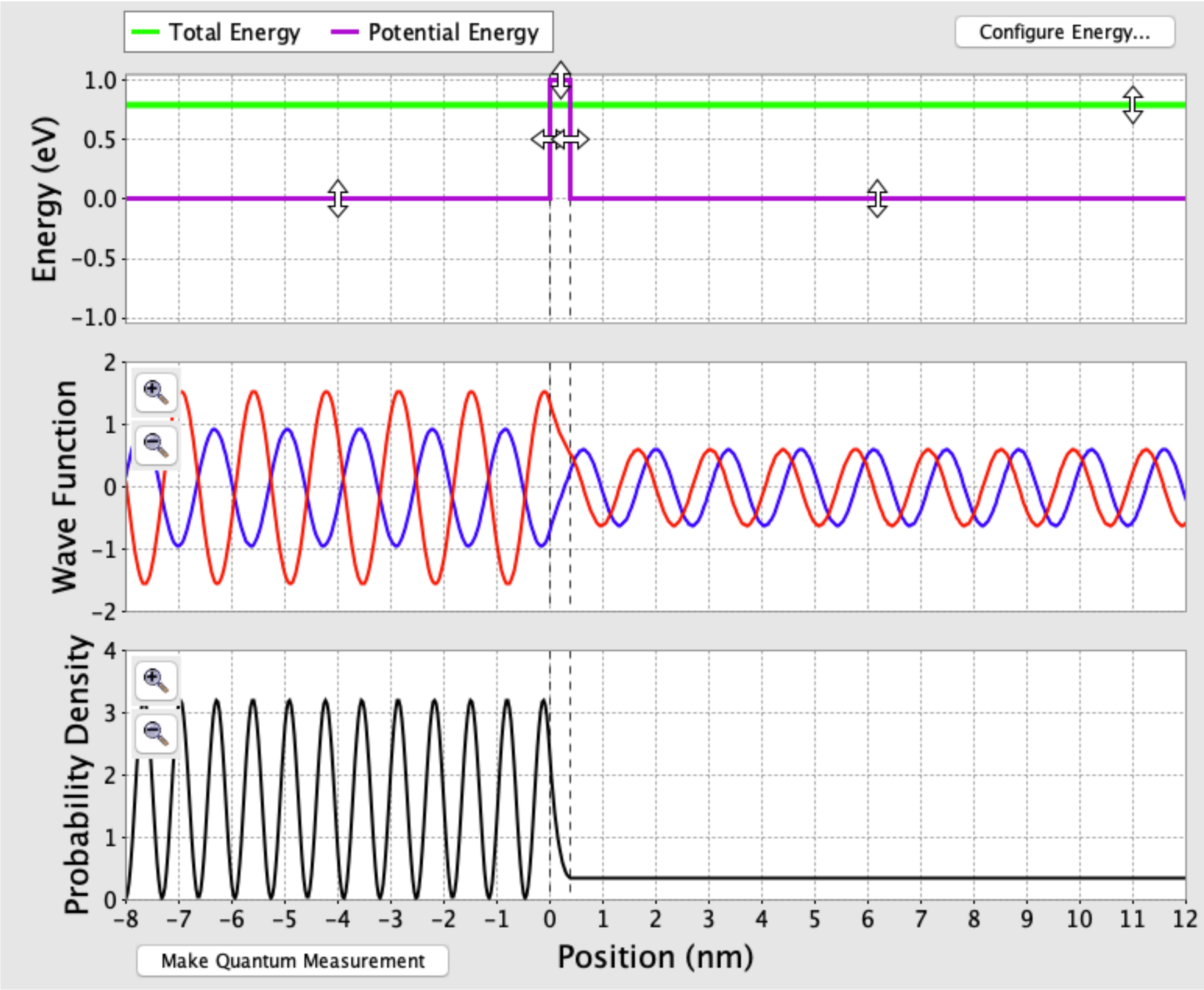


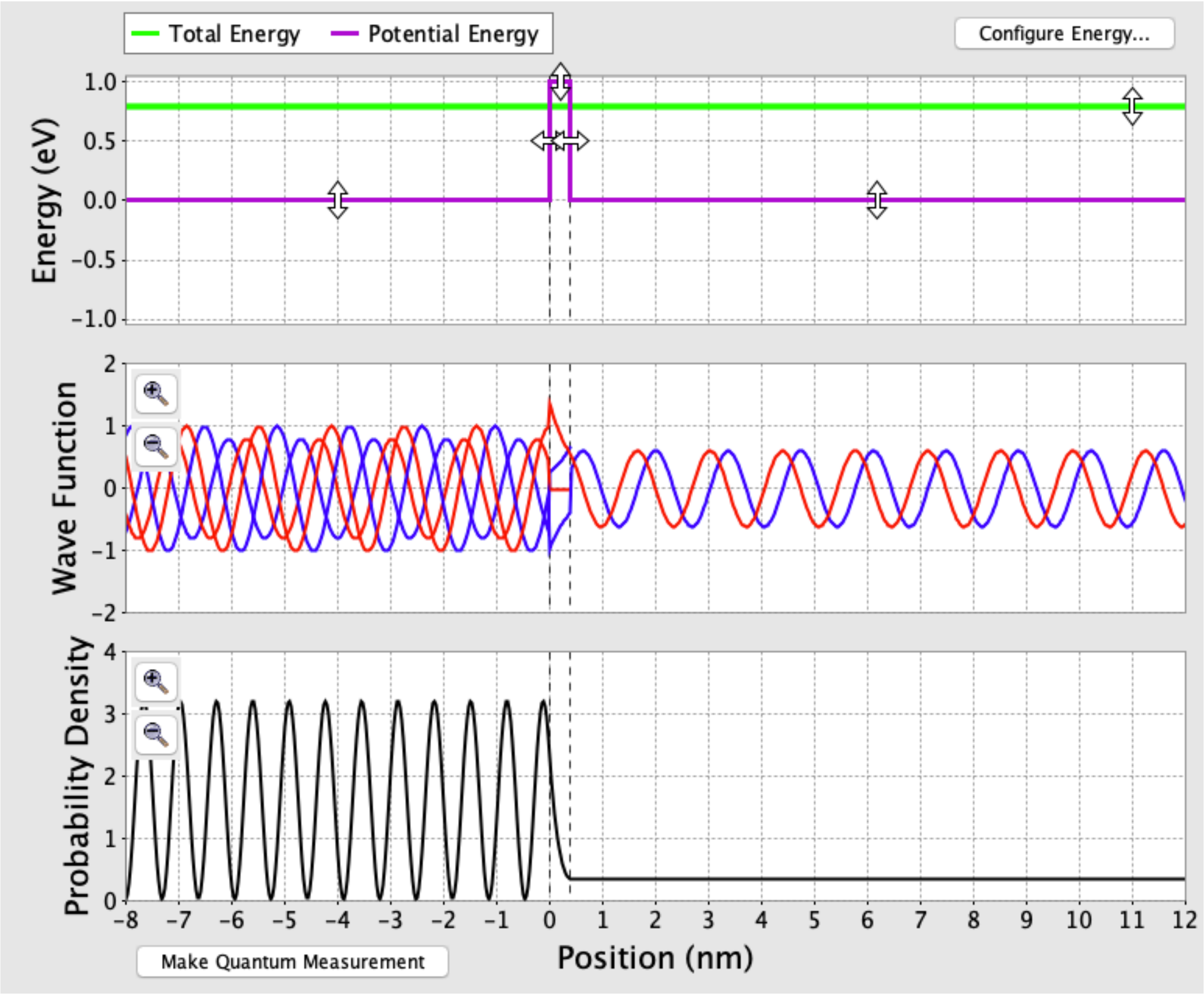
Step of 1.0 eV, $E = 0.8$ eV





Step of 1 eV up, then back down to 0 eV





Summary of Examples with E = 0.8 eV

V = 0.6 eV

Wave is transmitted, like the classical case.
There is also a reflected wave, which sums to a standing wave
(if the step were gradual, the reflection wouldn’t occur)

V = 1.0 eV

The incident wave is completely reflected as a standing wave, like the classical case.
But the wavefunction extends into the barrier a bit.

V = 1.0 eV, then back to V = 0

Unlike the classical case, some of the wave crosses the step.
The rest of the wave is reflected.

For Next Time

WebWork 3 is due at midnight

Midterm Exam at 5-6 PM Wednesday, in this room.
You may bring one page (both sides) of notes.
Group formula sheet is OK, but you learn more by making your own.
Any calculator, but no phones, tablets, laptops or anything wireless.

Today's (and Wednesday's) material on Schrodinger will <u>not</u> be on the exam.

Wednesday is Schrodinger bound states, Friday is tutorial worksheet.

Next week is Applications: Lasers and Semiconductors.