PHYS 250

Lecture 4.2

Schrodinger Equation with Potentials

Preview

Midterm and Final Exam Info
Review
Separating the Time-Dependence
Waves with Potential Step: Transmission, Reflection
Waves with Potential Barrier
Tunnelling
Infinite Square Well: Bound States
Finite Square Well: Bound States + Continuum
Symmetry of Solutions
Quantum Harmonic Oscillator

Midterm and Final Exam

Midterm is today at 5-6 PM, in this room.

Bring 1 page (both sides) of notes. I do not provide a formula sheet.

Bring any calculator. But no laptops, tablets, or anything wireless.

Final exam is Monday June 23 at 3:30-6 PM in BIOL 1000.

Bring two pages (both sides) of notes, and a calculator.

Review 1

Wave Equation $\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \cdot \frac{\partial^2 y}{\partial t^2}$ has a fixed velocity built in.

Solutions $y(x,t) = g(x \pm vt)$ or $\sin(kx - \omega t + \phi)$ with $k = \frac{2\pi}{\lambda}$, $\omega = 2\pi f$, $v = \frac{\omega}{k}$

Schrodinger sought a wave equation with different velocities,

consistent with de Broglie $\lambda = \frac{h}{p}$, Planck $E = hf$, and classical $E = \frac{p^2}{2m}$.

Time-Dependent Schrodinger Equation: $i\hbar \frac{\partial}{\partial t}\psi(x,t) = \frac{-\hbar^2}{2m}\frac{\partial^2}{dx^2}\psi(x,t) \quad \hbar = \frac{h}{2\pi}$

Plane-Wave Solutions: $\psi(x,t) = \exp\left[i(kx - \omega t)\right] = \exp\left[i\frac{px - Et}{\hbar}\right]$

with $p = \hbar k$, $E = \hbar\omega = \frac{(\hbar k)^2}{2m}$

Review 2

Both sides of Schrodinger are of the form $(E)\cdot\psi$

Include forces by adding a term $V(x)\cdot\psi$ where $V(x)$ is the potential function

related to the force by $V(x) = -\int F(x)\,dx$

Time-Dependent Schrodinger Equation with Potential

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

Review 3

The time-dependent wavefunction $\psi(x, t)$ is complex.

The complex conjugate is $\psi^*(x, t)$, which we get by changing i to $-i$ everywhere.

The product $\psi^*(x,t)\cdot\psi(x,t)$ is real and non-negative.

The relative probability of finding the particle at position x is $\psi^*(x,t)\cdot\psi(x,t)$.

We can multiply a Schrodinger solution $\psi(x, t)$ by any constant,
and it's still a solution.

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

Then $\int_{x1}^{x2}\psi^*\psi\, dx$ is the probability of finding the particle between x_1 and x_2.

Review 4

The Fourier Transform of a function $y(x)$ is $a(k)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} dx\; y(x)\exp(-ikx)$.

This decomposes $y(x)$ into plane waves $\exp(ikx)$ with amplitudes $a(k)$.

To reconstruct $y(x)$, use the inverse transform $y(x)=\int_{-\infty}^{+\infty} dk\; a(k)\exp(+ikx)$.

The Fourier Transform of a Gaussian in x-space $\exp\left(\frac{-x^2}{2\sigma_x^2}\right)$,

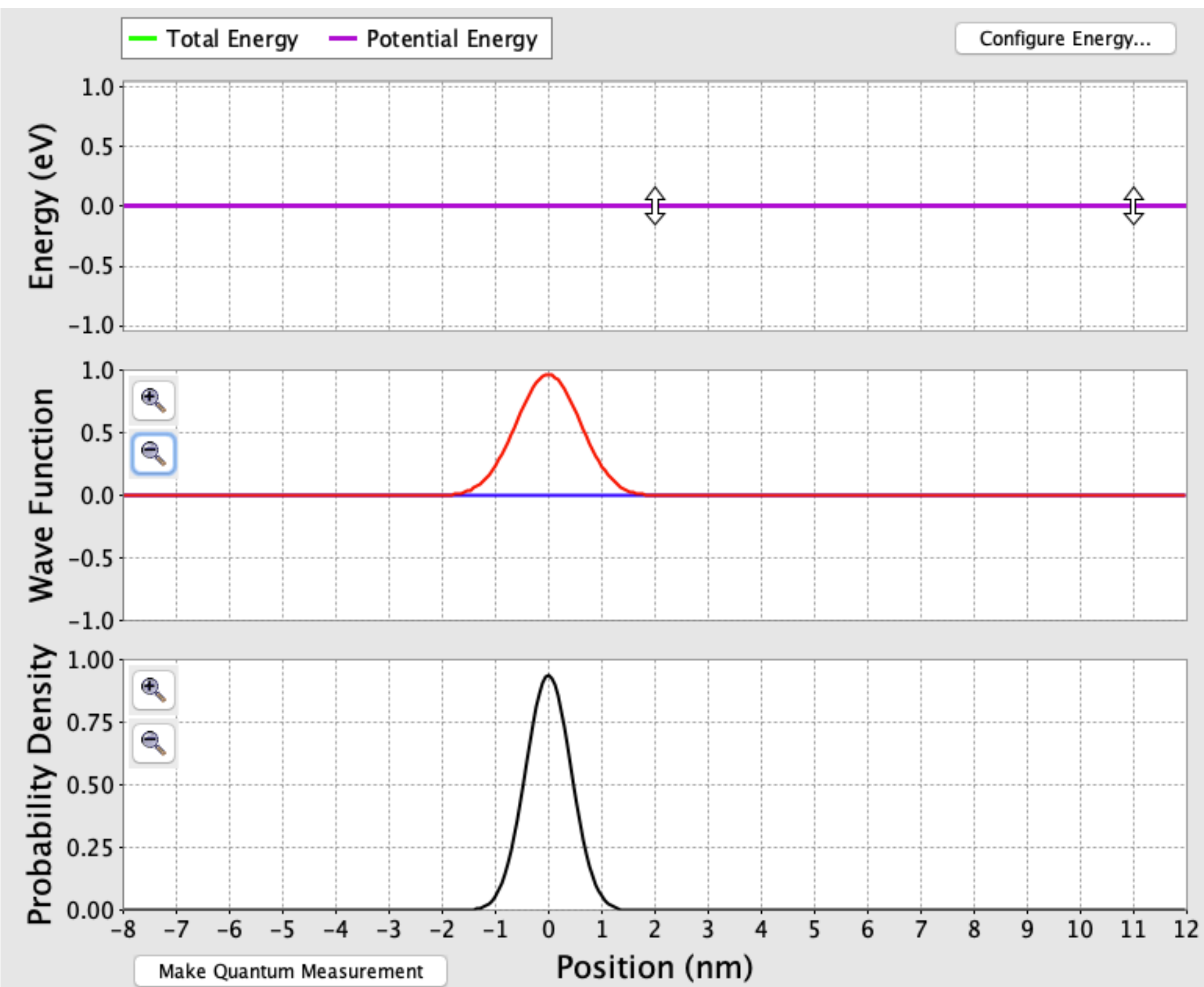
ignoring normalization, is a Gaussian in k-space $\exp\left(\frac{-k^2}{2\sigma_k^2}\right)$ with $\sigma_x \cdot \sigma_k = 1$

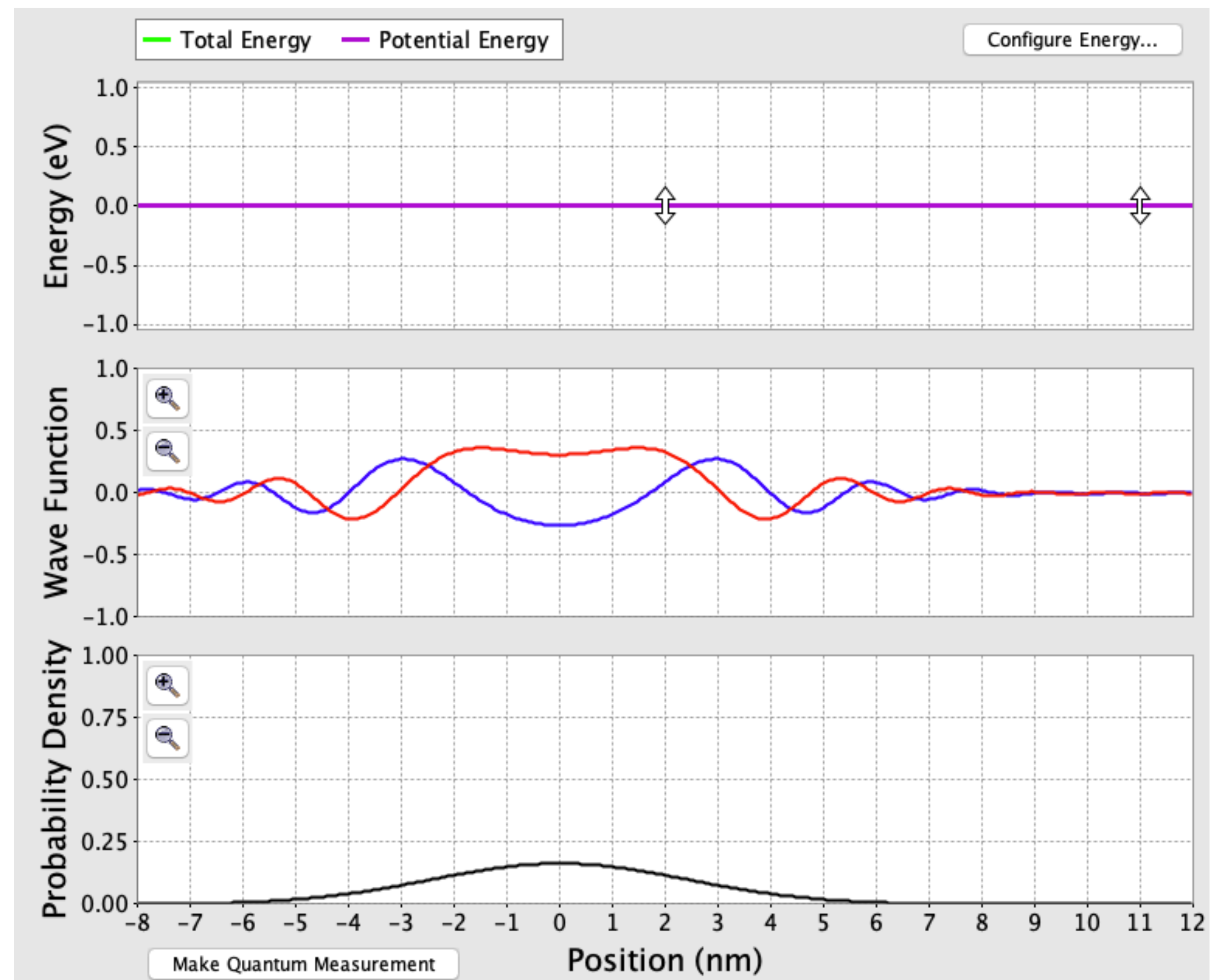
This leads to the Heisenberg Uncertainty Principle: $\sigma_x \sigma_p \geq \frac{\hbar}{2}$.

Review 5

A Gaussian wavefunction with zero velocity can be decomposed into components with positive and negative k, and thus positive and negative $p = \hbar k$.

So the Gaussian wavefunction spreads out over time.
The narrower it is in x-space, the wider it is in k-space, and the faster it spreads.

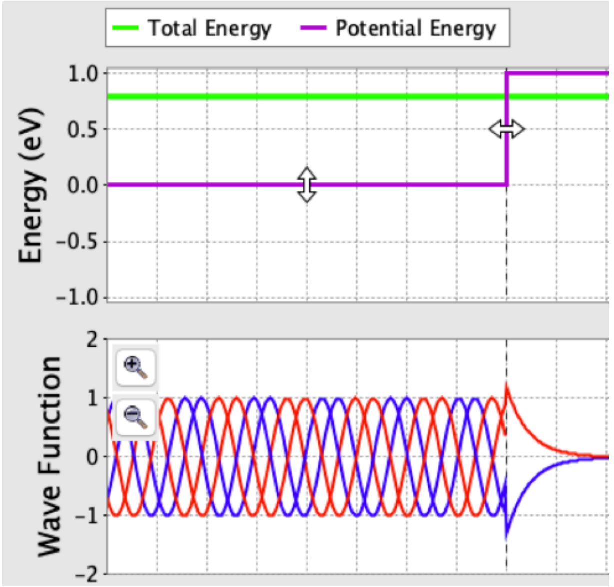




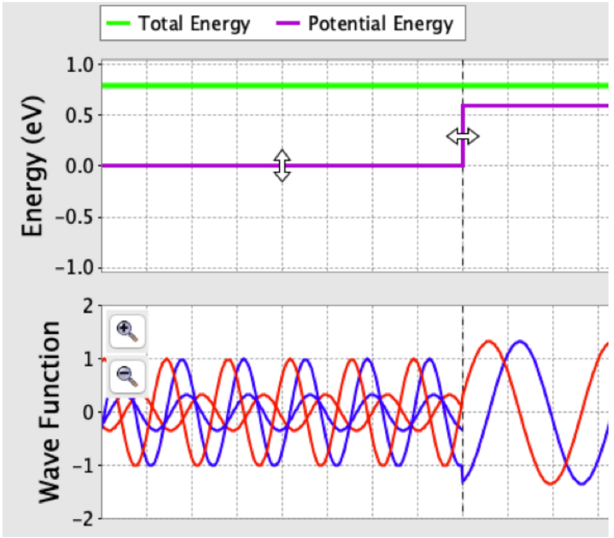
But the area under $\psi^*(x,t) \cdot \psi(x,t)$ stays constant.

Review 6

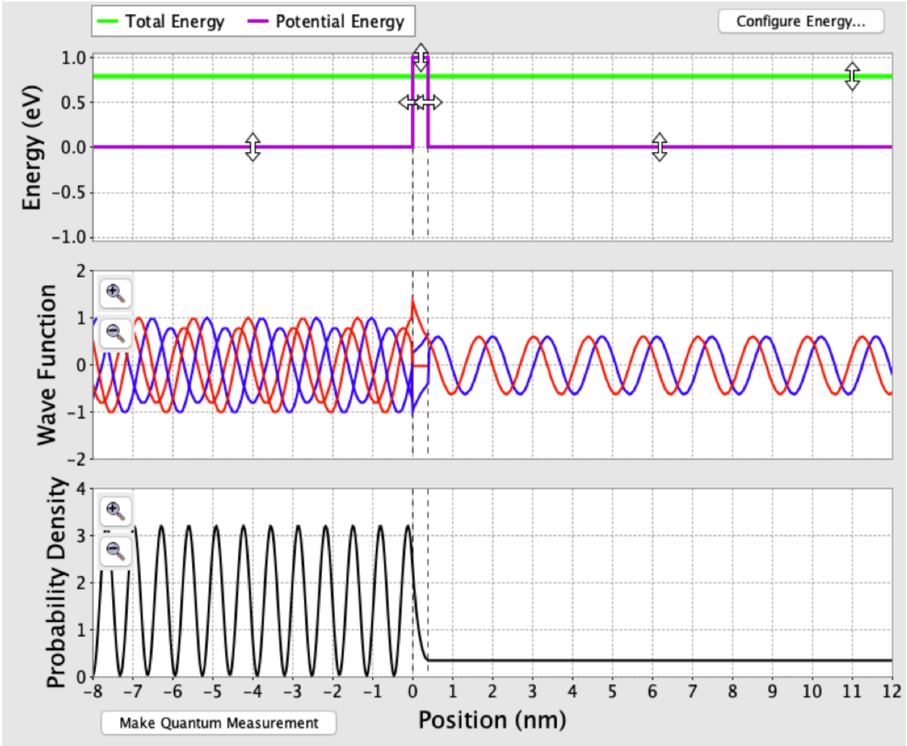
A plane wave incident on a potential step that is higher than its energy is completely reflected, like the classical case, but penetrates inside a bit.



A plane wave incident on a step lower than its energy is transmitted like the classical case, but there is also some reflection (artifact of infinitely steep step).



If the potential steps up above the particle energy, then steps back to zero, in a distance that is not long compared to the wavelength, then the wave is mostly reflected, but some penetrates the barrier. This is called tunnelling.



Review 7

An operator is something that turns a function into another function.

The momentum operator is $p_{op} = \frac{\hbar}{i}\frac{\partial}{\partial x}$.

Applying it to $\psi = \exp\left[i\frac{px - Et}{\hbar}\right]$ gives $\frac{\hbar}{i}\cdot i\frac{p}{\hbar}\cdot \exp\left[i\frac{px - Et}{\hbar}\right] = p\psi$.

We say that this ψ is an eigenfunction of p_{op} with eigenvalue p.

Separating Schrodinger

Many Schrodinger solutions can be written as the product of a function of space and a function of time: $\psi(x,t) = f(x)\cdot g(t)$. Plugging that into Schrodinger

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

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

Divide by $f(x)\cdot g(t)$: $$i\hbar\frac{1}{g}\cdot\frac{\partial g}{\partial t} = \frac{-\hbar^2}{2m}\frac{1}{f}\cdot\frac{\partial^2 f}{dx^2} + V(x)$$

The left side has no x-dependence, the right side has no t-dependence, so both sides must be equal to some constant we will call E:

$$i\hbar\frac{1}{g}\cdot\frac{\partial g}{\partial t} = E = \frac{-\hbar^2}{2m}\frac{1}{f}\cdot\frac{\partial^2 f}{dx^2} + V(x)$$

Separating Schrodinger 2

$$i\hbar \frac{1}{g} \cdot \frac{\partial g}{\partial t} = E = \frac{-\hbar^2}{2m} \frac{1}{f} \cdot \frac{\partial^2 f}{dx^2} + V(x)$$

The left equation is easy to solve:

$$i\hbar \frac{1}{g} \cdot \frac{\partial g}{\partial t} = E \rightarrow \frac{dg}{g} = \frac{E}{i\hbar} \cdot dt \rightarrow \int \frac{dg}{g} = \frac{E}{i\hbar} \int dt + C$$

$$\ln g = \frac{Et}{i\hbar} + C \rightarrow g(t) = \exp\left(-i \frac{Et}{\hbar} + C\right) = C' \exp\left(-i \frac{Et}{\hbar}\right)$$

$$g(t) = C' \exp(-i\omega t) \text{ with } \omega = \frac{E}{\hbar}$$

Separating Schrodinger 3

The right equation we just transform by multiplying by *f* and rearranging:

$$E = \frac{-\hbar^2}{2m}\frac{1}{f}\cdot\frac{\partial^2 f}{dx^2} + V(x) \rightarrow \frac{-\hbar^2}{2m}\cdot\frac{\partial^2}{dx^2} f(x) + V(x)\cdot f(x) = E\cdot f(x)$$

This is more commonly written with $\psi(x)$: $\frac{-\hbar^2}{2m}\cdot\frac{\partial^2\psi}{dx^2} + V\cdot\psi = E\psi$

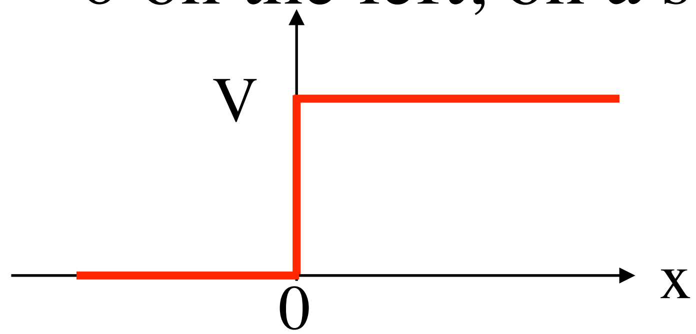
This is the Time-Independent Schrodinger Equation.

Note that this is a real equation (no i's) so it can have real solutions.

But it can also have complex solutions, and they are often convenient to use.

Simple Step Potential Problem

There is a wave with some momentum or energy,
incident from a region with $V = 0$ on the left, on a step to V at $x = 0$.



We find $p = \sqrt{2mE}$ if necessary, then $k = p/\hbar$.

The incident wave is $\psi_I(x,t) = \exp\left[i(kx - \omega t)\right]$, taking the amplitude to be 1.

There is a reflected wave with unknown amplitude and <u>opposite momentum</u>,
and a transmitted wave with unknown amplitude and different momentum k'.

There are boundary conditions at the step, that have to be satisfied at <u>all times</u>.
So all 3 waves must have the <u>same time-frequency ω</u>.

So they are $\psi_R(x,t) = R\exp\left[i(-kx - \omega t)\right]$ and $\psi_T(x,t) = T\exp\left[i(k'x - \omega t)\right]$

Simple Step Potential Problem 2

Since the time-dependence is the same, the energy $E = \hbar\omega$ is the same for all 3 waves, and we can use the time-independent Schrodinger Equation, and time-independent wavefunctions. So we have

$$\psi_I = \exp\left[ikx\right] \quad \psi_R = R\exp\left[-ikx\right] \quad \psi_T = T\exp\left[ik'x\right]$$

Now we use Schrodinger to figure out k':

$$\frac{-\hbar^2}{2m}\cdot\frac{\partial^2\psi_T}{dx^2} + V\cdot\psi_T = E\psi_T$$

$$\frac{-\hbar^2}{2m}\cdot\left(ik'\right)^2\cdot T\exp\left[ik'x\right] = \left(E-V\right)T\exp\left[ik'x\right]$$

$$\frac{-\hbar^2}{2m}\cdot\left(ik'\right)^2 = E-V$$

$$k' = \frac{\sqrt{2m\left(E-V\right)}}{\hbar} = \frac{\sqrt{2mc^2\left(E-V\right)}}{\hbar c}$$

Simple Step Potential Problem 3

One boundary condition is that the <u>sum</u> of the incident and reflected waves must be equal to the transmitted wavefunction at the boundary.

$$\psi_I(0) + \psi_R(0) = \psi_T(0)$$

$$\exp[ik0] + R\exp[-ik0] = T\exp[ik'0]$$

$$1 + R = T$$

The other condition is that the <u>slope</u> of the incident plus reflected waves must be equal to the slope of the transmitted wave at the boundary.

$$\left.\frac{d\psi_I}{dx}\right|_0 + \left.\frac{d\psi_R}{dx}\right|_0 = \left.\frac{d\psi_T}{dx}\right|_0$$

$$ik\exp[ik0] - ikR\exp[-ik0] = ik'T\exp[ik'0]$$

$$k - kR = k'T$$

Simple Step Potential Problem 4

We have $1+R=T$ and $k-kR=k'T$.

Multiply first equation by k and add:

$$\begin{array}{l} k+kR=kT \\ k-kR=k'T \\ \hline 2k=\left(k+k'\right)T \end{array}$$

$$T=\frac{2k}{k+k'}$$

Multiply first by k' and subtract:

$$\begin{array}{l} k'+k'R=k'T \\ k \quad -kR=k'T \\ \hline k'-k+k'R+kR=0 \end{array}$$

$$\left(k'+k\right)R=k-k'$$

$$R=\frac{k-k'}{k+k'}$$

Simple Step Potential Problem 5

So we have $R = \dfrac{k - k'}{k + k'}$ $T = \dfrac{2k}{k + k'}$ $k = \dfrac{\sqrt{2mE}}{\hbar}$ $k' = \dfrac{\sqrt{2m \cdot \left(E - V\right)}}{\hbar}$

The factor $\sqrt{2m}\big/\hbar$ cancels in T and R, so we don't need the mass or $\hbar$!

$$R = \frac{\sqrt{E} - \sqrt{E - V}}{\sqrt{E} + \sqrt{E - V}} \qquad T = \frac{2\sqrt{E}}{\sqrt{E} + \sqrt{E - V}}$$

If $V = 0$, then reflected $R = 0$, and transmitted $T = 1$.

If $V < E$, then $R > 0$, but transmitted $T > 1$??

If $V > E$, we get an imaginary k'! That makes R and T complex, which is OK.

And the transmitted wave becomes a <u>real</u> exponential $\psi_T = T\exp\left[-\left|k'\right|x\right]$.

Simple Step Potential Problem 6

$$R = \frac{\sqrt{E} - \sqrt{E-V}}{\sqrt{E} + \sqrt{E-V}} \quad T = \frac{2\sqrt{E}}{\sqrt{E} + \sqrt{E-V}}$$

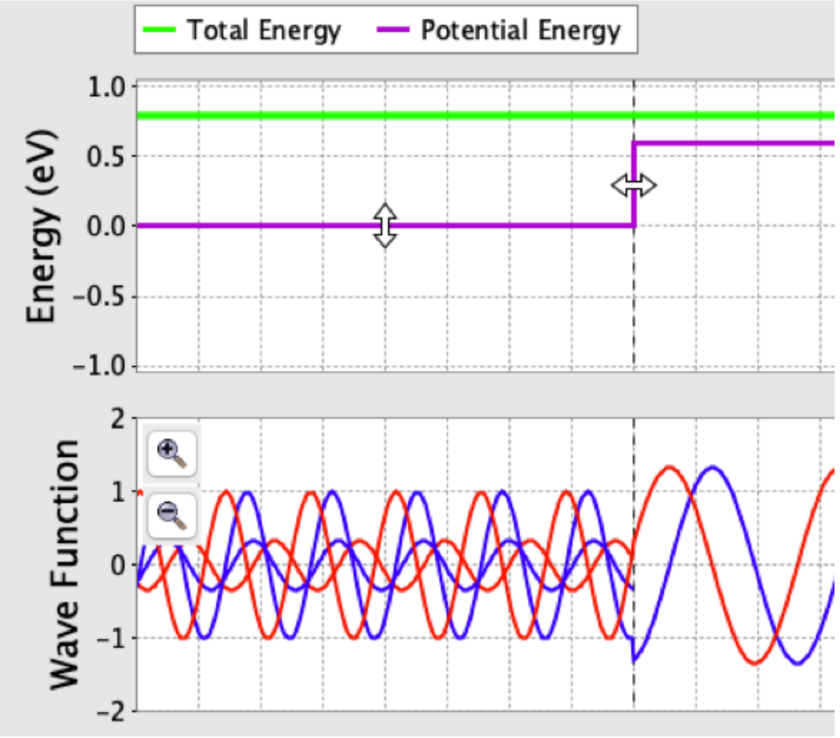
If V goes to + infinity, $\sqrt{E-V}$ becomes imaginary infinity.

That makes $R = -1$. The reflected wave has the same magnitude as the incident wave, but the opposite phase, so they add up to zero at the potential step. The transmitted amplitude T goes to zero.

If V is slightly less than E then $\sqrt{E-V}$ is real but small.
That makes T slightly less than 2. The transmitted probability is the square, or 4 !

What's going on?

Interpreting the Results



We already saw a similar thing with the simulation. When E and V are similar, the transmitted amplitude can be larger than the incident amplitude.

That <u>does</u> mean that the probability of finding a particle to the right of the step is larger than on the left of the step.

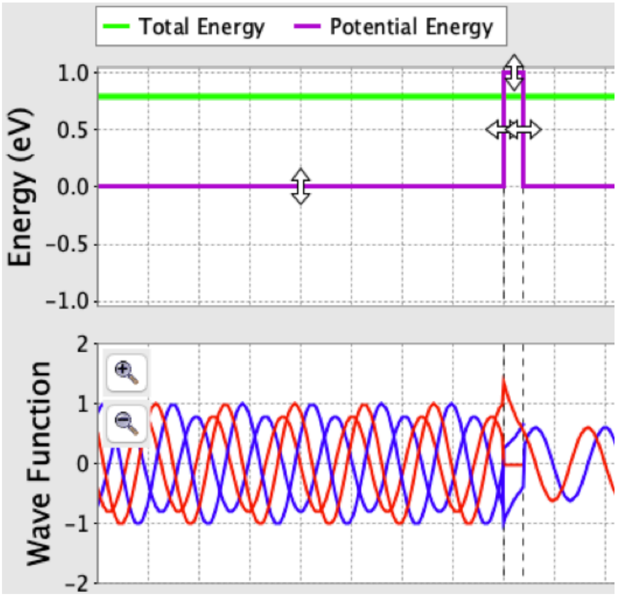
But that's because <u>the step slows the particle down</u>.

If particles with speed v enter separated by Δt, the density is $1/(v\Delta t)$.

If they slow down to 1/10 the speed, the density goes up by a factor of 10.

Potential Barrier

We will assume V in the barrier, and $V = 0$ outside. The barrier runs from $x = 0$ to $x = w$.



There is an incident wave, a reflected wave, a transmitted wave, but also a forward wave a backwards wave inside the barrier.

$$\psi_I = \exp\left[ikx\right] \qquad \psi_R = R\exp\left[-ikx\right] \qquad \psi_T = T\exp\left[ikx\right]$$

$$\psi_F = F\exp\left[ik'x\right] \qquad \psi_B = B\exp\left[-ik'x\right]$$

We compute k and k' the same way as for the simple potential step. The boundary condition equations are

$$1 + R = F + B \qquad F\exp\left[ik'w\right] + B\exp\left[-ik'w\right] = T\exp\left[ikw\right]$$

$$k - kR = k'F - k'B \qquad k'F\exp\left[ik'w\right] - k'B\exp\left[-ik'w\right] = kT\exp\left[ikw\right]$$

Potential Barrier 2

Four linear equations in 4 unknowns. Put variables in order.

$$-R + F + B = 1$$

$$kR + k'F - k'B = k$$

$$e^{ik'w}F + e^{-ik'w}B - e^{ikw}T = 0$$

$$k'e^{ik'w}F - k'e^{-ik'w}B - ke^{ikw}T = 0$$

Write in matrix form:

$$\begin{bmatrix} -1 & 1 & 1 & 0 \\ k & k' & -k' & 0 \\ 0 & e^{ik'w} & e^{-ik'w} & -e^{ikw} \\ 0 & k'e^{ik'w} & -k'e^{-ik'w} & -ke^{ikw} \end{bmatrix} \begin{bmatrix} R \\ F \\ B \\ T \end{bmatrix} = \begin{bmatrix} 1 \\ k \\ 0 \\ 0 \end{bmatrix}$$

Potential Barrier 3

Pick values to make the matrix pretty: $k=1,\ k'=0.5,\ w=\pi$, which gives

$$\begin{bmatrix} -1 & 1 & 1 & 0 \\ 1 & 0.5 & -0.5 & 0 \\ 0 & i & -i & 1 \\ 0 & 0.5i & 0.5i & 1 \end{bmatrix}\begin{bmatrix} R \\ F \\ B \\ T \end{bmatrix}=\begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

The solution is $R=0.6, F=1.2, B=0.4, T=-0.8i$

That means 60% reflection <u>amplitude</u>, or $60\%^2$ = 36% reflection <u>probability</u>.
And 80% transmission amplitude, or $80\%^2$ = 64% transmission probability.

There is a large internal forward wave, and a smaller backward wave.

Potential Barrier 4

If the barrier is higher than the particle energy, *k*' will be imaginary. Let's try $k' = 0.5i$, with the other values unchanged. The solution is

$$R = 0.53 - 0.79i \quad |R| = 0.944 \quad |R|^2 = 0.892$$

$$F = 1.54 - 0.85i \quad |F| = 1.765 \quad |F|^2 = 3.118$$

$$B = -0.01 + 0.07i \quad |B| = 0.076 \quad |B|^2 = 0.006$$

$$T = -0.27 - 0.19i \quad |T| = 0.328 \quad |T|^2 = 0.107$$

Note that $\frac{k'}{k} = 0.5i = \frac{\sqrt{2m\left(E-V\right)}\big/\hbar}{\sqrt{2mE}\big/\hbar} = \sqrt{\frac{E-V}{E}}$.

Square both sides: $-0.25 = \frac{E-V}{E} \rightarrow V = 1.25E$.

Tunnelling Approximation

There is a wave transmitted into the barrier, which is a decaying real exponential.

At the exit end of the barrier, some of that wave is transmitted out of the barrier as a complex exponential with the original k, and there is also a reflection.

The reflection decays as it travels back to the entry end.

Ideally, we calculate the transmission into the barrier from the incident wave, the transmitted wave, and the reflection from the exit end of the barrier.

But if the decay in the barrier is large, the reflected wave is tiny at the entry, so we neglect it.

We already know how to calculate the transmission T into the barrier.
And we know how to calculate the decay from entry to exit.
So we just need to calculate the transmission T_2 out at the exit,
and multiply it all together.

Tunnelling Approximation 2

At the exit end, we have forward and backward waves, and a transmitted wave

$$\psi_F = \exp\left[ik'x\right] \quad \psi_B = R_2 \exp\left[-ik'x\right] \quad \psi_{T2} = T_2 \exp\left[ikx\right]$$

For $V > E$, k is real but k' is imaginary. So ψ_F is a real decaying exponential, and ψ_B is a real exponential that grows toward $+x$, so it decays toward $-x$. But ψ_{T2} is a non-decaying complex wave.

The exit boundary is at some non-zero x, but that just gives a phase-factor that is the same for all 3 functions, and we can divide it out. So it's OK to treat the boundary as if it's at $x = 0$.

Matching the wavefunctions at $x = 0$ gives $1 + R_2 = T_2$.
Matching the derivatives gives $ik' - ik'R_2 = ikT_2$.
Multiply the first by ik' and add to get $2ik' = i\left(k + k'\right)T_2 \rightarrow T_2 = \dfrac{2k'}{k + k'}$

Tunnelling Approximation 3

Inside the barrier we have $\psi_{T1} = T_1 \exp\left[ik'x\right]$ with imaginary k' and $T_1 = \dfrac{2k}{k+k'}$.

We multiply that by $T_2 = \dfrac{2k'}{k+k'}$ then $\exp\left[ik\cdot\left(x+w\right)\right]$ for the transmitted wave, where w is the barrier width.

$$\psi_{T2} = T_1 \cdot \exp\left[ik'w\right]\cdot T_2 \cdot \exp\left[ik\cdot\left(x+w\right)\right] = \frac{2k}{k+k'}\cdot\frac{2k'}{k+k'}\cdot\exp\left[ik'w\right]\cdot\exp\left[ik\cdot\left(x+w\right)\right]$$

The matrix solution for $k=1,\ k'=0.5i,\ w=\pi$ was $T = \left(-0.27-0.19i\right)\cdot\exp\left[ikx\right]$.

This approximate solution is

$$\psi_{T2} = \left(\frac{2}{1+0.5i}\cdot\frac{2\cdot 0.5i}{1+0.5i}\cdot\exp\left[-\frac{\pi}{2}\right]\cdot\exp\left[i\cdot 1\cdot\pi\right]\right)\cdot\exp\left[ikx\right]$$

$$= \left(-0.266-0.199i\right)\cdot\exp\left[ikx\right]$$

Tunnelling Approximation 4

We can write the transmitted amplitude

$$T = \frac{2k}{k+k'} \cdot \frac{2k'}{k+k'} \cdot \exp\left[ik'w\right] = \frac{2}{1+k'/k} \cdot \frac{2}{1+k/k'} \cdot \exp\left[ik'w\right]$$

using $k = \frac{\sqrt{2mE}}{\hbar}$ and $k' = \frac{\sqrt{2m\cdot\left(E-V\right)}}{\hbar} = i \cdot \frac{\sqrt{2m\cdot\left(V-E\right)}}{\hbar}$.

Many factors of $\sqrt{2m}/\hbar$ cancel, so $T = \frac{2}{1+i\sqrt{\frac{V-E}{E}}} \cdot \frac{2}{1-i\sqrt{\frac{E}{V-E}}} \cdot \exp\left[ik'w\right]$

The transmission <u>probability</u> is

$$T^*T = \frac{4}{1+\frac{V-E}{E}} \cdot \frac{4}{1+\frac{E}{V-E}} \cdot \exp\left(2ik'w\right) = \frac{4}{1+\frac{V-E}{E}} \cdot \frac{4}{1+\frac{E}{V-E}} \cdot \exp\left(-2\frac{\sqrt{2m\cdot\left(V-E\right)}}{\hbar}w\right)$$

Tunnelling Approximation 5

If $V >> E$, we can introduce another approximation:

$$\frac{4}{1+\frac{V-E}{E}} \cdot \frac{4}{1+\frac{E}{V-E}} \approx \frac{4}{1+\frac{V}{E}} \cdot \frac{4}{1+\frac{E}{V}} \approx 16 \cdot \frac{E}{V} \cdot \left(1-\frac{E}{V}\right)$$

Then the transmission probability through thickness w is then

$$P(w) = 16 \cdot \frac{E}{V} \cdot \left(1-\frac{E}{V}\right) \cdot \exp\left(-2\frac{\sqrt{2m \cdot (V-E)}}{\hbar} w\right)$$

This the formula in Young and Friedman, and most other sources.

Tunnelling Approximation 6

If the barrier is not flat, then the wavefunction inside the barrier will not be exactly an exponential, and we have to solve Schrodinger.

But there is fairly simple approximation for that. We assume the wavefunction is of the form $\psi(x) = \exp[-f(x)]$, meaning the decay length is a function of x.
Then we manipulate Schrodinger into a differential equation for $f(x)$, that can be solved by doing an integration.

The approximate decaying wavefunction inside the barrier is

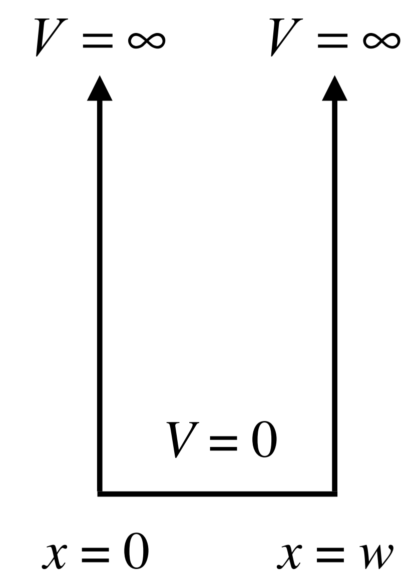
$$\psi(x) = \exp\left[-\frac{\sqrt{2m}}{\hbar}\int_{x=0}^{x} dx\sqrt{V(x) - E}\right]$$

The probability to tunnel through thickness w is then

$$P(w) = 16 \cdot \frac{E}{\langle V \rangle} \cdot \left(1 - \frac{E}{\langle V \rangle}\right)\exp\left[-2\frac{\sqrt{2m}}{\hbar}\int_{x=0}^{x=w} dx\sqrt{V(x) - E}\right]$$

Infinite Square Well 1

Imagine a potential that is + infinite for $x < 0$, zero for $0 < x < w$, and + infinite again for $x > w$.



The wave function must satisfy $E\psi = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\psi}{\partial x^2} + 0\cdot\psi$

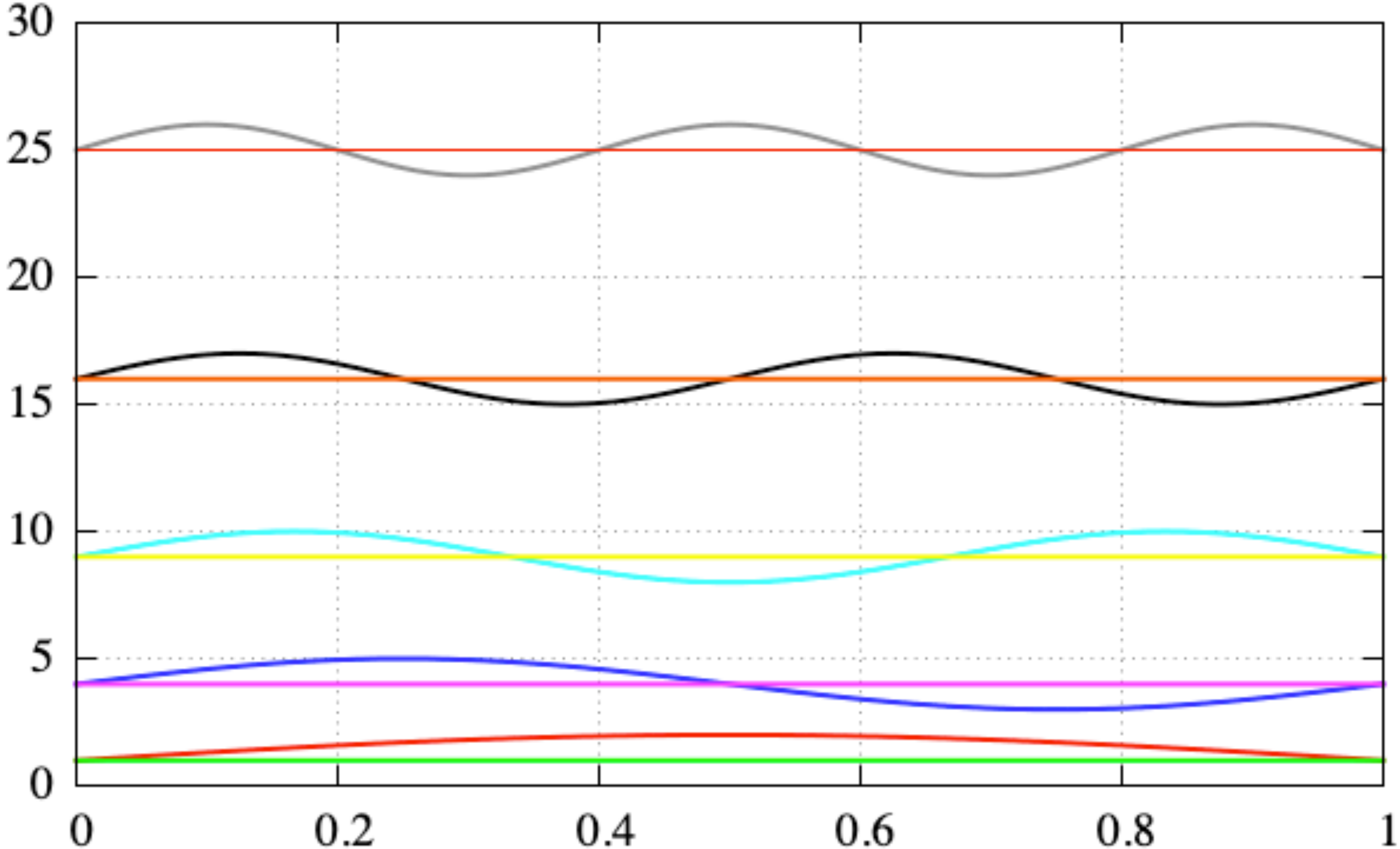
Solutions to that are sines, cosines, and complex exponentials.

The boundary conditions require the solution to be zero at $x = 0$ and at $x = w$.

The solutions are then $\psi(x) = \sin(k_n x)$ with $k_n = \dfrac{n\pi}{w}$ for $n = 1, 2, 3, \ldots$

Infinite Square Well 2

The solutions look like this:



The energies of the solutions are $E_n = \dfrac{\hbar^2 k_n^2}{2m} = \dfrac{\hbar^2 n^2 \pi^2}{2mw^2} = n^2 \dfrac{\hbar^2 \pi^2}{2mw^2}$

Infinite Square Well 3

The integral of the conjugate square (for normalization) is

$$\int_0^w dx\,\psi_n^*\psi_n = \int_{x=0}^{x=w} dx\,\sin^2\left(k_n x\right) = \int_{x=0}^{x=w} dx\,\frac{1-\cos\left(2k_n x\right)}{2}$$

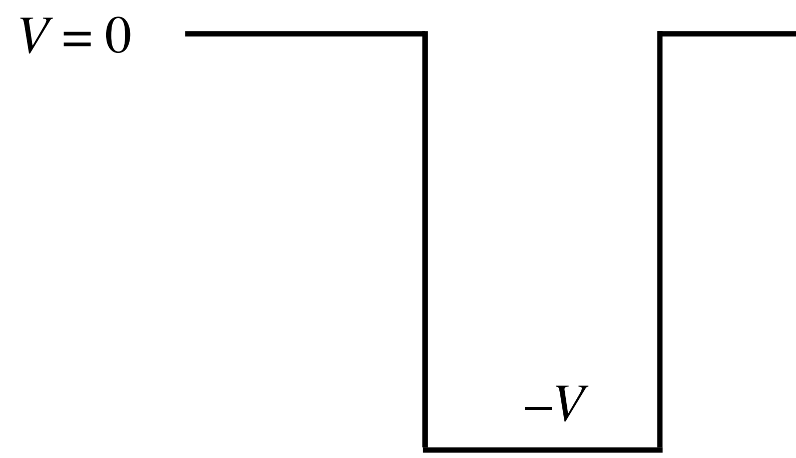
$$= \frac{1}{k_n}\int_{k_n x=0}^{k_n x=k_n w} d\left(k_n x\right)\frac{1-\cos\left(2k_n x\right)}{2} = \frac{1}{2k_n}\int_{u=0}^{u=k_n w} du\left[1-\cos\left(2u\right)\right]$$

$$= \frac{1}{2k_n}\left[u-\frac{1}{2}\sin\left(2u\right)\right]_{u=0}^{u=k_n w} = \frac{w}{2n\pi}\left[u-\frac{1}{2}\sin\left(2u\right)\right]_{u=0}^{u=\frac{n\pi}{w}w} = \frac{w}{2n\pi}\left[u\right]_{u=0}^{u=n\pi}$$

$$= \frac{w}{2n\pi}\cdot n\pi = \frac{w}{2} \qquad \rightarrow \qquad \psi_n = \sqrt{\frac{2}{w}}\sin\left(k_n x\right)$$

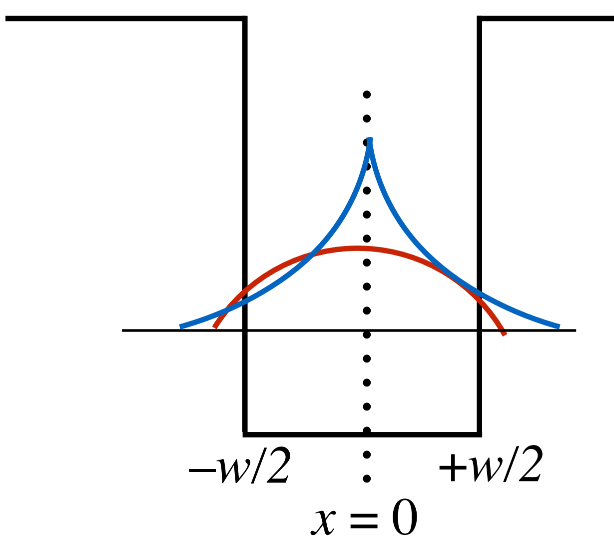
Finite Negative Square Well

The potential is zero everyplace,
except a region where it is flat and negative.



For the usual positive-energy plane wave,
this is just a barrier problem, with a negative potential.
There is a large transmitted wave, a small reflected wave,
and complex-exponential waves inside.

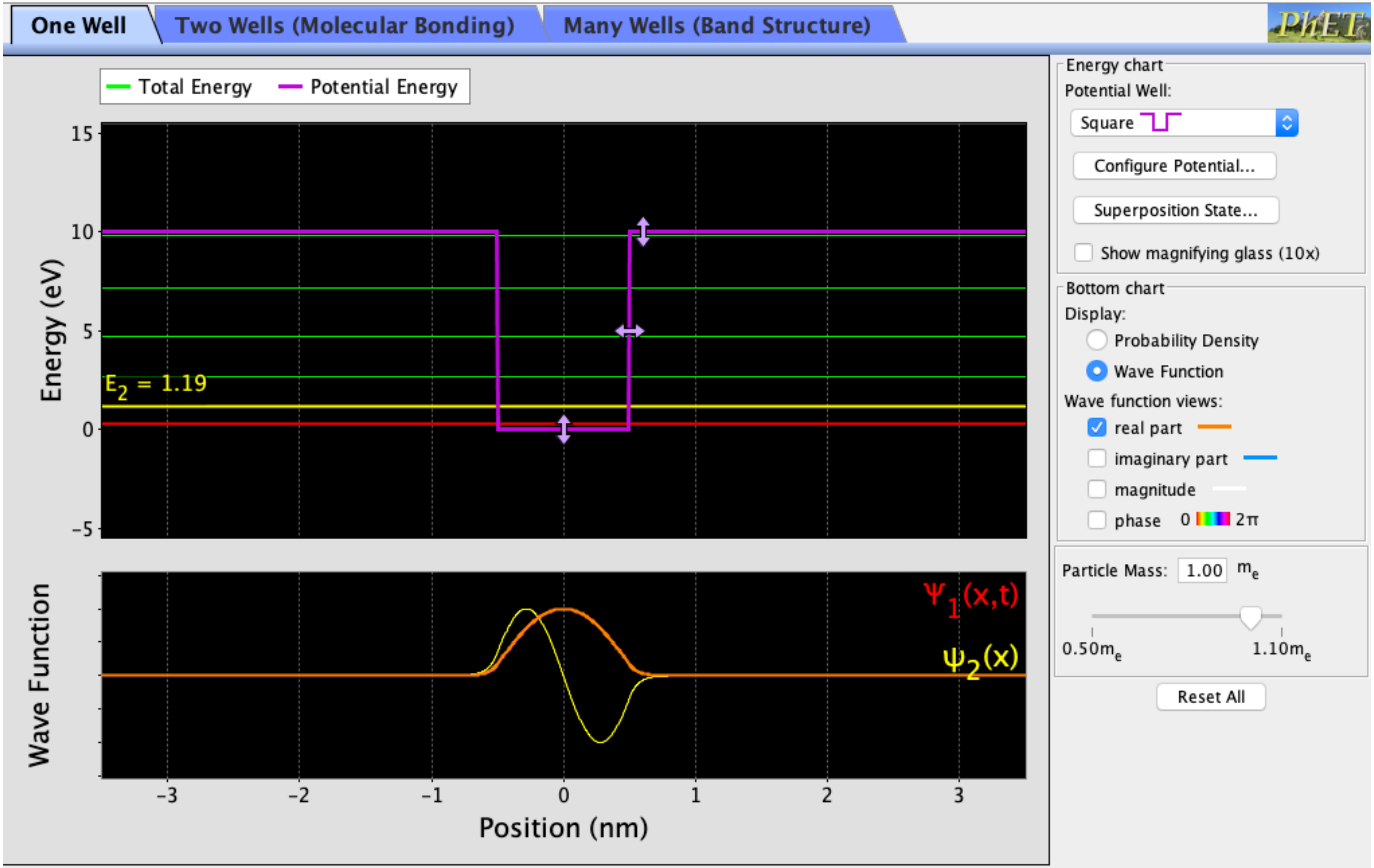
But there can also be bound states.



The lowest state is a half-cycle of sine wave,
but a bit wider than the well, and has exponential tails.
The higher states are a full cycle, 1.5 cycles, etc,
all with exponential tails.

The energies are approximately $E_n \approx -V + n^2 \dfrac{\hbar^2 \pi^2}{2mw^2}$.

The bound states have negative energy, and there are only a finite number.



One Well
Two Wells (Molecular Bonding)
Many Wells (Band Structure)
PhET
Total Energy
Potential Energy
Energy (eV)
15
10
5
0
−5
E2 = 1.19
Wave Function
Ψ1(x,t)
ψ2(x)
−3
−2
−1
0
1
2
3
Position (nm)
Energy chart
Potential Well:
Square
Configure Potential...
Superposition State...
Show magnifying glass (10x)
Bottom chart
Display:
Probability Density
Wave Function
Wave function views:
real part
imaginary part
magnitude
phase 0 2π
Particle Mass: 1.00 me
0.50me
1.10me
Reset All

Hamiltonian Operator

The right-hand side of $i\hbar\frac{\partial\psi}{\partial t}=\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{dx^2}+V(x)\cdot\psi$ or $E\psi=\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{dx^2}+V(x)\cdot\psi$

is an operator: it takes the ψ function as an input, and returns another function.

This is called the <u>Hamiltonian operator</u> $H_{op}=\frac{-\hbar^2}{2m}\frac{\partial^2}{dx^2}+V(x)$.

When you take more advanced classical mechanics, the Hamiltonian
is the sum of the kinetic and potential energy. This is the quantum version.

Reflection Symmetry

If we change x to $-x$ in a derivative, $\dfrac{\partial}{\partial x} \to \dfrac{\partial}{\partial(-x)} = -\dfrac{\partial}{\partial x}$.

For a second derivative, we get two minus signs, so $\dfrac{\partial^2}{\partial x^2} \to \dfrac{\partial}{\partial(-x)}\dfrac{\partial}{\partial(-x)} = +\dfrac{\partial^2}{\partial x^2}$.

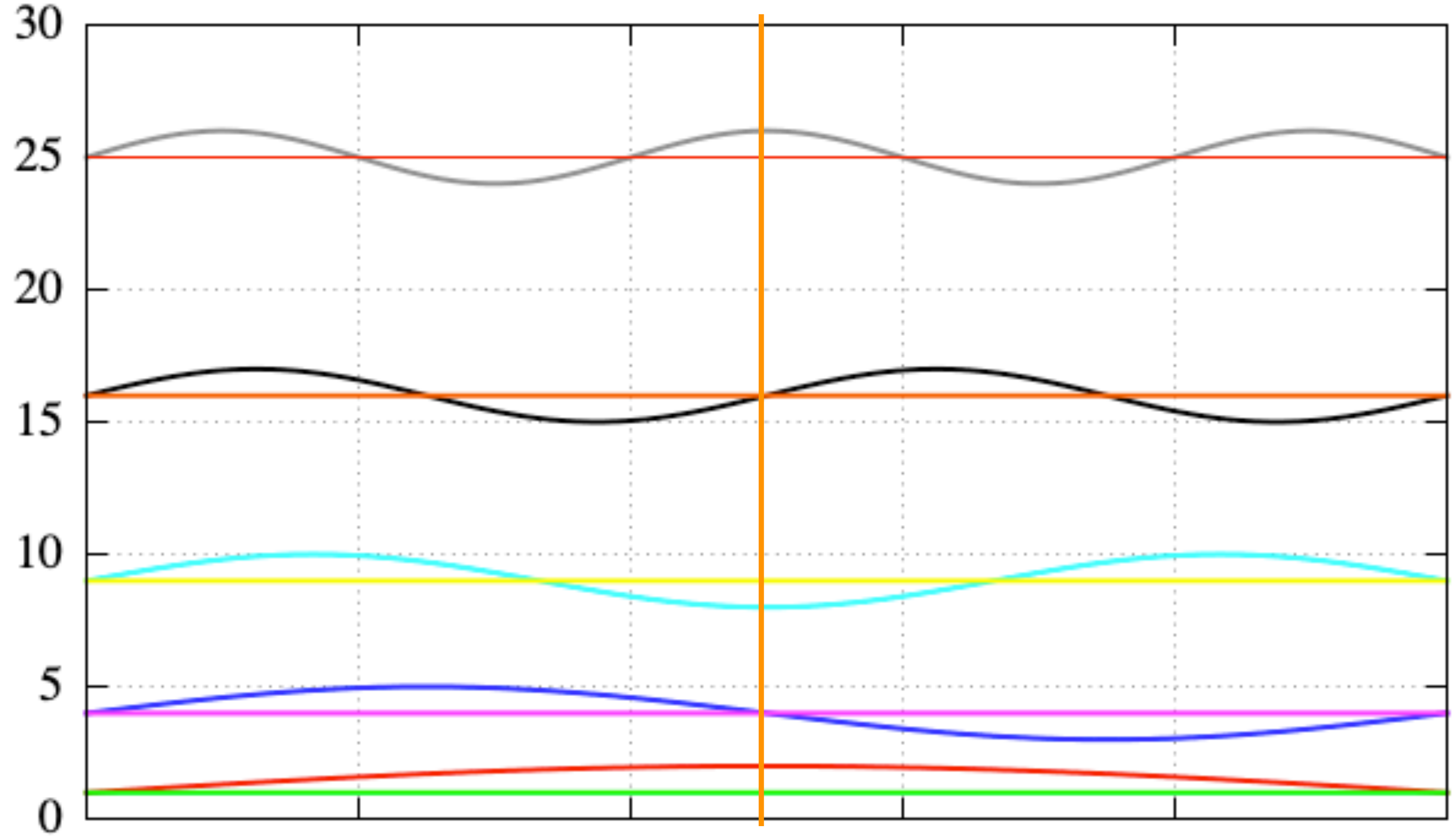
So changing from x to $-x$ doesn't change a second derivative.

If we put the x-origin at the center of an infinite or finite square well, then the potential has the property that $V(-x) = V(x)$.

So if the potential $V(-x) = V(x)$ has reflection symmetry, changing from x to $-x$ doesn't change the Hamiltonian.

Reflection Symmetry of Solutions

Here are some solutions for the infinite square well:



$x = 0$

They are all either <u>symmetric</u> around $x = 0$ so $\psi(-x) = \psi(x)$,
or <u>anti-symmetric</u> so $\psi(-x) = -\psi(x)$.

This is a general property: if $V(x)$ is symmetric so H_{op} is symmetric,
then the solutions will be either symmetric or anti-symmetric.

Quantum Harmonic Oscillator 1

We just plug $V(x) = \frac{1}{2}kx^2$ into Schrodinger:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}kx^2 \cdot \psi = E\psi$$

At large enough $\pm x$, $V(x) = \frac{1}{2}kx^2 >> E$, so let's drop $E\psi$ for a while.

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{1}{2}kx^2 \cdot \psi$$

So we need a function whose second derivative is proportional to x^2 times the function. We also want the function to go to zero at $x = \pm$ infinity.

Quantum Harmonic Oscillator 2

Let's guess a Gaussian: $\psi(x) = \exp\left(-\frac{x^2}{2b^2}\right)$ and work out the derivatives

$$\frac{\partial}{\partial x}\exp\left(-\frac{x^2}{2b^2}\right) = \frac{-2x}{2b^2}\exp\left(-\frac{x^2}{2b^2}\right) = \frac{-x}{b^2}\exp\left(-\frac{x^2}{2b^2}\right)$$

$$\frac{\partial^2}{\partial x^2}\exp\left(-\frac{x^2}{2b^2}\right) = \left[\frac{-x}{b^2}\right]^2 \exp\left(-\frac{x^2}{2b^2}\right) + \frac{-1}{b^2}\exp\left(-\frac{x^2}{2b^2}\right) = \frac{1}{b^2}\left[\frac{x^2}{b^2} - 1\right]\psi(x)$$

Plug into the full equation: $\frac{-\hbar^2}{2m}\frac{1}{b^2}\left[\frac{x^2}{b^2} - 1\right]\psi + \frac{1}{2}kx^2 \cdot \psi = E\psi$

Divide out ψ and collect powers of x: $\left[\frac{-\hbar^2}{2m}\frac{1}{b^4} + \frac{1}{2}k\right]x^2 + \left[\frac{\hbar^2}{2m}\frac{1}{b^2} - E\right] = 0$

Each square bracket must equal zero for this to work.

Quantum Harmonic Oscillator 3

Set the bracket for the coefficient of x^2 to zero:

$$\left[\frac{-\hbar^2}{2mb^4}+\frac{1}{2}k\right]=0\rightarrow\frac{\hbar^2}{mb^4}=k\rightarrow b^2=\sqrt{\frac{\hbar^2}{km}}=\frac{\hbar}{\sqrt{km}}$$

Plug that into the bracket for the coefficient of x^0 and set that to zero:

$$\left[\frac{\hbar^2}{2m}\frac{1}{b^2}-E\right]\rightarrow\left[\frac{\hbar^2}{2m}\frac{\sqrt{km}}{\hbar}-E\right]=0\rightarrow E=\frac{1}{2}\hbar\sqrt{\frac{k}{m}}=\frac{1}{2}\hbar\omega_{\text{classical}}$$

So our guess of $\psi(x)=\exp\left(-\frac{x^2}{2b^2}\right)$ is a Schrodinger solution,

with $E=\frac{1}{2}\hbar\sqrt{\frac{k}{m}}=\frac{1}{2}\hbar\omega_{\text{classical}}$ and $b^2=\frac{\hbar}{\sqrt{km}}$.

Quantum Harmonic Oscillator 4

For any potential, the lowest energy solution tends to have "one bump."

Our Gaussian has one bump. It's probably the lowest energy solution.

For symmetrical potentials, like this one, solutions are even or odd.
Our Gaussian is even, so the next solution should be odd.

We can try a simple odd function $\psi(x) = x \cdot \exp\left(-\frac{x^2}{2b^2}\right)$ and take derivatives

$$\frac{\partial}{\partial x} x \cdot \exp\left(-\frac{x^2}{2b^2}\right) = 1 \cdot \exp\left(-\frac{x^2}{2b^2}\right) + x \cdot \frac{-x}{b^2} \exp\left(-\frac{x^2}{2b^2}\right) = \left[1 - \frac{x^2}{b^2}\right] \exp\left(-\frac{x^2}{2b^2}\right)$$

Quantum Harmonic Oscillator 5

Plug that in to work out the second derivative:

$$\frac{\partial^2}{\partial x^2} x \cdot \exp\left(-\frac{x^2}{2b^2}\right) = \frac{\partial}{\partial x}\left[1-\frac{x^2}{b^2}\right]\exp\left(-\frac{x^2}{2b^2}\right)$$

$$= \left[\frac{-2x}{b^2}\right]\exp\left(-\frac{x^2}{2b^2}\right) + \left[1-\frac{x^2}{b^2}\right]\cdot\frac{-x}{b^2}\exp\left(-\frac{x^2}{2b^2}\right)$$

$$= \left[\frac{-2x}{b^2}-\frac{x}{b^2}+\frac{x^3}{b^4}\right]\exp\left(-\frac{x^2}{2b^2}\right) = \left[\frac{x^3}{b^4}-\frac{3x}{b^2}\right]\exp\left(-\frac{x^2}{2b^2}\right)$$

$$= \left[\frac{x^2}{b^4}-\frac{3}{b^2}\right]\cdot x\cdot\exp\left(-\frac{x^2}{2b^2}\right) = \left[\frac{x^2}{b^4}-\frac{3}{b^2}\right]\psi(x)$$

Then plug into Schrodinger and pray

Quantum Harmonic Oscillator 6

Plug into Schrodinger:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}kx^2 \cdot \psi = E\psi$$

$$\frac{-\hbar^2}{2m}\left[\frac{x^2}{b^4} - \frac{3}{b^2}\right]\psi + \frac{1}{2}kx^2 \cdot \psi = E\psi$$

Divide out ψ and collect powers of x:

$$\left[\frac{-\hbar^2}{2mb^4} + \frac{1}{2}k\right]x^2 + \left[\frac{3\hbar^2}{2mb^2} - E\right] = 0$$

Setting the left bracket to zero gives us exactly what we got before for b^2:

$$\left[\frac{-\hbar^2}{2mb^4} + \frac{1}{2}k\right] = 0 \rightarrow \frac{\hbar^2}{mb^4} = k \rightarrow b^2 = \sqrt{\frac{\hbar^2}{km}} = \frac{\hbar}{\sqrt{km}}$$

Quantum Harmonic Oscillator 7

Setting the right bracket to zero gives us

$$\left[\frac{3\hbar^2}{2m}\cdot\frac{1}{b^2}-E\right]=0\rightarrow\frac{3\hbar^2}{2m}\cdot\frac{\sqrt{km}}{\hbar}-E=0\rightarrow E=\frac{3}{2}\cdot\hbar\sqrt{\frac{k}{m}}=\frac{3}{2}\cdot\hbar\omega_{\text{classical}}$$

So our second solution is $\psi(x)=x\cdot\exp\left(-\frac{x^2}{2b^2}\right)$

with the same $b^2=\frac{\hbar}{\sqrt{km}}$ but higher energy $E=\frac{3}{2}\hbar\sqrt{\frac{k}{m}}=\frac{3}{2}\hbar\omega_{\text{classical}}$,

compared to $E=\frac{1}{2}\hbar\omega_{\text{classical}}$ for the first state.

The energy is higher by $\Delta E=\hbar\omega_{\text{classical}}$.

More Solutions

$$0 \quad E_0 = (0+1/2)\hbar\omega \quad \psi_0 = e^{-\frac{y^2}{2}}$$

$$1 \quad E_1 = (1+1/2)\hbar\omega \quad \psi_1 = ye^{-\frac{y^2}{2}}$$

$$2 \quad E_2 = (2+1/2)\hbar\omega \quad \psi_2 = \left(y^2 - 1/2\right)e^{-\frac{y^2}{2}}$$

$$3 \quad E_3 = (3+1/2)\hbar\omega \quad \psi_3 = \left(y^3 - 3/2 \cdot y\right)e^{-\frac{y^2}{2}}$$

$$4 \quad E_4 = (4+1/2)\hbar\omega \quad \psi_4 = \left(y^4 - 3y^2 + 3/4\right)e^{-\frac{y^2}{2}}$$

$$y = \frac{x}{b} \qquad b^2 = \frac{\hbar}{\sqrt{km}} \qquad \omega = \sqrt{\frac{k}{m}}$$

Harmonic Oscillator Wavefunctions

The wavefunctions are

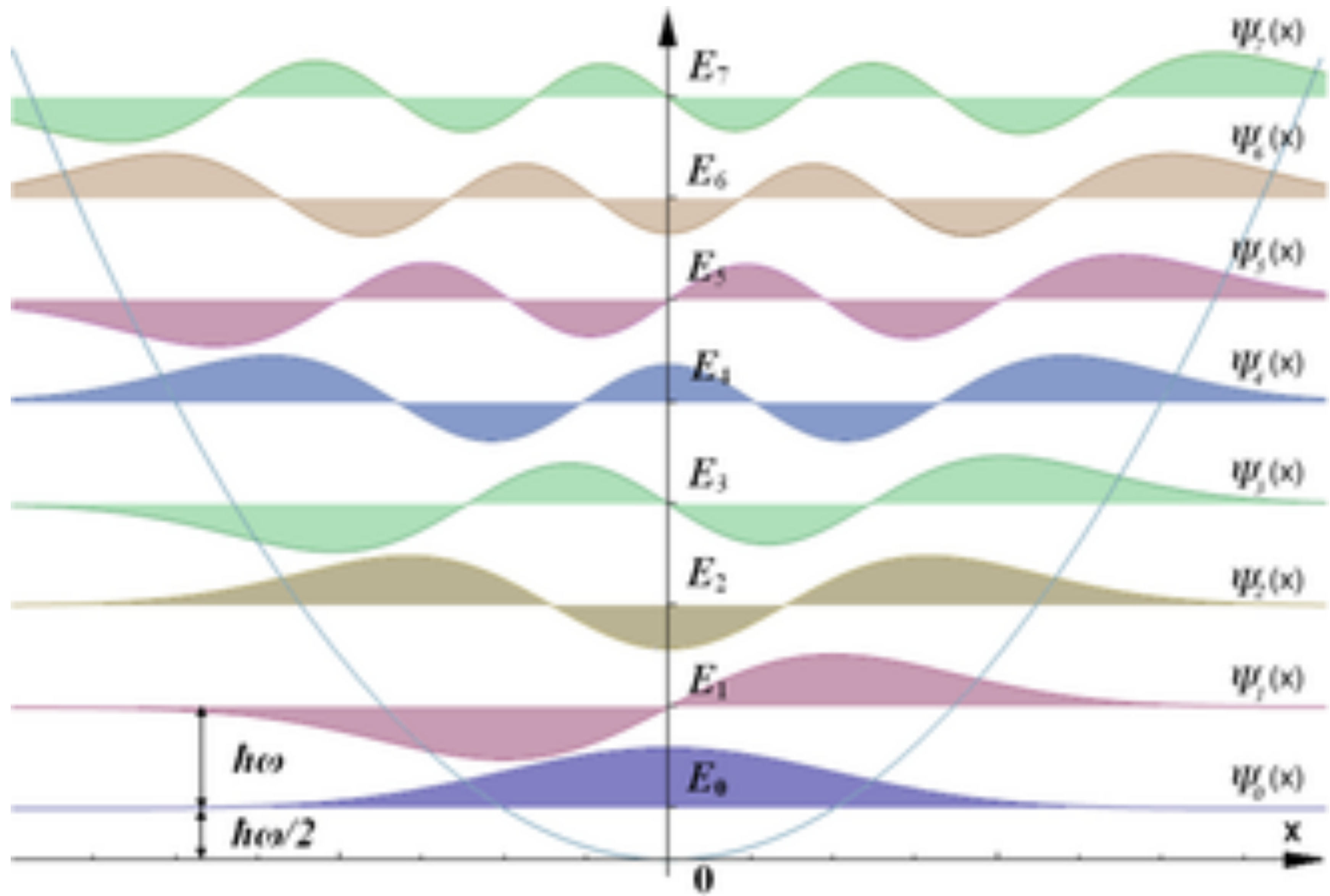
$$\psi_n(y) = H_n(y) \cdot \exp\left(-\frac{y^2}{2}\right)$$

They are a polynomial H_n of order n times a Gaussian.

The index n starts at 0.

The polynomials alternate between even and odd.

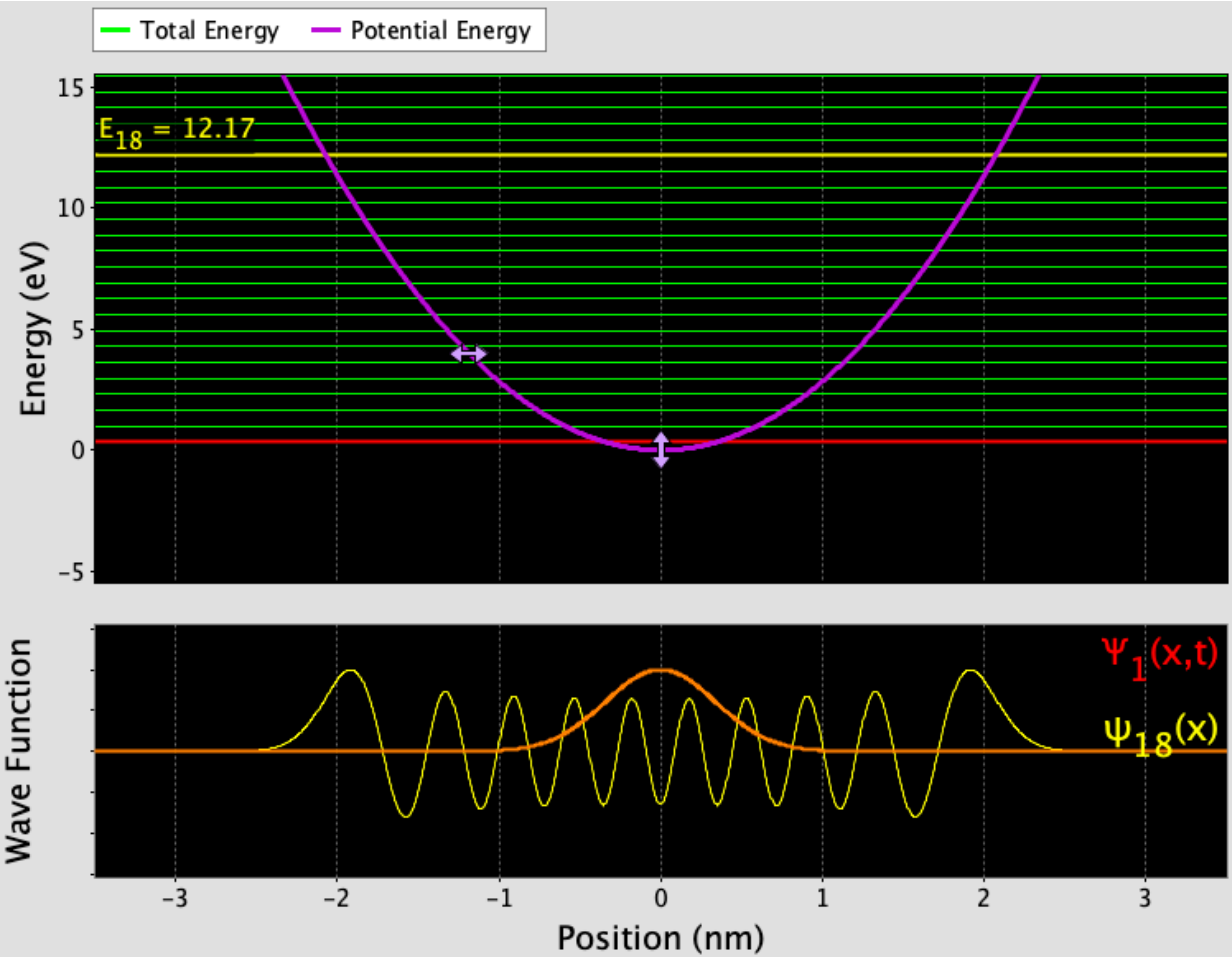
The polynomials have either all-even or all-odd powers.



Hermite Polynomials

The polynomials are called the (physicists) Hermite Polynomials.
One normalization convention is for the first coefficient to be 2^n.
With this normalization, the "wiggles" in ψ are all about the same size.

$$
\begin{aligned}
H_0(x) &= 1, \\
H_1(x) &= 2x, \\
H_2(x) &= 4x^2 - 2, \\
H_3(x) &= 8x^3 - 12x, \\
H_4(x) &= 16x^4 - 48x^2 + 12, \\
H_5(x) &= 32x^5 - 160x^3 + 120x, \\
H_6(x) &= 64x^6 - 480x^4 + 720x^2 - 120, \\
H_7(x) &= 128x^7 - 1344x^5 + 3360x^3 - 1680x, \\
H_8(x) &= 256x^8 - 3584x^6 + 13440x^4 - 13440x^2 + 1680, \\
H_9(x) &= 512x^9 - 9216x^7 + 48384x^5 - 80640x^3 + 30240x, \\
H_{10}(x) &= 1024x^{10} - 23040x^8 + 161280x^6 - 403200x^4 + 302400x^2 - 30240.
\end{aligned}
$$


Total Energy
Potential Energy
E18 = 12.17
Energy (eV)
15
10
5
0
−5
Wave Function
Ψ1(x,t)
ψ18(x)
−3
−2
−1
0
1
2
3
Position (nm)

For Next Time

Midterm today at 5-6 PM, in this room.

Bring 1 page (both sides) of notes, and a calculator.

Homework will be posted tomorrow, due Monday.

Tutorial worksheet on Friday as usual.

Next week will be Lasers and Semiconductors.