Example one-dimensional quantum systems

Notes on Quantum Mechanics

http://quantum.bu.edu/notes/QuantumMechanics/Example1DQuantumSystems.pdf
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We have learned that the one dimensional Schrödinger equation,

$$\text{curvature of } \psi \text{ at } x = -\frac{2\,m}{\hbar^2} \times \text{kinetic energy at } x \times \psi \text{ at } x,$$

implies the oscillatory nature of wavefunctions in allowed regions, their divergent behavior in forbidden regions, and that, when combined with the Born recipe for finding probability densities from wavefunctions, these behaviors account for the quantization of energies whenever a particle is confined by forbidden regions of infinite spatial extent. This is all we need to understand the properties of any one dimensional quantum system.

We have already studied the simplest one dimensional system, a particle of mass m confined by infinite potential walls to the region $0 \le x \le L$. There are an infinite number of possible quadratically spaced energies,

$$E_j = \frac{j^2\,\pi^2\,\hbar^2}{2\,m\,L^2} = \frac{j^2\,\pi^2 (h/2\,\pi)^2}{2\,m\,L^2} = \frac{j^2\,h^2}{8\,m\,L^2},$$

indexed by $j = 1, 2, \ldots$, the number of loops in the wavefunction

$$\psi_j = \sqrt{2/L}\,\sin(j\,\pi\,x/L).$$

Here we will explore the effect of distorting the potential energy in various ways. We will do this using the curvature form of the Schrödinger equation to find the possible energies and wavefunctions.

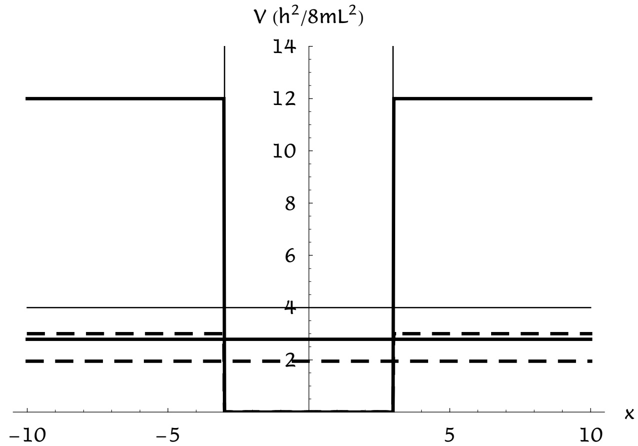
> In calculations with the Schrödinger equation it is very convenient to work in units of energy and length that are natural to the problem at hand. The implementation of the stepwise solution to Schrödinger equation that we use assumes that units of energy and length are chosen so that the proportionality constant, $2\,m/\hbar^2$, is equal to one. In terms of the energies of the infinite potential well case, this means that

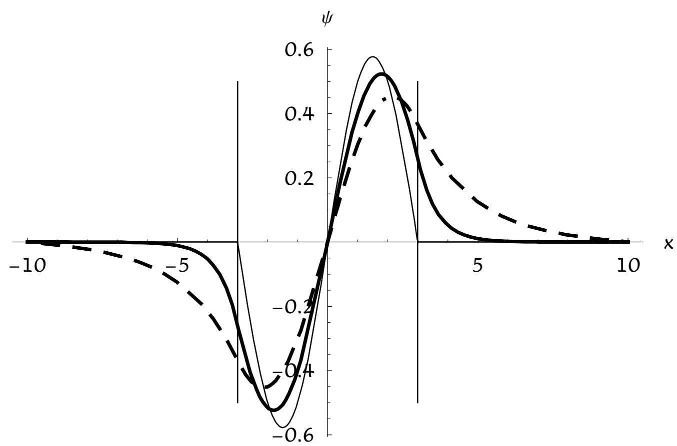
$$\frac{2\,m}{\hbar^2} = 1 = 4\,\pi^2\,\frac{2\,m}{h^2} = \left(\frac{\pi}{L}\right)^2\,\frac{8\,m\,L^2}{h^2},$$

> and so that the lowest infinite potential well energy value in these dimensionless units is $h^2/(8\,m\,L^2) = (\pi/L)^2$. For example, in these dimensionless energy units an infinite well of width $L = 6$ will have lowest (zero point) energy $(\pi/6)^2 = 0.27416$. This means that to express energies in multiples of the zero point energy of an infinite potential well, $h^2/(8\,m\,L^2)$, we need to divide the dimensionless energies by $(\pi/6)^2$.

■ Effect of wall "softness"

What happens if the potential walls confining the particle are not infinite? Here are three different $L = 6$ wide wells and their corresponding second lowest energy wavefunctions. One well is the infinitely deep well, for which the energy of the second lowest state is 4, in units of the infinite well zero point energy, $h^2/(8\,m\,L^2)$; one well is 12 units deep, and the energy of the second lowest state is lowered to 2.79 units; and the third well is 3 units deep, and the energy of its second lowest state is lowered further to 1.95 units. The successive lowering of the energy value is due to the increasing penetration of the wavefunction into the wall of the potential, and hence its increasing loop length, as shown in the figure below.



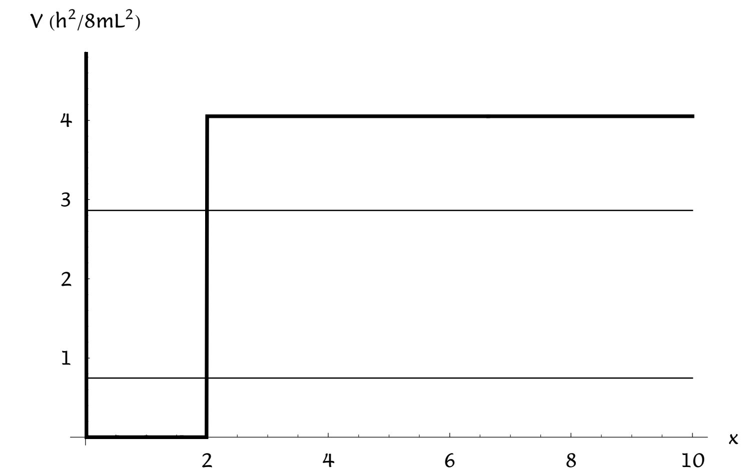


Three different $L = 6$ wide wells and their corresponding second lowest energy wavefunctions and energy value. Energies are units of the infinite well zero point energy, $h^2/(8\,m\,L^2) = h^2/(32\,m)$. One well and it wavefunction (thin solid lines) is the infinitely deep well, for which the energy of the second lowest state is 4 (thin horizontal line); one well is 12 units deep (thick solid lines), and the energy of the second lowest state is lowered to 2.79; and the third well only 3 units deep (thick dashed lines), and the energy of its second lowest state is lowered further to 1.95 units. Vertical lines at $x = \pm 3$ mark the classical turning point on the wavefunction figure.

The shallower the potential well, the greater the penetration of the wavefunction into the forbidden regions, and so the greater the leakage of probability density out of the potential wells. We can quantify this leakage by calculating the fraction of the wavefunction in the allowed region. The results are 75% for the shallowest well, 96% for the intermediate depth well, and 100% for the infinite depth well. From this we achieve the intuition that the the shallower the well, the "softer" its walls.

■ Semi-infinite potential well

We have seen that the smaller are potential walls are, the softer they are in the sense that wavefunctions penetrate more deeply. What if one potential wall is not infinitely high? Here is an example of such a potential

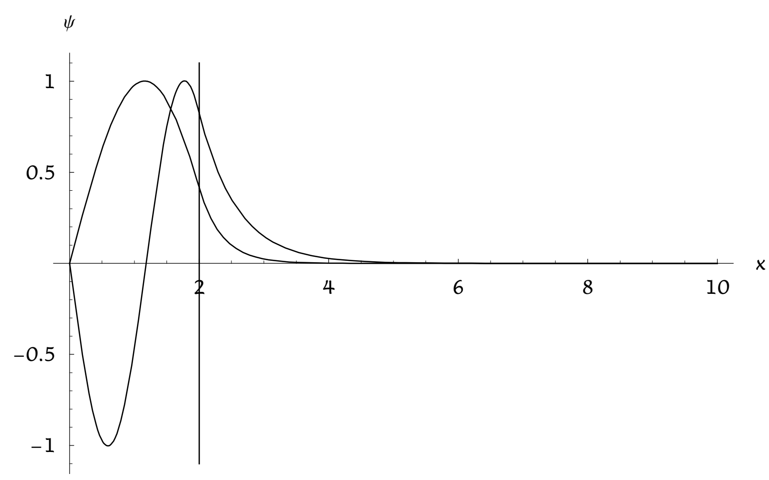


Semi-infinite potential of width $L = 2$ (thick line).. The two horizontal thin lines are the energies, 0.75 and 2.86, of the two bound states of the potential. Energies are units of the infinite well zero point energy, $h^2 / (8\, m\, L^2) = h^2 / (32\, m)$.

The potential energy is infinite for $x < 0$. This means there can be no wavefunction penetration into this forbidden region. The potential energy is 4, in units of the infinite well zero point energy, $h^2 / (8\, m\, L^2) = h^2 / (32\, m)$, for $2 < x \leq \infty$, and so energies are quantized in this potential for energies less that its height. These energies are 0.75 and 2.86.

> What would these energies be if the potential were infinitely high for $2 < x \leq \infty$? Answer: 1 and 4.

Here are the corresponding wavefunctions.



Wavefunctions of the lowest tow energy states of the semi-infinite well potential. The vertical line at $x = 2$ marks the right classical turning point.

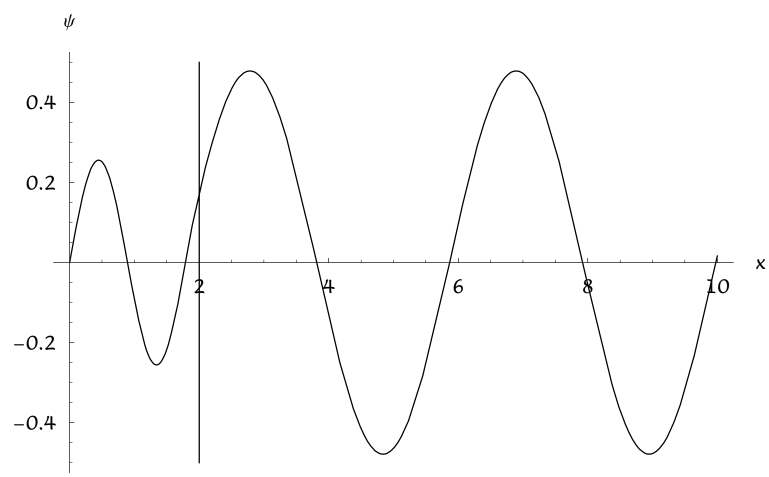
> Explain why the wavefunction with two loops penetrates more into the right forbidden region of the potential indicated by the dotted line.

> Explain why are there only two quantized energies of the potential indicated by the dotted line. Hint: Sketch the solution to the Schrödinger equation with energy just below the right hand potential energy.

> Explain whether the a particle can exist for energies greater than 4, that is, for energies above the potential energy of the right forbidden region.

■ Energy continuum

For energies above the potential energy of the right forbidden region, the wavefunction is oscillatory for all value $x > 0$ and so the particle can have any energy above 4. Here is the wavefunction for energy 5 units, that is, 1 unit above the potential energy for $x > 2$.



Wavefunction of the energy continuum of the semi-infinite potential, with energy 5. Energy is units of the infinite well zero point energy, $h^2/(8\,m\,L^2) = h^2/(32\,m)$. The vertical line at $x = 2$ marks the right classical turning point.

> Sketch how this wavefunction would change if its energy were 9 units, that is, 5 units above the potential energy for $x > 2$.

> Sketch how this wavefunction would change if its energy were 4.25 units, that is, 0.25 units above the potential energy for $x > 2$.

Because amy energy is possible above 4, the potential energy at $x > 2$, these energies form an *energy continuum*.

> What is the lowest energy (in zero point energy units) that can be absorbed if the particle is initial in its lowest energy state? Answer 2.11.

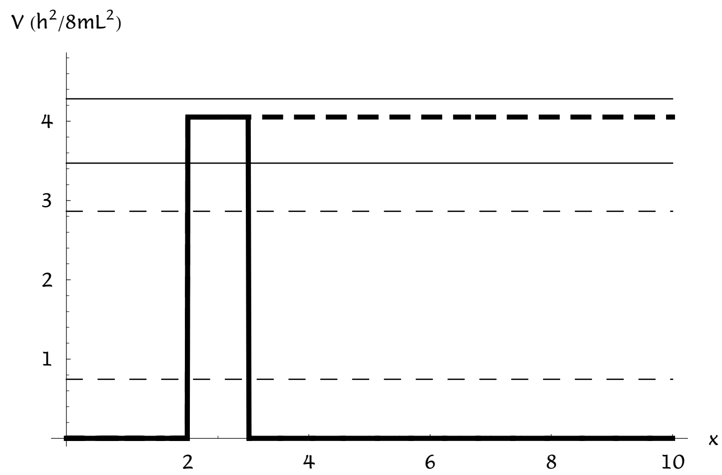
> What is the next lowest energy (in zero point energy units) that can be absorbed if the particle is initial in its lowest energy state? Answer 3.25.

> Explain whether it is possible for the system to absorb energy 3.26?

> Explain whether the system has an ionization energy.

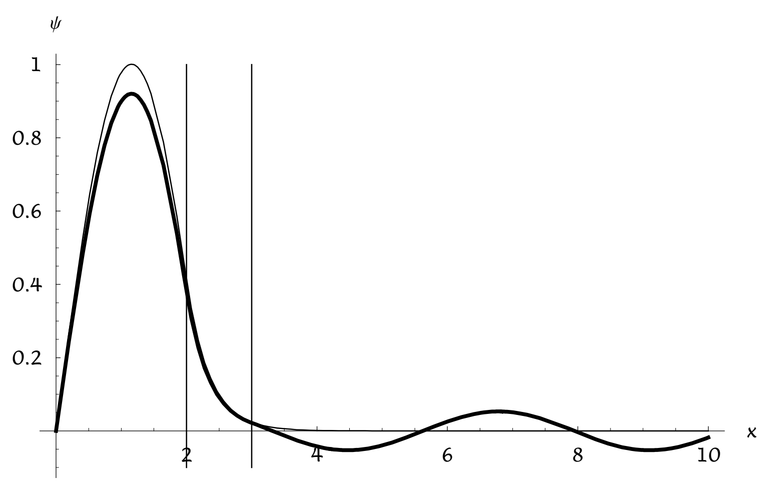
■ Field ionization

A scanning tunneling microscope (STM) works by distorting the potential energy confining electrons to atoms, molecules, or the surface of a solid. Here is an example modification of the semi-infinite potential above.



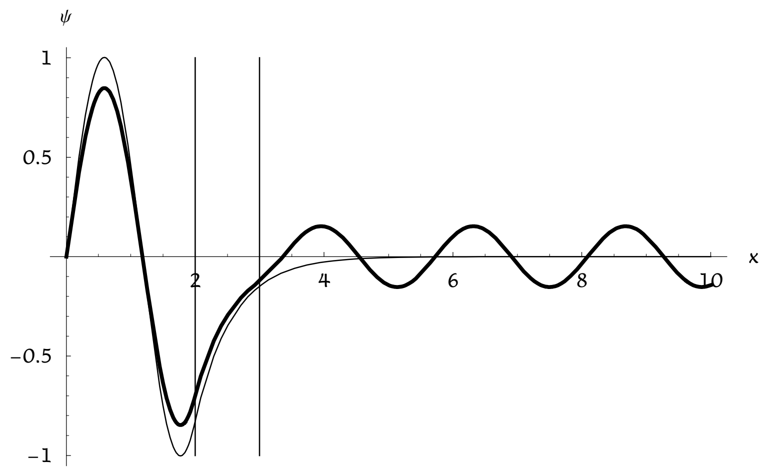
Distorted semi-infinite potential (thick solid line) and unmodified potential (thick dashed line). The two horizontal thin dashed lines are the energies, 0.75 and 2.86, of the unmodified potential. The lowest horizontal thin solid line the energy of a wavefunction possible for the modified potential but not for the unmodified potential. The highest horizontal thin line is a possible energy of both potentials. Energies are units of the infinite well zero point energy, $h^2/(8\,m\,L^2) = h^2/(32\,m)$.

The effect of the modification is to make the right forbidden region only 1 unit wide. Here is the effect on the wavefunctions of the lowest energy wavefunction.



Lowest energy wavefunction of a semi infinite well before (thin line) and after (thick line) modification by an applied potential. The vertical lines at $x = 2$ and $x = 3$ mark the finite width forbidden region of the modified potential.

And here is the effect on the wavefunctions of the second lowest energy wavefunction.

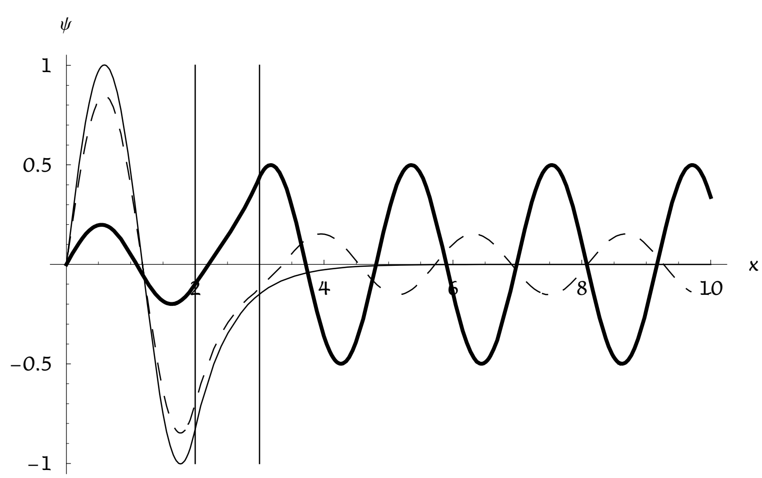


Second lowest energy wavefunction of a semi infinite well before (thin line) and after (thick line) modification by an applied potential. The vertical lines at $x = 2$ and $x = 3$ mark the finite width forbidden region of the modified potential.

In both cases the wavefunction has "leaked" out of the potential well into the exterior allowed region. The wavefunction of the lowest energy state is now only 96% confined and the wavefunction of the second energy state is now only 78% confined.

This effect of passing through a finite width forbidden region is called *tunnelling* and we say the potential has become *permeable*.

Another consequence of the potential being made permeable is that there is no longer quantization of energy, since there is no longer any confinement by two infinite forbidden regions. This means that there are now physically sensible solutions to the Schrödinger equation at every energy. As example, here is a solution at an energy 0.5 units above the second bound energy of the unmodified potential, together with the bound state wavefunction and its changed form in the modified potential.



Wavefunction (thick line) of a semi-infinite well after modification by an applied potential at energy 0.5 units above the second bound state of the unmodified potential, together with the bound state wavefunction (thin line) and its changed form in the modified potential (thin dashed line). The vertical lines at $x = 2$ and $x = 3$ mark the finite width forbidden region of the modified potential.

The effect is that now the wavefunction is only 4% confined, that is, most of the wavefunction is now outside the original well.

It is a general feature of potentials that have been made permeable by external potentials that only near energies of bound states of the unmodified potential is there appreciable probability density in the originally bound region.