Implementing curvature based solution of Schrödinger equations

Notes on Quantum Mechanics

http://quantum.bu.edu/notes/QuantumMechanics/ImplementingCurvatureBasedSolutionOfSchrodingerEquations.pdf
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The best way to understand the curvature form of the Schrödinger equation,

$$\text{curvature of } \psi \text{ at } x \propto -\text{kinetic energy at } x \times \psi \text{ at } x,$$

is to see how it works for an example. To keep things simple, we will do this for now omitting units, since we are interested in the qualitative details. To begin we need to specify the kinetic energy variation, and then to choose starting values for the function ψ.

Note that there are two aspects to what follows. First are the details of using the Schrödinger equation to determine successive values of the wavefunction once two initial values are chosen. Second is the implementation of these details. Here the implementation is done in *Mathematica*, since this allows us to express things in a way that follows closely the equations. If you do not yet know *Mathematica*, following along may help you see by example how *Mathematica* can be used. However, you do not need to understand the *Mathematica* details to understand the ideas developed here.

■ Choose the kinetic energy variation

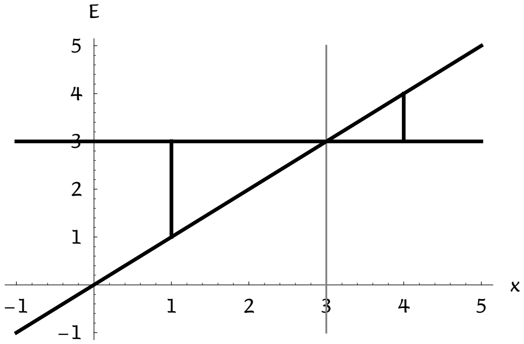
The starting point in working with the Schrödinger equation is always the same, namely to specify how the kinetic energy changes with position. This is usually done indirectly by specifying how the potential energy changes with position. Let's choose a ramp potential, that increases at a constant rate, say

$$V(x) = x.$$

In general, the absolute value of the potential energy and the location of the zero value of position are arbitrary. What is important is the potential energy *relative* to the total energy, for this determines the kinetic energy, as

$$T(x) = E - V(x).$$

As example, let's set the total energy at $E = 3$ units and then graph the potential energy (red line) and total energy (blue line).



Variation of kinetic energy with position for an upward sloping ramp potential energy, $V(x)$. The horzontal line is the total energy, E. The vertical lines are the kinetic energy, $E - V(x)$. The classical turning point is at $x = 3$ (thin vertical line). To the right of the classical turning point the kinetic energy is *negative* (thick vertical line) and so not realizable classically.

The kinetic energy at each point is the difference of the values of the blue line and red line at that point. For example, the vertcial line at $x = 1$ represents the kinetic energy of two units at that point. The kinetic energy decreases as position moves to more positive values of x, since the potential increases in this direction.

The thin vertical line is the position at which the total energy is entirely potential energy. This is the rightmost position a classical particle with total energy E can have. To the right of this line the kinetic energy is *negative*! For example, the vertical line at $x = 4$ represents the kinetic energy of negative one unit.

Regions of negative kinetic energy are not possible in ordinary, everyday experience, but they turn out to be very important in the quantum world. Such regions are called *forbidden regions*. Regions of positive kinetic energy are called *allowed regions*.

■ Use the Schrödinger equation to determine the wavefunction

Once we have specified the kinetic energy, we next need to choose starting values for the wavefunction ψ at two adjacent positions. Let's do this for $x = 0$ and $x = 0.4$,

$$x_1 = 0,\ \psi(x_1) = 0,$$

$$x_2 = 0.4,\ \psi(x_2) = 0.4,$$

> Show that these values mean we are assigning an initial slope of 1 to the wavefunction.

With these starting values of $\psi(x)$, together with the kinetic energy function $T(x)$, we have everything we need to use the Schrödinger equation to determine $\psi(x)$ for all other values of x. Here is the recipe.

From two adjacent values of ψ, we can determine its slope. The slope corresponding to the first two points we have chosen is

$$\text{slope}(x_1) = \frac{\psi(x_2) - \psi(x_1)}{x_2 - x_1} = \frac{0.4 - 0}{0.4 - 0} = 1$$

From the Schrödinger equation and the kinetic energy we can determine the rate at which the slope changes (the slope of the slope),

$$\text{curvature of } \psi \text{ at } x_2 = \frac{\text{slope}(x_2) - \text{slope}(x_1)}{x_2 - x_1} = -T(x_2)\,\psi(x_2)$$

Here, for simplicity, we have omitted from Schrödinger equation the constant factor $2\,m/\hbar^2$. This "curvature" tells us how the slope changes moving from x_1 to x_2. We can use change in slope to get the value of the function ψ at a nearby new point 0.4 units away,

$$x_3 = x_2 + 0.4.$$

To do this, first we use the Schrödinger equation to evaluate that the initial slope is changing at the rate

$$-T(x_2)\,\psi(x_2) = -(E - V(x)\,\psi(x_2) = -(3 - 0.4) \times 0.4 = -1.04$$

That is, for each unit change of x the slope increases by -1.04. The negative sign means that over a distance 0.4 the slope decreases by

$$\text{slope}(x_2) - \text{slope}(x_1) = -T(x_2)\,\psi(x_2)\,(x_2 - x_1) = -1.04 \times (0.8 - 0.4) = -0.416.$$

and so at position x_3 the slope has changed to

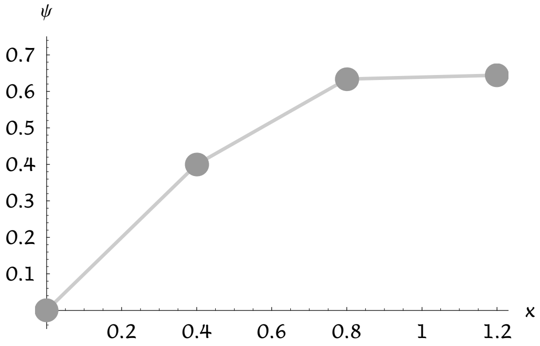
$$\text{slope}(x_3) = \text{slope}(x_2) - T(x_2)\,\psi(x_2)\,(x_2 - x_1) = 1 - 0.416 = 0.584$$

Finally, since this new slope is given by $(\psi_3 - \psi_2)/(x_3 - x_2)$, we can use it to determine the value of the ψ at x_3 to be

$$\psi(x_3) = \psi(x_2) + \text{slope}(x_2)\,(x_3 - x_2) = 0.4 + 0.584 \times (0.8 - 0.4) = 0.634.$$

> Show that the wavefunction changes to $\psi(x_4) = 0.644$ at $x_4 = x_3 + 0.4$.

Here is an illustration showing the successive function values.



The rightmost value of the wavefunction is computed from the change in slope connecting the first two points. According to the Schrödinger equation, this change in slope is given by the negative of the product of the kinetic energy and the value of the wavefunction at the second point.

The successive values of the function ψ are indicated by the grey circles. The line connecting the first and second values of the function has the initial slope 1. The line connecting the second and third values of the function has the new, lower slope. The difference in these two slopes reflects the curvature of the function, determined by the Schrödinger equation.

We have seen how to use the Schrödinger equation to find a next value of the function ψ from two adjacent, preceding values. Once we have the new value of ψ we can use it, and the immediately preceding value, to get a next new value of ψ. We can continue in this way to determine the how the function ψ changes along a set of successive positions.

To implement the process we need to collect together the steps we have taken above to determine ψ_3,

$$\begin{aligned}
\psi_3 & \\
&= \text{newSlope} \times (x_3 - x_2) + \psi_2 \\
&= (\text{initialSlope} + \text{changeInSlope}) * (x_3 - x_2) + \psi_2 \\
&= \left\{ \frac{\psi_2 - \psi_1}{x_2 - x_1} + \text{slopeOfSlope}[x_2] \times (x_3 - x_2) \right\} \times (x_3 - x_2) + \psi_2 \\
&= \left\{ \frac{\psi_2 - \psi_1}{x_2 - x_1} - T(x_2) \times \psi_2 \times (x_3 - x_2) \right\} \times (x_3 - x_2) + \psi_2 \\
&= \left\{ \frac{\psi_2 - \psi_1}{x_2 - x_1} - [E - V(x_2)] \times \psi_2 \times (x_3 - x_2) \right\} \times (x_3 - x_2) + \psi_2.
\end{aligned}$$

This last expression shows that each new value, $\psi_{3,}$ depends on: the previous two values, $\psi_1$and ψ_2; the previous two positions, $x_1$and x_2; the new position, x_3; the potential energy at the immediately preceding position, $V(x_2)$; and the total energy, E.