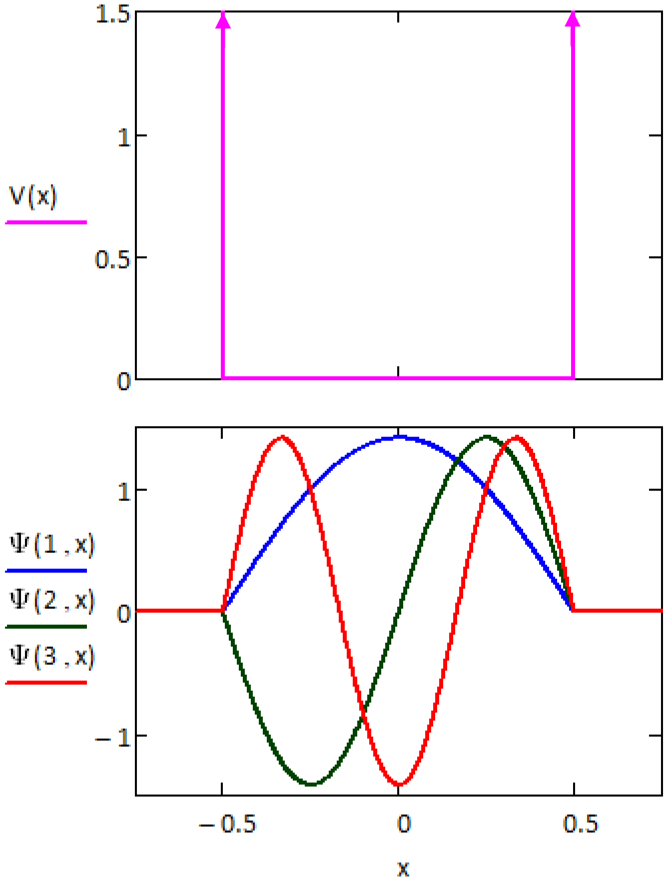
Today in Physics 237: solving the Schrödinger equation, I

- Separation of variables
- Solution of the 1-D time-independent Schrödinger equation
- Properties of the solutions



See problem 2.1c, page 7.

Separation of variables

- Our first recourse to solution of a partial differential equation is to try to **separate the equation into a number of ordinary differential equations**, one for every independent variable.
- There is no guarantee in general that this will work – plenty of partial differential equations important to physics do not separate, and must be solved by other means.
- But the Schrödinger equation in 1-D and spherically-symmetrical 3-D does separate for time-independent potentials V, and thus separation of variables is all we'll need for the next couple months.
  - Victims of PHYS 217 are already intimately familiar with this technique, so they can be permitted to daydream for the next few minutes.
- 1-D first.

Separation of variables (continued)

- Suppose that the solution to the 1-D Schrödinger equation can be written as $\Psi(x,t)=\psi(x)\varphi(t)$. Then we have

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\Psi(x,t) \quad \Rightarrow \quad \psi(x)i\hbar\frac{d}{dt}\varphi(t)=\varphi(t)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x) \quad .$$

- Divide through by $\psi(x)\varphi(t)$, and the partial derivatives change to simple derivatives:

$$\frac{1}{\varphi(t)}i\hbar\frac{d}{dt}\varphi(t)=\frac{1}{\psi(x)}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x) \quad .$$

- The LHS is a function only of *t*; the RHS, only of *x*. The only way for the equality to hold for arbitrary *x* and *t* is for both LHS and RHS to be constant, independent of *x* and *t.* We shall call the constant *E*:

$$\frac{1}{\varphi(t)}i\hbar\frac{d}{dt}\varphi(t)=\frac{1}{\psi(x)}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E \quad .$$

Separation of variables (continued)

- And thus we are left with two ordinary differential equations:

$$i\hbar\frac{d}{dt}\varphi(t)=E\varphi(t) \quad , \quad \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x) \quad .$$

- The time equation can be separated and integrated directly:

$$\int\frac{d\varphi}{\varphi}=-\frac{iE}{\hbar}\int dt \quad \Rightarrow \quad \ln\varphi=-\frac{iEt}{\hbar}+C' \quad \Rightarrow \quad \boxed{\varphi(t)=Ce^{-iEt/\hbar}} \quad ,$$

where *C* is a constant, independent of *x* and *t,* which can be evaluated if given a boundary value or initial condition.

- The other equation can be solved if supplied with a definite $V(x)$ and two boundary values:

$$\boxed{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x)} \quad .$$

Time-independent Schrödinger equation (1-D)

Separation of variables (continued)

- Since we're doing physics here, the potential energy $V(x)$ is real-valued, so a solution to the time-independent Schrödinger equation certainly **exists**, as you might have seen proven in a math class like MATH 173.
- If supplied with two boundary conditions and a value of *E*, a solution of this equation (or its 3-D version) is also **unique**.
  - We defer the proof of uniqueness to PHYS 217; this proof would be similar to that of uniqueness of solutions of the Poisson and Laplace equations, as recent victims of PHYS 217 will remember.
  - Uniqueness of solutions is not trivial. It justifies solution shortcuts like separation of variables.
    - It may seem a drastic and arbitrary assumption to take the time-dependent Schrödinger equation to be separable.
    - Thus it should be substantial comfort that a solution obtained in this fashion is the **only** solution, not just one among many.
    - Physicists use dirty tricks like this all the time, and lean hard upon uniqueness of solutions. It therefore behooves us to be familiar with uniqueness proofs, and to produce them on demand by our math colleagues. (We leave the existence proofs to them, though.)

Properties of separation solutions to the 1-D Schrödinger equation

- They are **stationary** states, because $\Psi^*\Psi = (\varphi^*\varphi)(\psi^*\psi) = \psi^*\psi$ and $\langle Q\rangle = \int \Psi^*\hat{Q}\Psi dx = \int \psi^*\hat{Q}\psi dx$. (No *t*.)

- They are states of definite **energy** *E*.
  - Classically, energy is given by the **Hamiltonian**, $H = p^2/2m + V(x)$. Quantum mechanically this is represented by $\hat{H} = \frac{\hat{p}^2}{2m} + V(x) = \frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$, so the time-independent Schrödinger equation is $\hat{H}\psi = E\psi$, and the expectation value of the Hamiltonian is $\langle H\rangle = \int \psi^*\hat{H}\psi dx = E\int \psi^*\psi dx = E\int \Psi^*\Psi dx = E$. That's why we chose *E* for the separation constant.

- For given boundary conditions: at each value of energy, say E_n, there is a unique wavefunction $\Psi_n(x,t) = \psi_n(x)e^{-iE_nt/\hbar}$. The **general** solution is the linear combination of all these wavefunctions:

$$\Psi(x,t) = \sum_n c_n\psi_n(x)e^{-iE_nt/\hbar} \quad .$$

Properties of separation solutions to the 1-D Schrödinger equation (cont'd)

- For normalizable $\Psi_n(x,t)$, E_n is real (Problem 2.1a).

- $\psi_n(x)$ can always be taken to be real (Problem 2.1b).

- If $V(x)=V(-x)$ – that is, if V is an **even** function of x – then $\psi(x)$ is either even $\left(\psi(x)=\psi(-x)\right)$ or odd $\left(\psi(x)=-\psi(-x)\right)$. (Problem 2.1c; see page 1).

  Proof: compare the time-independent Schrödinger equation to that with $x \to -x$:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x) \quad ; \quad \left[-\frac{\hbar^2}{2m}\frac{d^2}{d(-x)^2}+V(-x)\right]\psi(-x)=\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(-x)\right]\psi(-x)=E\psi(-x)$$

  So if V is even, then $\psi(x)$ and $\psi(-x)$ are both solutions for the same E. And any linear combination is too, such as $\psi_+=\left(\psi(x)+\psi(-x)\right)/2$ – even – or $\psi_-=\left(\psi(x)-\psi(-x)\right)/2$ – odd. But $\psi(x)=\psi_+(x)+\psi_-(x)$, so a solution $\psi(x)$ can always be decomposed into a linear combination of an even function and an odd function, q.e.d.

- E must exceed the minimum of $V(x)$, if $\psi(x)$ is normalizable (Problem 2.2).