

SCHROEDINGER WAVE EQUATION

*Reading:
Course packet Ch 5.7*



$$\hat{H}\psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t}$$

*(both images from
Wikipedia.com)*

Schrödinger Wave Equation

Schrödinger Wave Equation:

$$\hat{H}\psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t}$$

More-or-less “god-given”, just like Newton’s law $F(x) = dp/dt$.
It works, and if we can show that it fails, we’ll refine or discard.

You learned in PH425 that the solution to the time-dependent SE is, in terms of the eigenstates of the Hamiltonian:

$$|\psi(t)\rangle = \sum_n |\varphi_n\rangle e^{-iE_n t / \hbar} \quad \text{where} \quad \hat{H}|\varphi_n\rangle = E_n |\varphi_n\rangle$$

$$\psi(x,t) = \sum_n \varphi_n(x) e^{-iE_n t / \hbar} \quad \text{where} \quad \hat{H}\varphi_n(x) = E_n \varphi_n(x)$$

Notice the parallels to the rope problem we solved last week?

How did this solution to the SWE come about?

$$\hat{H}\psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t}$$

How do we solve this for $\psi(x,t)$? The operator H , the *Hamiltonian* or energy operator, is clearly special. So representing the kets or the wave function in the energy basis for expanding a general wave function is important! Note that the energy eigenstates are time INdependent if H is time independent. Write down the eigenvalue equation for the the Hamiltonian:

$$\hat{H}\varphi_n(x) = E_n\varphi_n(x) \qquad \hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle$$

We'll spend much of the class solving this equation for the energy eigenstates and energy eigenvalues, but just for a few minutes, let's not, and say we did! So now you know values for the E 's and functions for the φ 's.

What follows is cast in terms of wave functions to give you practice, but in fact the ket notation can be used just as easily. The ket version of this discussion is in your text (Ch. 3) and was discussed in PH425.

Expand wave function in energy basis; time dependence comes from coefficients:

$$\psi(x,t) = \sum_n c_n(t) \phi_n(x)$$

$$\hat{H}\psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t}$$

Substitute
$$\hat{H} \sum_n c_n(t) \phi_n(x) = i\hbar \frac{\partial}{\partial t} \sum_n c_n(t) \phi_n(x)$$

$$\sum_n c_n(t) E_n \phi_n(x) = i\hbar \frac{\partial}{\partial t} \sum_n c_n(t) \phi_n(x)$$

Expand wave function in energy basis; time dependence comes from coefficients:

$$\psi(x,t) = \sum_n c_n(t) \phi_n(x)$$

Substitute

$$\sum_n c_n(t) E_n \phi_n(x) = i\hbar \frac{\partial}{\partial t} \sum_n c_n(t) \phi_n(x)$$

$$\left(-\frac{iE_n}{\hbar} \right) c_n(t) \phi_n(x) = \frac{\partial c_n(t)}{\partial t} \phi_n(x)$$

$$c_n(t) = e^{-\frac{iE_n}{\hbar}t}$$

$$\psi(x,t) = \sum_n e^{-\frac{iE_n}{\hbar}t} \phi_n(x)$$

So we have solved Schrödinger's time dependent equation! We know the time dependence, because we already know the eigenstates and energies, which we obtained from solving the eigenvalue equation.

$$\psi(x,t) = \sum_n e^{-\frac{iE_n t}{\hbar}} \phi_n(x)$$

$$\hat{H}\varphi_n(x) = E_n \varphi_n(x)$$

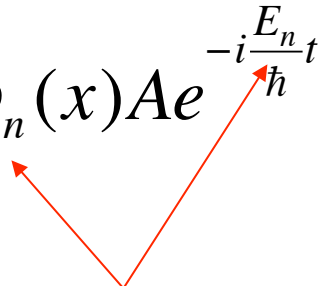
$$\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle$$

$$\hat{H}\varphi_n(x) = E_n\varphi_n(x)$$

$$\hat{H}|\varphi_n\rangle = E_n|\varphi_n\rangle$$

There are usually many functions that solve the eigenvalue problem, each function with its own associated eigenvalue. Label them with index n .

In general, the state of particle is NOT an eigenstate of the Hamiltonian, but a superposition of eigenstates ...

$$\Psi(x,t) = \sum_n \varphi_n(x) A e^{-i\frac{E_n}{\hbar}t}$$


Very important that the energy in the exponent matches the corresponding eigenstate.

Example: $V(x) = 0$ (free particle)

$$\hat{H}\varphi_n(x) = E_n\varphi_n(x)$$

$$-\frac{\hbar^2}{2m} \frac{d^2\varphi(x)}{dx^2} = E\varphi(x)$$

$$\varphi(x) = C' e^{i\frac{\sqrt{2mE}}{\hbar}x} + Ce^{-i\frac{\sqrt{2mE}}{\hbar}x}$$

$$\psi(x,t) = C' e^{i\left(\frac{\sqrt{2mE}}{\hbar}x - \frac{E}{\hbar}t\right)} + Ce^{-i\left(\frac{\sqrt{2mE}}{\hbar}x + \frac{E}{\hbar}t\right)}$$

1st term is traveling wave (to right) and 2nd is traveling to left. Same eigenvalue E - “degenerate”

Note the relationship between ω and k for a free particle
DISPERSION RELATION:

$$E = \hbar\omega \qquad E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

$$\omega(k) = \frac{\hbar k^2}{2m}$$

$$\frac{\omega}{k} = \frac{\hbar k}{2m}$$

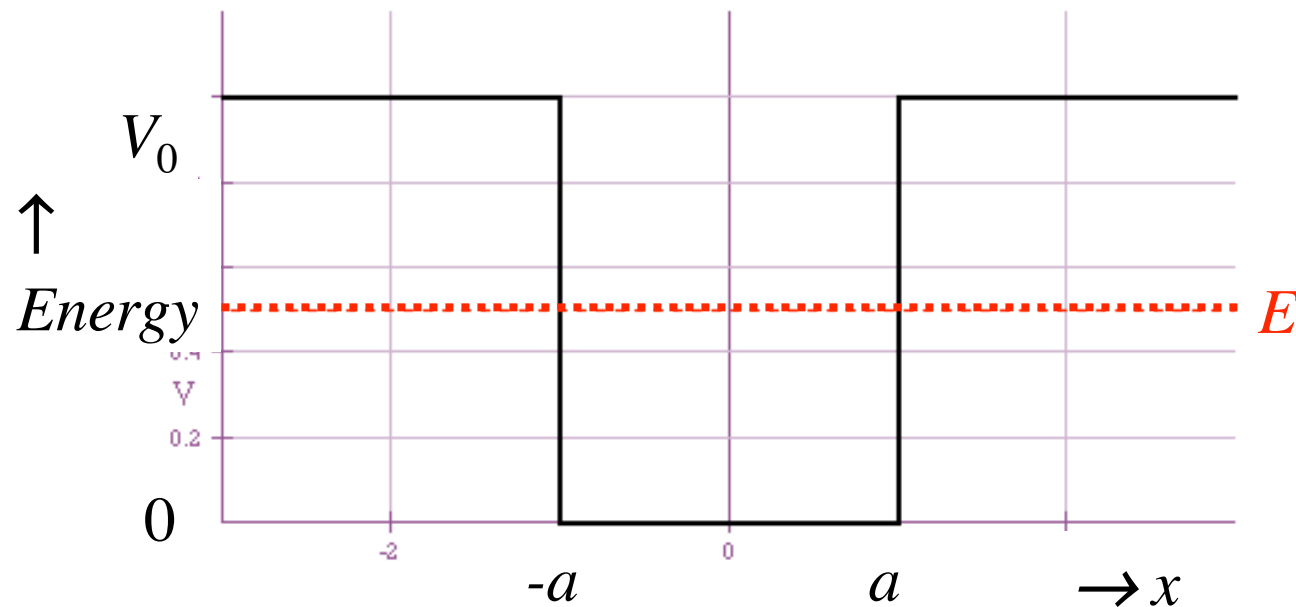
Phase velocity

Not the same!!!

$$\frac{d\omega}{dk} = \frac{\hbar k}{m}$$

Group velocity

Now solve the TISE for different potentials and find examples where there are many solutions with different energies



$$V(x) = \begin{cases} V_0 & |x| > a \\ 0 & |x| < a \end{cases}$$

Schrödinger Wave Equation

SCHROEDINGER WAVE EQUATION REVIEW

- *Time dependent Schrödinger equation*
- *Energy eigenvalue equation (time independent SE)*
- *Eigenstates*
- *Time dependence*
- *(Connection to separation of variables)*
- *Mathematical representations of the above*

The following treatment parallels the discussion of the 1-D wave equation more closely, but I like the approach earlier better.

Schrödinger wave equation:

$$\hat{H}\psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t}$$

As in 1-D non-dispersive eqn, use technique of separation of variables.

$$\psi(x,t) = \varphi(x)T(t)$$

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \quad \text{is function of } x \text{ only}$$

$$\hat{H}\psi(x,t) = i\hbar \frac{\partial \psi(x,t)}{\partial t}$$

$$\hat{H}\varphi(x)T(t) = i\hbar \frac{\partial \varphi(x)T(t)}{\partial t}$$

$$T(t)\hat{H}\varphi(x) = i\hbar \varphi(x) \frac{\partial T(t)}{\partial t}$$

$$\frac{1}{\varphi(x)} \hat{H}\varphi(x) = i\hbar \frac{1}{T(t)} \frac{\partial T(t)}{\partial t}$$

What shall we call the separation constant?

$$\frac{1}{\varphi(x)} \hat{H}\varphi(x) = i\hbar \frac{1}{T(t)} \frac{\partial T(t)}{\partial t} = E$$

$$\hat{H}\varphi(x) = E\varphi(x)$$

$$\hat{H}|\varphi\rangle = E|\varphi\rangle$$

Eigenvalue problem! Solutions (and there are many in general) depend on particular $V(x)$. E represents the energy of a particle in that particular eigenstate, and there are many E values.

$$\frac{\partial T(t)}{\partial t} = -i \frac{E}{\hbar} T(t)$$

$$T(t) = Ae^{-i\frac{E}{\hbar}t}$$

$$T(t) = Ae^{-i\omega t} ; \omega = \frac{E}{\hbar}$$

Most general solution is:

$$\psi(x, t) = \sum_n \varphi_n(x) e^{-iE_n t / \hbar}$$