Lectures 1-2

Phys 521

Schrödinger equation

Lectures 1-2. Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{r})\psi = i\hbar\frac{\partial\psi}{\partial t}$$

Theme: Linearity or superposition principle

Stationary states (normal modes of linear system):

$\psi_n(\vec{r},t) = \varphi_n(\vec{r})\, e^{-i\omega_n t}$ ⟵ nothing happens

$$-\frac{\hbar^2}{2m}\nabla^2\varphi_n + V(\vec{r})\varphi_n = \underbrace{\hbar\omega_n}_{E_n}\varphi_n$$ ⟵ eigenvalue problem Hermiticity

General solution: $\psi(\vec{r},t) = \sum_n c_n \varphi_n(\vec{r})\, e^{-i\omega_n t}$ linearity + completeness

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DeBroglie waves

$p = \frac{h}{\lambda} = \hbar k$, $k = \frac{2\pi}{\lambda}$

$E = h\nu = \hbar\omega$, $\omega = 2\pi\nu$

$\hbar = h/2\pi$

$\hbar = 1.05\times10^{-34}$ J-s

$= 1.05\times10^{-27}$ erg-s

$= 0.66$ eV-fs

Small. What mean?

$L \propto \frac{ML}{T}$ action ang mom

Photons: $E = cp \Leftrightarrow \omega = ck$ $\omega/k = c$

Non-rel particles: $E = \frac{p^2}{2m} \Leftrightarrow \omega = \frac{\hbar k^2}{2m}$ $\omega/k = \frac{\hbar k}{2m} = \frac{p}{2m}$

$\hbar = 0.66$ eV-fs

$= 0.66 \frac{\text{eV}}{\text{nm/fs}} - \text{nm}$

Plane wave: $\psi(x) = e^{ikx} = e^{(i/\hbar)px}$

Should we take complex numbers seriously?

Real waves

Wave to right $\qquad t=0$

$\text{l.i.} \leftarrow \begin{cases} \cos(kx-\omega t) & \cos kx \\ \sin(kx-\omega t) & \sin kx \end{cases}$

gen $\quad \cos(kx-\omega t-\theta) \qquad \cos(kx-\theta)$

phase

Wave to left

$\text{l.i.} \leftarrow \begin{cases} \cos(kx+\omega t) & \cos kx \\ \sin(kx-\omega t) & \sin kx \end{cases}$

gen $\quad \cos(kx-\omega t-\theta) \qquad \cos(kx-\theta)$

phase

Need ψ and $\partial\psi/\partial t$

E $\qquad$ B

2nd order diff eq in t

Complex waves

Wave to right $\qquad t=0$

$e^{i\theta} e^{i(kx-\omega t)} \qquad e^{i\theta} e^{ikx}$

irrelevant phase

Wave to left

$e^{i\theta} e^{i(kx+\omega t)} \qquad e^{i\theta} e^{-ikx}$

Need ψ only

1st order diff eq in t

$$\psi(\vec{r},t) = e^{i(\vec{k}\cdot\vec{r}-\omega t)}$$

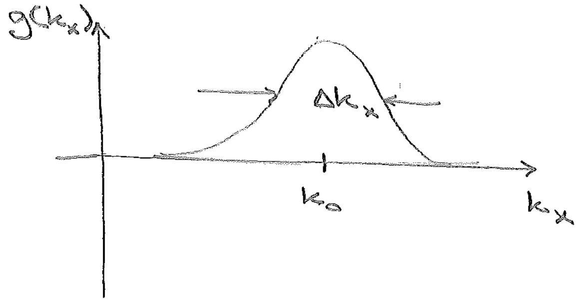
Wave packets:

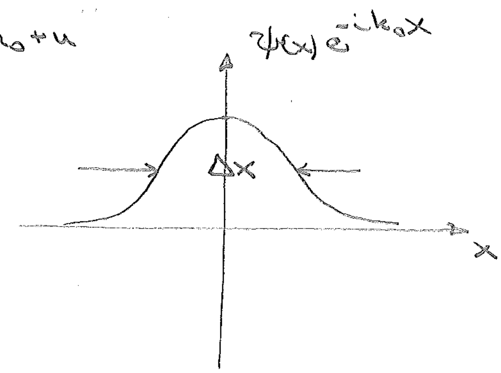
$$\psi(\vec{r},t) = \int \frac{d^3k}{(2\pi)^{3/2}}\, g(\vec{k})\, e^{i(\vec{k}\cdot\vec{r}-\omega t)} = \int \frac{d^3p}{(2\pi\hbar)^{3/2}}\, \underset{\displaystyle \frac{g(\vec{k})}{\hbar^{3/2}}}{\underset{\shortparallel}{\tilde{\psi}(\vec{p})}}\, e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{r}-Et)}$$

1-d: $\psi(x,t) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, g(k)\, e^{i(kx-\omega t)}$

$t=0$: $\psi(x) = \int_{-\infty}^{\infty} \frac{dk_x}{\sqrt{2\pi}}\, g(k_x)\, e^{ik_x x} = e^{ik_0 x} \int_{-\infty}^{\infty} \frac{du}{\sqrt{2\pi}}\, g(k_0+u)\, e^{iux}$

$k_x = k_0 + u$





$$\Delta x\, \Delta k_x \gtrsim 1$$

Uncertainty relation: $\Delta x\, \Delta p_x \gtrsim \hbar$

How get a wave packet displaced to x_0?
$g(k_x) \to g(k_x)\, e^{-ik_x x_0}$

$t>0$: $\psi(x,t) = \int_{-\infty}^{\infty} \frac{dk_x}{\sqrt{2\pi}}\, g(k_x)\, \exp\left[\underbrace{i(k_x x - \omega(k_x)t)}\right]$

dispersionless propagation

$$i\Big(k_x x - \omega(k_0)t - \overbrace{\underbrace{\frac{d\omega}{dk_x}\Big|_{k_x=k_0}}_{\to\, v_{g0}} (k_x-k_0)t} -$$

$$\underbrace{- \frac{1}{2}\frac{d^2\omega}{dk_x^2}\Big|_{k_x=k_0} (k_x-k_0)^2 t - \ldots}_{\text{wave-packet spreading (dispersion)}}$$

dispersion-free propagation $= e^{-i\omega_0 t}\, e^{ik_0 x} \int_{-\infty}^{\infty} \frac{du}{\sqrt{2\pi}}\, g(k_0+u)\, e^{iu(x-v_{g0}t)}$

Maximum moves to right at group velocity

$$v_{g0} = \left.\frac{d\omega}{dk_x}\right|_{k_x = k_0} = \frac{\hbar k_0}{m} = \frac{p_0}{m}.$$

Spreading: $\Delta x_t \sim \frac{\Delta p_0}{m} t \gtrsim \frac{\hbar}{m(\Delta x)_0} t$

Gaussian wave packets – important example

Contracting wave packets

Key point: <u>superposition</u> (required if all those wave packets are allowed)

Statistical interpretation:

$$|\psi(\vec{r},t)|^2 d^3x = \left(\frac{\text{probability to find particle}}{\text{within } d^3x \text{ at time } t} \right)$$

$$\langle f(x) \rangle_t = \int d^3x \; f(x) \, |\psi(x,t)|^2$$

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dp_x}{\sqrt{2\pi\hbar}} \, \bar{\psi}(p_x) \, e^{\frac{i}{\hbar}(p_x x - Et)} = \int_{-\infty}^{\infty} \frac{dp_x}{\sqrt{2\pi\hbar}} \underbrace{\bar{\psi}(p_x)\, e^{-i\omega t}}_{\bar{\psi}(p_x,t)} e^{\frac{i}{\hbar}p_x x}$$

$$\bar{\psi}(p_x,t) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi\hbar}} \, \psi(x,t) \, e^{-\frac{i}{\hbar}p_x x}$$

$$\left[\begin{aligned} \psi(x,t) &= \int \frac{dp_x}{\sqrt{2\pi\hbar}} \, e^{\frac{i}{\hbar}p_x x} \int \frac{dx'}{\sqrt{2\pi\hbar}} \, e^{-\frac{i}{\hbar}p_x x'} \psi(x',t) \\ &= \int dx' \, \psi(x',t) \underbrace{\int \frac{d(p_x/\hbar)}{2\pi} \, e^{i\frac{p_x}{\hbar}(x-x')}}_{\delta(x-x')} \\ &= \psi(x,t) \end{aligned} \right]$$

$$|\overline{\Phi}(\vec{p},t)|^2 d^3p = \left(\begin{array}{l}\text{probability for particle to have}\\ \text{momentum within } d^3p \text{ at time } t\end{array}\right)$$

Normalization: $1 = \int d^3x\, |\psi(\vec{x},t)|^2 = \int d^3p\, |\overline{\Phi}(\vec{p},t)|^2$

$$\langle p_x \rangle_t = \int dp_x\, |\overline{\Phi}(p_x,t)|^2\, p_x$$

$$= \int dp_x\, p_x \int \frac{dx}{\sqrt{2\pi\hbar}}\, \psi(x,t)\, e^{-\frac{i}{\hbar}p_x x} \int \frac{dx'}{\sqrt{2\pi\hbar}}\, \psi^*(x',t)\, e^{\frac{i}{\hbar}p_x x'}$$

$$= \underbrace{\int dx'\, \psi^*(x',t) \int dx\, \psi(x,t) \underbrace{\int \frac{d(p_x/\hbar)}{2\pi}\, p_x\, e^{-i\frac{p_x}{\hbar}(x-x')}}_{-\frac{\hbar}{i}\frac{\partial}{\partial x}\delta(x-x')}}_{\int dx\, \frac{\hbar}{i}\frac{\partial\psi}{\partial x}\,\delta(x-x')}$$

$$= \int dx\, \psi^*(x,t)\, \frac{\hbar}{i}\frac{\partial}{\partial x}\, \psi(x,t)$$

$$\langle f(p_x) \rangle_t = \int dx\, \psi^*(x,t)\, f\!\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \psi(x,t)$$

Rigorous uncertainty relation: $\Delta x\, \Delta p_x \geq \frac{\hbar}{2}$

uncertainties

Schrödinger equation:

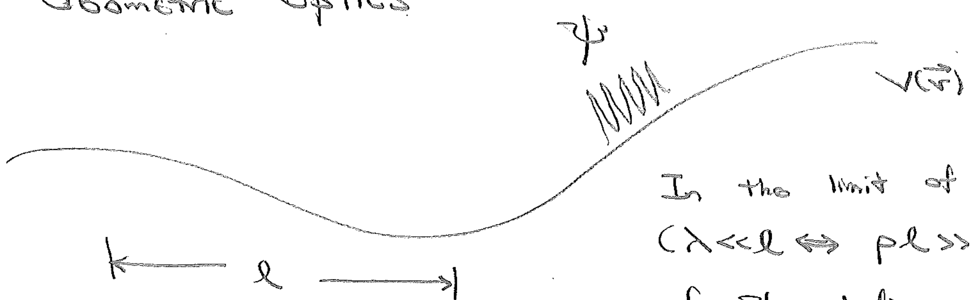
Free particle: $-\frac{\hbar^2}{2m}\nabla^2\psi = i\hbar\frac{\partial\psi}{\partial t}$

FT $\quad \frac{p^2}{2m}\bar{\psi} = i\hbar\frac{\partial\bar{\psi}}{\partial t} \Rightarrow \bar{\psi}(\vec{p},t) = e^{-\frac{i}{\hbar}Et}\,\bar{\psi}(\vec{p},0)$

What about a potential $V(\vec{r},t)$?

① Follow a wave packet to see if it follows a classical trajectory. Ehrenfest's theorem. Wave-packet spreading defeats.

② Geometric optics



In the limit of short wavelengths ($\lambda \ll \ell \Leftrightarrow p\ell \gg h$), the rays of ψ define classical trajectories

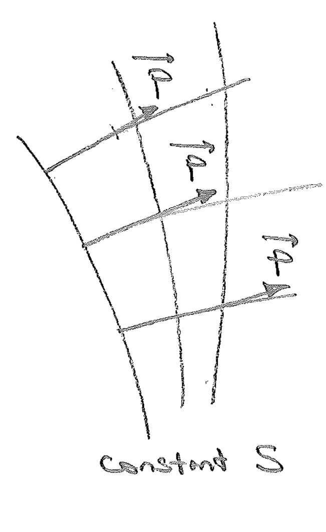
Here ψ defines a congruence of trajectories.

$\psi(\vec{r},t) = A(\vec{r},t)\exp\left(\frac{i}{\hbar}S(\vec{r},t)\right)$

$P(\vec{r},t) = A^2(\vec{r},t) = \begin{pmatrix}\text{probability}\\ \text{density}\end{pmatrix}$

$\frac{1}{\hbar}S(\vec{r},t) = (\text{phase})$

$\vec{p} = \nabla S$



$$0 = \overset{(1)}{-\frac{\hbar^2}{2m}\nabla^2\psi} + \overset{(3)}{V\psi} - \overset{(2)}{i\hbar\frac{\partial\psi}{\partial t}}$$

$$= e^{iS/\hbar}\left(\underset{\frac{\hbar^2}{\lambda^2 m}}{A}\left(\overset{(1)}{\frac{|\nabla S|^2}{2m}} + \overset{(3)}{V} + \overset{(2)}{\frac{\partial S}{\partial t}}\right) - \underset{\frac{\hbar^2}{mR^2}}{\overset{(1)}{\frac{\hbar^2}{2m}\nabla^2 A}}\right.$$

$$\left. - \underset{\frac{\hbar^2}{mR\lambda}}{i\hbar}\underbrace{\left(\overset{(1)}{\frac{\nabla A\cdot\nabla S}{m}} + \overset{(1)}{\frac{A\nabla^2 S}{2m}} + \overset{(2)}{\frac{\partial A}{\partial t}}\right)}_{\frac{1}{2A}\left(\frac{\partial P}{\partial t} + \frac{\nabla P\cdot\vec{p}}{m} + P\frac{\nabla\cdot\vec{p}}{m}\right)}\right)$$

$$= \frac{1}{2A}\left(\underbrace{\frac{\partial P}{\partial t} + \frac{\nabla\cdot(P\vec{p})}{m}}_{=0}\right)$$

(conservation of probability)

Classical trajectories: $\frac{|\nabla S|^2}{2m} + V + \frac{\partial S}{\partial t} = 0$

$$\frac{d\vec{p}}{dt} = \frac{\vec{p}(\vec{r}+\Delta\vec{r}, t+\Delta t) - \vec{p}(\vec{r},t)}{\Delta t}$$

$$= \sum_j \frac{\partial\vec{p}}{\partial x^j}\frac{\Delta x^j}{\Delta t} + \frac{\partial\vec{p}}{\partial t}$$

$$= \frac{1}{m}\sum_j \frac{\partial(\nabla S)}{\partial x^j}\frac{\partial S}{\partial x^j} + \frac{\partial}{\partial t}\nabla S$$

$$= \frac{1}{2m}\nabla\left(\sum_j \frac{\partial S}{\partial x^j}\frac{\partial S}{\partial x^j}\right) + \nabla\frac{\partial S}{\partial t}$$

$$= \nabla\left(\frac{\nabla S\cdot\nabla S}{2m} + \frac{\partial S}{\partial t}\right)$$

1-d, $\partial V/\partial t = 0$:

$S = -Et + W(x)$

$p_x = \frac{\partial S}{\partial x} = \frac{\partial W}{\partial x}$

(1) $\frac{p_x^2}{2m} + V = E$

(2) $\frac{\partial}{\partial x}(P p_x) = 0$

$P(x) \propto \frac{1}{v_x}$

$P(x)\,dx \propto dt$

$$-\nabla V = \frac{d\vec{p}}{dt} = \nabla\left(\frac{\nabla S\cdot\nabla S}{2m} + \frac{\partial S}{\partial t}\right)$$

$$0 = \nabla\left(\frac{\nabla S\cdot\nabla S}{2m} + V + \frac{\partial S}{\partial t}\right)$$

Quantum: $$\frac{|\nabla S|^2}{2m} + V \underbrace{- \frac{\hbar^2}{2m}\frac{1}{A}\nabla^2 A}_{\text{Quantum potential}} = -\frac{\partial S}{\partial t}$$

① Responsible for wave-packet spreading

Spreading is biggest when A gets large. Singularities in A at classical turning points are eliminated.

Feedback from A to S, absent in H-J theory

② Responsible for superposition by making Schrödinger equation linear.

Makes ψ nonzero in classically forbidden regions: discrete bound states; tunneling.

Schrödinger equation and H-J theory

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$$\psi = A(\vec{r},t)\, e^{\frac{i}{\hbar}S(\vec{r},t)}$$

$$P(\vec{r},t) = A^2(\vec{r},t)$$

$$\vec{p}(\vec{r},t) = \nabla S$$

$$\nabla\psi = \left(\nabla A + \frac{i}{\hbar} A\nabla S\right) e^{\frac{i}{\hbar}S}$$

$$\nabla^2\psi = \left(\nabla^2 A + \frac{2i}{\hbar}\nabla A\cdot\nabla S + \frac{i}{\hbar}A\nabla^2 S - \frac{1}{\hbar^2}A|\nabla S|^2\right) e^{\frac{i}{\hbar}S}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \left(A\frac{|\nabla S|^2}{2m} - i\frac{\hbar}{m}\nabla A\cdot\nabla S - i\frac{\hbar}{2m}A\nabla^2 S - \frac{\hbar^2}{2m}\nabla^2 A\right) e^{\frac{i}{\hbar}S}$$

$$\frac{\partial\psi}{\partial t} = \left(\frac{\partial A}{\partial t} + \frac{i}{\hbar}A\frac{\partial S}{\partial t}\right) e^{\frac{i}{\hbar}S}$$

$$i\hbar\frac{\partial\psi}{\partial t} = \left(-A\frac{\partial S}{\partial t} + i\hbar\frac{\partial A}{\partial t}\right) e^{\frac{i}{\hbar}S}$$

$$0 = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi - i\hbar\frac{\partial\psi}{\partial t}$$

$$
\begin{aligned}
0 = e^{iS/\hbar} \overbrace{\Bigg(A \underbrace{\left(\frac{|\nabla S|^2}{2m} + V + \frac{\partial S}{\partial t} \right)}_{=0 \ \text{(H-J equation)}} - \underbrace{\frac{\hbar^2}{2m} \nabla^2 A}_{\substack{\text{quantum potential} \\ \text{(wave-packet spreading)}}}}^{=0 \ \text{(QM)}} \\
- i\hbar \underbrace{\left(\frac{\nabla A \cdot \nabla S}{m} + A \frac{\nabla^2 S}{2m} + \frac{\partial A}{\partial t} \right)}\Bigg)
\end{aligned}
$$

$$
\frac{1}{2A} \left(\frac{\partial \rho}{\partial t} + \frac{\nabla \rho \cdot \vec{p}}{m} + \rho \frac{\nabla \cdot \vec{p}}{m} \right)
$$

$$
= \frac{1}{2A} \underbrace{\left(\frac{\partial \rho}{\partial t} + \frac{\nabla \cdot (\rho \vec{p})}{m} \right)}_{=0 \quad \text{(continuity equation)}}
$$

Harmonic oscillator

H-J theory:

$$\frac{S'^2}{2m} + \frac{1}{2}m\omega^2x^2 = E$$

$$S' = p = \hbar k = \pm\sqrt{2m}\left(E - \frac{1}{2}m\omega^2x^2\right)^{1/2} = \pm\sqrt{2mE}\left(1 - \frac{m\omega^2x^2}{2E}\right)^{1/2}$$

$$k = \pm\frac{\sqrt{2mE}}{\hbar}\left(1 - \frac{m\omega^2x^2}{2E}\right)^{1/2} = \pm k_0\left(1 - x^2/x_0^2\right)^{1/2}$$

$$\frac{p_0}{\hbar} = k_0 \equiv \frac{\sqrt{2mE}}{\hbar}, \quad x_0 = \sqrt{\frac{2E}{m\omega^2}} \qquad \frac{x_0p_0}{\hbar} = \frac{2E}{\hbar\omega}$$

$$\text{constant} = P(x)\,k \Rightarrow P(x) = A^2(x) = \frac{\text{const}}{k} = \frac{\text{const}}{\sqrt{1 - x^2/x_0^2}}$$

$$S(x) = \pm\hbar k_0\int_0^x dx'\left(1 - x'^2/x_0^2\right)^{1/2} = \pm k_0x_0\int_0^{\sin^{-1}(x/x_0)} du\,\cos^2 u$$

$$x' = x_0 \sin u$$

$$S(x) = \pm\frac{1}{2}\hbar k_0x_0\underbrace{\int_0^{\sin^{-1}(x/x_0)} du\,(1 + \cos 2u)}_{\sin^{-1}(x/x_0) + \frac{1}{2}\sin 2u\Big|_0^{\sin^{-1}(x/x_0)}}$$

$$S(x) = \pm\frac{1}{2}\hbar k_0x_0\left(\sin^{-1}(x/x_0) + \frac{x}{x_0}\cos\left(\sin^{-1}(x/x_0)\right)\right), \quad |x| \le x_0$$

$$\psi(x) = \frac{\text{const}}{\sqrt{1 - x^2/x_0^2}}\exp\left[\pm\frac{i}{2}k_0x_0\left(\sin^{-1}(x/x_0) + \frac{x}{x_0}\cos\left(\sin^{-1}(x/x_0)\right)\right)\right]$$

Superpose $\pm$ to get standing waves