

I. Basics + Logistics

① According to the Online Schedule, Final is in 101 LSA at 8:00 AM, Tuesday, December 19<sup>th</sup>!

② Basic Info - Final is 5-6 problems, most involve little computation - mostly conceptual, physical. It covers wave mechanics, uncertainty principle, one-dimensional problems (1D-SHO, infinite square well), angular momentum / Hydrogen Atom, + perturbation theory. I'll cover the first three topics today + the last two along with solutions to the review problems next Sunday.

③ There will certainly be a cheat sheet allowed.

II. Fundamental Principles of QM I: Schrödinger's Eq<sup>n</sup>

Time dependent Schrödinger's Equation:  $i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$  describes the time evolution of any state/wave-function which describes some physical system. Two very important facts!

① This equation is linear! Thus, if  $\Psi$  and  $\chi$  are both solutions, so is:  $a\Psi + b\chi$  for  $a, b \in \mathbb{C}$ . In particular, suppose I have a set of solutions  $\{\Psi_n\}$  which, at time  $t=0$ , form a complete + orthonormal set of functions,

This  $\Rightarrow$  is why the space of states is a vector space. This is equiv. to the superposition principle!

(i.e.  $\int \Psi_n^*(x, t=0) \Psi_m(x, t=0) dx = \delta_{nm}$  and  $\exists \{c_n\}$  st. for any  $\Psi(x)$ ,  $\Psi(x) = \sum_{n=0}^{\infty} c_n \Psi_n(x, t=0)$ ), then for any initial condition,  $\Psi(x, t=0)$ , we can find its time evolution:

(a) Expand  $\Psi(x, t=0)$  in terms of the  $\Psi_n$ :  
 $\Psi(x, t=0) = \sum_{n=0}^{\infty} c_n \Psi_n(x, t=0)$ , where  $c_n = \int \Psi_n^*(x, t=0) \Psi(x, t=0) dx$   
 (b) The time dependent solution with initial condition  $\Psi(x, t=0)$  is then just:

$\Psi(x, t) = \sum_{n=0}^{\infty} c_n \Psi_n(x, t) \Rightarrow$  so finding a set  $\{\Psi_n\}$  allows us to solve Schr. Eq<sup>n</sup> completely!  
 ② Special Case: suppose  $H$  is time independent. Then, we can use separation of variables + the time independent Schrödinger equation to find and solve for a particular set of solutions  $\{\Psi_n\}$  which are complete + orthonormal, and by ① above, we've solved our problem! Note: This will not work if  $H$  is time dependent!!!

In particular, let's work this out. We make the ansatz that  $\Psi_n(x, t) = \chi_n(t) \psi_n(x) \Rightarrow H\psi_n(x) = E_n \psi_n(x)$ ,  $\chi_n(t) = e^{-iE_n t/\hbar}$

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Thus, we see that this complete set  $\{\Psi_n(x,t) = \psi_n(x)e^{-iE_n t/\hbar}\}$  is just the set of normalized eigenfunctions of the Hamiltonian! Thus, we find: Given  $\Psi(x,t=0)$ ,  $H$ , we should:

- Ⓐ Solve  $H\psi_n(x) = E_n\psi_n(x)$  to obtain  $\{\Psi_n(x,t) = \psi_n(x)e^{-iE_n t/\hbar}\}$  a complete set of orthonormal eigenfunctions of  $H$ .
- Ⓑ Expand  $\Psi(x,t=0) = \sum_{n=0}^{\infty} c_n \psi_n(x)$   $c_n = \int \psi_n^*(x) \Psi(x,t=0) dx$
- Ⓒ We're done! Our solution is:  $\Psi(x,t) = \sum_{n=0}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$

### III. Fundamentals II: Measurement, Observables, Uncertainty.

Observables in QM are represented by Hermitian operators

$\hat{O}$ , acting on the vector space ( $\infty$ -dim'l Hilbert space) of states of the physical system. For example:

$$x, H = \frac{\hat{p}^2}{2m} + V(x) = \frac{\hat{p}_x^2}{2m} + V(x), \quad \hat{p}_x = -i\hbar \frac{\partial}{\partial x}, \quad \vec{L} = \vec{r} \times \vec{p}$$

$$L_z = (x p_y - y p_x) = -i\hbar (x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x}) = -i\hbar \frac{\partial}{\partial \phi}$$

The fact that they are Hermitian means that  $\hat{O}^\dagger = \hat{O}$ , where  $\hat{O}^\dagger$  is defined by the condition that:

$$\langle \hat{O}\psi | \chi \rangle = \int (\hat{O}\psi)^* \chi dx \stackrel{\text{def}}{=} \int \psi^* (\hat{O}^\dagger \chi) dx = \langle \psi | \hat{O}^\dagger \chi \rangle$$

[I've used bra-ket notation here:  $\chi(x) \mapsto |\chi\rangle$  while  $\int \psi^*(x) \cdot dx \mapsto \langle \psi |$ , so  $\langle \psi | \chi \rangle = \int \psi^*(x) \chi(x) dx$ !]

Given an observable  $\hat{O}$ , we'd like to know what values it can take in a given state, how probable each of them are and the average value of  $\hat{O}$  for any given state. To do this, we do the following:

- ① Find a complete set of eigenvectors of  $\hat{O}$ , i.e.  $\{\phi_n(x)\}$  (or  $\{|\phi_n\rangle\}$ , s.t.  $\hat{O}\phi_n(x) = \lambda_n\phi_n(x)$ ). The set  $\{\lambda_n\}$  is the set of all possible outcomes of a measurement of  $\hat{O}$  (for any possible ~~initial~~ state)!
- ② For a given state  $\Psi(x,t)$ , (or  $|\Psi\rangle$ ), the probability of measuring the value  $\lambda_n$  for the observable  $\hat{O}$  is given by:
 
$$P(\lambda_n) = |\langle \phi_n | \Psi \rangle|^2 = \left| \int \phi_n^*(x) \Psi(x,t) dx \right|^2$$
- ③ The average value (expectation value) of  $\hat{O}$  in a state  $\Psi$  is just:
 
$$\langle \Psi | \hat{O} | \Psi \rangle = \int \Psi^*(x,t) \hat{O} \Psi(x,t) dx = \sum_{n=0}^{\infty} P(\lambda_n) \lambda_n = \langle \hat{O} \rangle$$
- ④ The uncertainty in  $\hat{O}$  is given by:
 
$$\sqrt{\langle (\hat{O} - \langle \hat{O} \rangle)^2 \rangle} = \sqrt{\langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2} = \Delta \hat{O}$$

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IV. Fundamentals III: Wave Packets, Dispersion, Heisenberg Uncertainty.

It is worthwhile reviewing Budker's HW3, problems 1 + 2.

1D Free particle:  $V(x) = 0$   $\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E \psi$ ,  $k \equiv \frac{\sqrt{2mE}}{\hbar}$

The solutions are  $\psi(x) = A e^{ikx} + B e^{-ikx}$ , we get time dep. by adding  $e^{-iEt/\hbar}$ ,

$$\Rightarrow \psi(x,t) = A \exp(ik(x - \frac{\hbar k}{2m}t)) + B \exp(-ik(x + \frac{\hbar k}{2m}t))$$

↑ right moving wave
↑ left moving wave

Apparently, these are moving at the velocity  $v_p = \pm \frac{\hbar k}{2m}$  (phase velocity)

But this makes no sense! Their kinetic energy is:

$$E = \frac{\hbar^2 k^2}{2m} = \frac{1}{2} m v^2 \Rightarrow v = \frac{\hbar k}{m} \neq \frac{\hbar k}{2m} ? ! ?$$

What's going on? First, note that this wave  $\psi$  is NOT normalizable

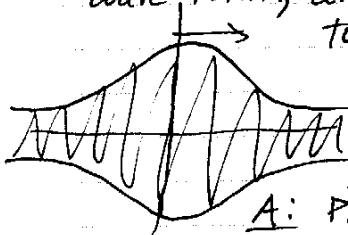
$\Rightarrow \int \psi^* \psi = \infty$ ! Thus it isn't a physic. realizable state!

We need to construct a wave packet, a sum of these eigenstates!

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int \phi(k) e^{i(kx - \frac{\hbar k^2}{2m}t)} dk$$

which is normalizable for an appropriate choice of  $\phi(k)$ .

It turns out that a particle is represented by a localized wave form; and the speed of the particle should be related



to the speed of the motion of the wave form itself, not of any particular  $e^{i(kx - \omega t)}$  term in this superposition.

Q: What is the speed of the wave form?

A: Principle of Stationary phase tells us that

an integral of the form  $\int \phi(k) \exp(i\beta(k)) dk$  is dominated by the region of the integral where  $\beta$  is stationary (either minimum or maximum). Why? IF  $\beta$  is near a min or max,  $\frac{\partial \beta}{\partial k} = 0$ , so  $\beta$  is nearly constant, ~~so~~ Thus,

the ~~integral doesn't~~ integrand isn't oscillating very much (as it would any where that  $\beta$  is varying), and won't cancel out to 0. In our case, we have:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int \phi(k) \exp(i(kx - \omega(k)t)) dk \quad \omega(k) = \frac{\hbar k^2}{2m}$$

$$\Rightarrow \text{dominated by } \frac{\partial}{\partial k} (kx - \omega(k)t) = 0 \Rightarrow x - \frac{\partial \omega}{\partial k} t = 0 \Rightarrow \frac{x}{t} = \frac{\partial \omega}{\partial k}$$

Thus,  $\psi(x,t)$  is dominated by values ~~at~~ where  $\frac{x}{t} = \frac{\partial \omega}{\partial k} \equiv v_g$ , and thus looks like a wave form travelling at group velocity  $v_g = \frac{\partial \omega}{\partial k}$ , rather than the phase velocity  $v_p = \frac{\omega}{k}$ .

In particular, in QM, we have for a free particle  $\omega(k) = \frac{\hbar k^2}{2m}$

$\Rightarrow v_g = \frac{\hbar k}{m}$ ,  $v_p = \frac{\hbar k}{2m}$ , so a wave packet moves at the speed we'd expect!

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Q: What are the group + phase velocities for a relativistic particle of mass  $m$ ?

A: In this case  $E^2 = p^2 c^2 + m^2 c^4 = \hbar^2 k^2 c^2 + m^2 c^4$

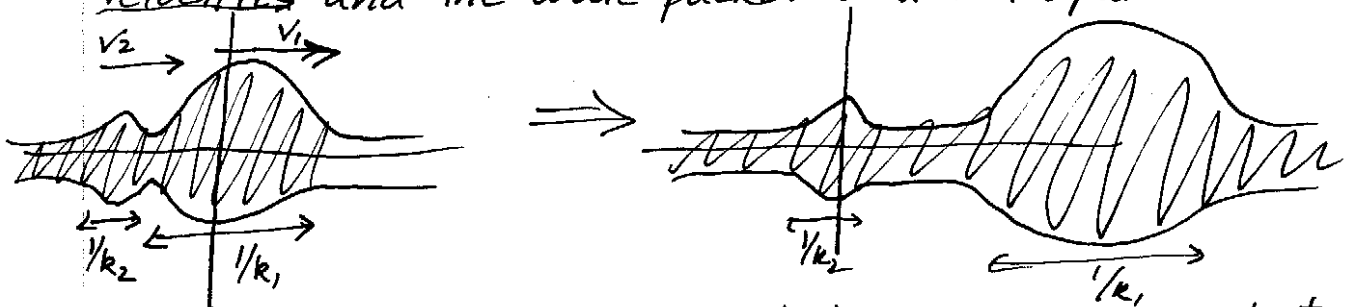
So, using the relations  $E = \hbar \omega$ ,  $p = \hbar k$ , we have:

$$\hbar^2 \omega(k)^2 = \hbar^2 k^2 c^2 + m^2 c^4 \Rightarrow \omega(k) = c \sqrt{k^2 + \frac{m^2 c^2}{\hbar^2}}$$

Thus,  $v_p = \frac{\omega(k)}{k} = \frac{c \sqrt{k^2 + (mc/\hbar)^2}}{k}$  while  $v_g = \frac{c}{2} \frac{2k}{\sqrt{k^2 + (mc/\hbar)^2}} = \frac{ck}{\sqrt{k^2 + (mc/\hbar)^2}}$

Q: Does a relativistic wave packet generally disperse? What about an ultra-relativistic wave packet  $p \gg mc$ ?

A: The dispersion of a wave packet is related to the question of whether the group velocity is constant as a function of  $k$ ! If the group velocities of wave-forms ~~with~~ with different values of  $k$  are different, then features with size  $\sim 1/k_1$  and those with size  $1/k_2$  will move at different velocities and the wave packet will fall apart!



Thus, we require the group velocity,  $v_g$  to be constant as a function of  $k$ !

No Dispersion  $\iff \frac{\partial v_g}{\partial k} = 0 \iff \frac{\partial^2 \omega}{\partial k^2} = 0$ !

Clearly, a relativistic wave packet disperses

as  $\frac{\partial^2 \omega}{\partial k^2} = \frac{c}{\sqrt{k^2 + (mc/\hbar)^2}} - \frac{ck^2}{(k^2 + (mc/\hbar)^2)^{3/2}} = (mc/\hbar)^2 (k^2 + (mc/\hbar)^2)^{-3/2}$

However, in the ultra relativistic limit,  $k^2 \gg (mc/\hbar)^2$ ,

$\frac{\partial^2 \omega}{\partial k^2} \rightarrow 0$ , so we expect little or no dispersion!