

## H) Simple Harmonic Oscillator (SHO)

Most important problem in QM. Why?

1) One of the only practical problems that is exactly solvable.

2) because the annihilation/creation operators and algebra provide the basis for Quantum Field Theory.

Start by first discussing these op's:

Suppose two operators  $a, a^\dagger$  who have the following commutation algebra.

$$[a, a^\dagger] = 1$$

(hey not very different from  $[x, p] = i\hbar \rightarrow$  and same as classical commutator!)

Then immediately we have

$$\begin{aligned} [a^\dagger, a]a &= -a = [a^\dagger a, a] \\ a^\dagger [a, a^\dagger] &= a^\dagger = [a^\dagger a, a^\dagger] \end{aligned}$$

which is to say if we define an Operator

$$N = a^\dagger a$$

that has eigenbasis states  $|n_n\rangle$  such that

$$N|n_n\rangle = n_n|n_n\rangle$$

(Let's just call it  $n$ , the same way we call  $A|a\rangle = a|a\rangle$ )

Then playing same game as w/ translation operator, we have the following interesting relation

$$\begin{aligned} N a |n\rangle &= (a N - a) |n\rangle = (n-1) a |n\rangle \\ N a^\dagger |n\rangle &= (a^\dagger N + a^\dagger) |n\rangle = (n+1) a^\dagger |n\rangle \end{aligned}$$

$$a^\dagger a |n\rangle = n |n\rangle$$

PURELY derived because of the commutator algebra:

Which of course IMPLIES:

$a |n\rangle$  is eigenket w/ eigenvalue  $n-1$

$a^\dagger |n\rangle$  is eigenket w/ eigenvalue  $n+1$

So if we start with any eigenstate  $|n\rangle$  we can always "generate" a new state  $|n-1\rangle$

$$a |n\rangle = c_n |n-1\rangle$$

This process has to stop because

$$n = \langle n | a^\dagger a |n\rangle = \langle a n | a n \rangle \geq 0$$

ALWAYS for all  $n$  (we require this to be so—because we want only positive definite normalizations)

This is only possible if there exists a zero eigenvalue

$$N |0\rangle = 0$$

remains zero after further lowering

$$N |0\rangle = a^\dagger a |0\rangle = 0$$
$$\Rightarrow a |0\rangle = 0$$

**$a$  called "annihilation" operator.** it "kills"  $|0\rangle$  and always decrements  $n$

**$a^\dagger$  called "creation" operator.** it cannot "resurrect" a killed state ( $a^n |0\rangle$ ) --"creation" bad term?--but it always increments  $n$

Actually the reason for these terms is because we think of each increment of energy  $N$  as a excitation above some base state  $|0\rangle$ . It is also part of general quantum thinking (e.g. including wave

mech) to think of any discrete excitation as a **particle**. In this case the particles would be called **phonons** of the SHO.

In Quantum Field Theory (QFT) the situation is generalized for ALL REAL fields, e.g. electromagnetic or particles. In place of our momentum states in this class  $|p\rangle$ , we construct new basis states that carry an “number of particles” for a given momentum  $\rightarrow |P\rangle = |p\rangle |n\rangle$ . E.g. for a propagating free electromagnetic field,  $n$  is the number of “photons” with momentum  $|p\rangle$ . In exactly the same way,  $n$  could be the number of electrons if the state describes electrons—and conversely electrons are thought of as just excitations in a some global “electron field”.

Now we’ve established that **N has eigenvalues that are**

- **chosen as integers**
- and as **only positive**

At least most conveniently—otherwise we need new postulates...

**Why is this relevant?**

Of course we **know the answer already for the SHO**. It’s because our **Hamiltonian** for the **SHO** is can be written **in terms of the N operator only—ie with no other “non-trivial” operator**. Done by **forming linear combinations of x,p** that satisfy the above requirements for **a,a†**

But **before** we show **that...**

**DIGRESSION:**

**Neat: Note** that we **don’t** even **need** to consider any **Hamiltonian at all** really.

The above actually works for ANY linear combination of  $x, p$  that fulfill this algebraic requirement.

Q: what’s the most trivial example, thinking of  $[x,p] = i\hbar$  ?  $\rightarrow [x,p/i\hbar] = [x,k/i] = 1$ .

(using  $a'$  so as not to confuse w/ SHO  $a$ ) Thus if we can simply define  $a' = x, a'^{\dagger} = p/i\hbar, N' = xp/i\hbar$

Means instead of our continuous bases,  $|x\rangle, |p\rangle$  we can always define a discrete basis of the operator  $xp/i\hbar$

What is this operator ? I don’t know. It almost looks like a reasonable observable (pos\*mom), but it probably isn’t. In fact it almost looks like angular momentum is  $L = \mathbf{x} \times \mathbf{p} = \epsilon_{ijk} x_i p_j$  but it’s  $\propto x_i p_i$

Who cares! point is we always can define at least one operator who has a discrete eigenbasis spanning the same Hilbert space as our  $|x\rangle, |p\rangle$  basis

**You will note that the in this case  $a^{\dagger}$  is not actually the hermitian conjugate of  $a$ :** true, but this only actually affects the requirement in the derivation that the states have positive integer eigenvalues of  $xp/i\hbar$ . Still we can think of a discrete basis of  $xp$  states.

We can fix this problem by considering Hermitian combinations of  $xp$ ,  $x$ ,  $p$  for our “N” ( e.g.  $\{x,p\}/2 = xp+px / 2$  is automatically Hermitian—not that that fixes this by itself). Actually we still likely need  $x \pm ip$  -like combinations to fully solve this issue. But still there are many such combinations, not just the SHO’s Hamiltonian/Number operators.

Also note there is likely some technicalities regarding which space we’re talking about since  $|x\rangle$ ,  $|p\rangle$  we said themselves weren’t actually vectors of the Hilbert space.

### END DIGRESSION

Point: We’ve gotten very far without actually even mentioning the actual Hamiltonian of the SHO.

### First define it: what is SHO?

Answer: a system with the following Hamiltonian:

$$H = p^2/2m + V(x) = p^2/2m + m\omega^2/2$$

(ie  $V(x) = x^2$  remember  $\omega = \sqrt{k/m}$  so that Force =  $dV/dx = -kx$ )

Immediately we see  $a^2-b^2 \rightarrow$  think of perfect square  $(a+b)(a-b)$  (remember  $a^2+b^2 = a^2 - (ib)^2$ )

Problem set: define an  $a, a^\dagger$  in terms of  $x$ ,  $p$  so that we can write  $H$  above in the form

$$H = K(a^\dagger a + a a^\dagger) = K(2N + 1)$$

So  $H$  commutes with  $N$  obviously— $\rightarrow$  same eigenbasis

And  $K$  works out such that energy eigenvalues are  $H_n = E_n = \hbar\omega (n+1/2)$  Ground state—lowest  $E = \hbar\omega/2$

$H$  is an observable quantity in this case obviously!

### I) Using the Position/Momentum Basis in the Formalism

So we see that the first, “most important” application of using the  $p$ ,  $x$  operators avoided using the  $|x\rangle$ ,  $|p\rangle$  basis at all! and preferred switching to a discrete basis.

Generally true for all Bound State problems in Wave Mech.

**For what are the position / momentum basis states useful ?**

### Answer 1) Approximation Schemes

The momentum basis will be most useful for approximation schemes especially particle scattering applications/approximations. Exactly solvable results not usually encountered in real world. Approximation schemes are necessary.

Notice two things about the Hamiltonian:  $H = p^2/2m + V(x) = T + V(x)$

- 1) Obviously with  $V(x) = 0$  The momentum basis is also the basis of the Hamiltonian.
- 2) We should usually be able to approximate potentials  $V(x)$  as some sort of series sum

Most obvious such expansion  $\rightarrow V(x) = V_1(x) + V_2(x) + \dots$  like Taylor expansion where other later terms are relatively smaller and smaller, so we can drop them.

### Separable Potentials

But we can also do expansions of a kind that is more convenient towards using a particular set of basis states:

Following the idea of making a general operator out of ket-bra outer products (e.g. we said in its own eigenbasis an operator  $A$  has the form  $\sum a_n |a_n\rangle\langle a_n|$ ) it can be useful to approximate using arbitrary potentials in the form

$$V = |g\rangle\lambda_{gf}\langle f|$$

Where  $g, f$  can be some state, which can of course be written as linear combinations of basis states, possibly momentum kets  $|p\rangle$  or position kets  $|x\rangle$  and  $\lambda$  is some number.

Potentials are called **separable** if they can be written as a combination of such terms (e.g. most commonly a discrete sum )

$$V_{\text{sep}} = \sum_{kn} |k\rangle\lambda_{kn}\langle n|$$

I think that word is used because it acts on each combination of basis states "separately."

A convenient choice for these could be the momentum basis states

$$\int dp dp' |p\rangle\lambda_{pp'}\langle p'|$$

Why ? Because then the entire Hamiltonian including the  $p^2/2m$  operator (sometimes called  $T$ ) is entirely composed of operators which act directly on  $|p\rangle$  basis kets !!!

YESTERDAY NUCLEAR SEMINAR: EXACTLY ONE EXAMPLE!!!

DIGRESSION: Why momentum kets instead of position?

Greater question: Perfect symmetry between  $p$ ,  $x$ ? PSET: The Position Operator in the  $|p\rangle$  Basis—  
also fulfills derivative relation

$$\langle p|x|\alpha\rangle \propto d/dp (\langle p|\alpha\rangle) = d\phi(p)/dp$$

So everything looks very symmetric.

Answer: **no** generally because of free Hamiltonian “preference” for  $p$  operator.  $p$  is likely the usually the preferred basis (in lieu of exact Hamiltonian basis).

Actually for separable potentials, it is actually usually angular momentum basis states.

end DIGRESSION

### **Perturbation Theory:**

More generally there is perturbation theory which we will not discuss this quarter. But we discussed it during the Wave Mech review (please go back and take a look)—its generalization in the bra/ket formalism should not be hard to imagine.

For high energy scattering problems, it is most convenient to treat the “base Hamiltonian” as

$$H_0 = p^2/2m = T$$

and because by assumption the  $T = KE$  is so high, treat the entire potential  $V(x)$  as a perturbation. Thus again the base states you want to start w/ for  $H_0$  are obviously the  $|p\rangle$  states.

The main difference between Perturbation Theory though is that PT is a full expansion of the STATES of the full Hamiltonian, in terms of the states of the base  $H$ , not just an approximate expansion of the potential.

### **Answer 2) “Artificial” Construction of States**

Another reason  $|p\rangle$ ,  $|x\rangle$  basis useful is it’s easy to construct arbitrary states using them—through the wave functions themselves. Sometimes we may not know or care what the Hamiltonian is, but we have a better idea how to describe the state in terms of the  $|x\rangle$  or  $|p\rangle$  states.

Examples:

-Suppose we know a particle is localized to some area

- Suppose we know its momentum

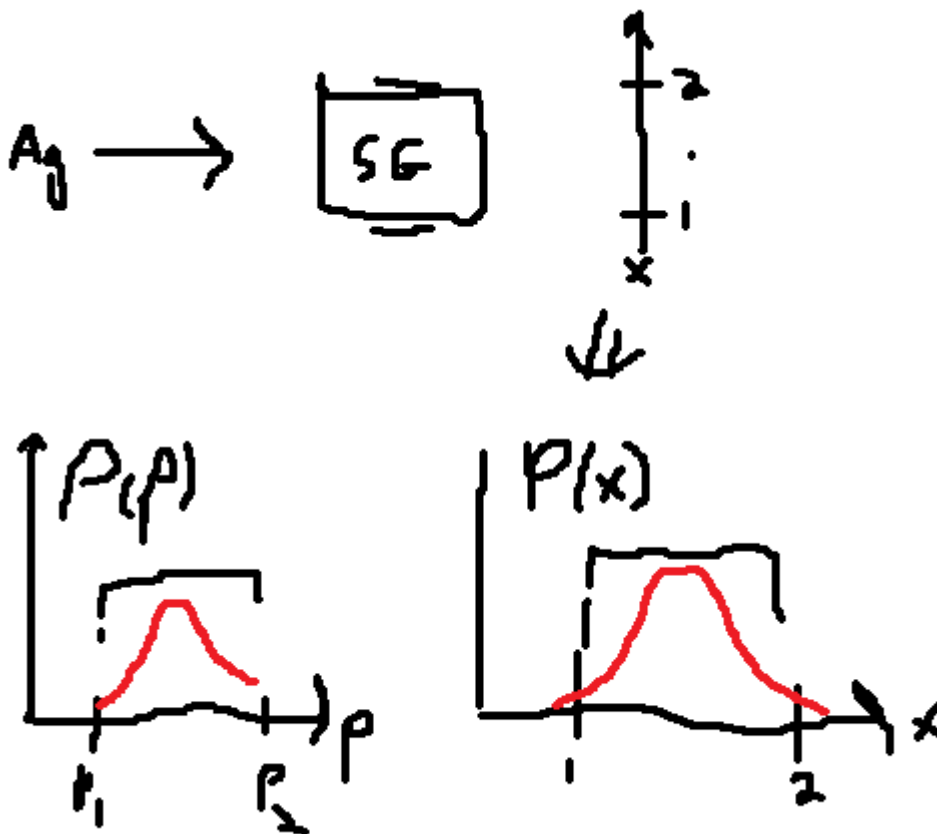
This is especially useful for the question of initial state.

**Remember question:** What is the state of the particle before it hits the SG device? Spin states may not be determined, but there is also a momentum/position state for the atom: this we do have some idea how it should look.

**A) it has some fixed momentum.** (this has to be tuned right to “see” the splitting due to spin) within some uncertainty range

**B) it has some fixed position** (changing w/ time) (this is what allows us to say it is going through the SG device)—within some uncertainty range.

This is demonstrated in this plot:



#### DIGRESSION:

CENTRAL LIMIT THEOREM (CLM): (classical thinking, not just QM) for some derived quantity (Observable)  $F(a,b,c,\dots)$ , ( $F$  depends on  $a,b,c,\dots$ ) no matter what the probability distributions of  $a, b, c,$  inputs are, the probability distribution of  $F$  will always tend towards a Gaussian.

POINT: All uncertainties/experimental errors tend to be Gaussian because they are usually due to some many microscopic inputs.

**end DIGRESSION**

Thus following the example set by the CLT we may reasonably assume it's also true for  $x, p$  in SG. Thus the following construction works very nicely to describe this situation:

**Gaussian Wave Packets**

So just CONJECTURE that the state initial space state for the SG looks like this:

$$\Psi_{\alpha}(x) = \frac{1}{\sqrt{\pi} \sqrt{d}} e^{ikx - \frac{x^2}{2d}}$$

=definite momentum eigenstate  $\exp(ikx)$  "smeared" around  $x = 0$ . (by this choice we have put our  $x$  origin @ 0)

Called a "PACKET" (group) of  $x$  states. It has a Gaussian form. ( $\propto \exp(-x^2)$ )

Has the right form for  $P(x)$  then because

$$P(x) = \Psi^* \Psi \propto \exp(-x^2/d^2)$$

We would choose  $d$  according to the box size. So we are PICKING the form of the WAVE FN first! This is what I mean by "artificial". Not any operator or eigenket that the state might be related to. Could  $|\alpha\rangle$  be the eigenstate of some other observable? Who knows! Is it a Discrete sum over eigenstates of some other observable? Who knows!

Actually we will show that the SHO ground state has this form.

Now the NEAT property of this state is that we already said

$$\langle x' | \alpha \rangle = \int dp' \underbrace{\langle x' | p' \rangle}_{\psi_{\alpha}(x')} \langle p' | \alpha \rangle$$

$\psi_{\alpha}(x') = N \int dp' e^{ip'x'/\hbar} \Phi_{\alpha}(p')$   
 which is the Fourier expansion of  $\psi_{\alpha}(x')$  in eigenfunctions  $N e^{ip'x'/\hbar}$  to  $p$ . The wave function of  $|\alpha\rangle$  in  $p$ -space is

$$\Phi_{\alpha}(p') = \langle p' | \alpha \rangle = \int dx' \langle p' | x' \rangle \langle x' | \alpha \rangle = N \int dx' e^{-ip'x'/\hbar} \psi_{\alpha}(x')$$

i.e. the Fourier transform is contained in the Dirac formalism.



DIGRESSION: Remembering Properties of the Fourier Transform (FT): The FT of a Gaussian form, is another Gaussian form.

$$\text{FT}(\text{Gaus}(x)) = \text{Gaus}(p)$$

$$\text{FT}(\text{Gaus}(p)) = \text{Gaus}(x)$$

end DIGRESSION

Thus for our artificial state  $|\alpha\rangle$  It's momentum wave function must also be a Gaussian in  $p$ :

Form is given in Sak. eq 1.7.42:

$$\langle p | \alpha \rangle = \sqrt{\frac{d}{\hbar \pi}} \exp\left[-\frac{(p' - \hbar k)^2 d^2}{2\hbar^2}\right]$$

Obviously this is a state with mean value  $p = \hbar k$  but with some uncertainty around it.

Why? because we can just read the value off From "Wikipedia: Gaussian distribution" Gaussian of  $x$  has form:

$$\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right)$$

where  $\sigma_x^2 = \langle \Delta x^2 \rangle$  and  $\mu = \langle x \rangle$

Thus matching symbols, by inspection,  $\langle p \rangle = \hbar k$

Our probability distribution  $P(p) = \langle \alpha | p \rangle \langle p | \alpha \rangle \propto \exp(-2(p - \hbar k)^2 d^2 / 2\hbar^2)$  so

$$\langle \Delta p^2 \rangle = \hbar^2 / 2d^2$$

NOTE THAT SAKURAI DERIVES THESE USING THE DERIVATIVE FORM OF  $p$  in sect. 1.7  $\rightarrow$  ie w/ wave mechanics. YOU SHOULD BE COMFORTABLE DOING THAT TO... (YOU MAY WANT TO PRACTICE). E.g.  $\langle x \rangle = 0$  is easy to see: because  $\exp(-x^2) * x$  odd

Anyway, the conjectured form of  $|\alpha\rangle$  fulfills what we want expected for our SG experiment. And actually even predicts something: based on the input requirement for the distribution of  $x$  we see what the  $P(p)$  of  $p$  must look like!

### Note about Uncertainty Relation

While we're add it let's read off uncertainty value for  $\langle \Delta x^2 \rangle$

$$\psi_{\alpha}(x) = \frac{1}{\sqrt{\hbar} \sqrt{d}} e^{i\alpha x - \frac{x^2}{2d}}$$

$$P(x) = \psi^* \psi \langle \alpha | x \rangle \langle x | \alpha \rangle \propto \exp(-x^2/d^2)$$

So it must be just  $\sigma = d^2/2$ .

So we have

$$\Rightarrow \langle (\Delta x)^2 \rangle \langle (\Delta p)^2 \rangle = \frac{\hbar^2}{4}$$

Gaussian Wave Functions always satisfy **minimum** uncertainty relation.

## V. Unfinished Business Regarding the Formalism

### A) Direct Product Spaces/States and Entanglement

### B) Implications of Measurement Postulates EPR Paradox

### C) Mixed States

The notes for the above are available on the website in a pdf. Please see there. One thing I forgot to point out in our discussion of Product Spaces was perhaps the most familiar example: the construction of our 3-D position/momentum kets from Direct Product Kets of the 1-D kets.

## Lecture 2/16/2010

**Reading Assignment: (by ~2/17 [tomorrow]: Sakurai Sections 2.1-2.2)**

**There will be a Problem Set due next week, but negotiated to have it due Wed: (posted Wed 2/17)**

In what follows below I give kind of a long winded Conceptual Intro: move forward to my scanned notes for the short version...

## VI) Time Dependence In Formalism

### A) Conceptual Intro (Pictures of Pictures of Pictures)

The best way to start thinking of how time enters into our formalism is as a parameter that has no physical significance.

In this way of thinking, the parameter  $t$  will simply label two different sets of kets AND associated operators.

This is because time will not correspond to an operator, (ie there is no  $t$  operator and no associated  $|t\rangle$  basis kets) so this label is NOT like when we label kets by their eigenvalues, which is also clear because we said the label is applied to operators themselves.

Picturing the following situation of two different operators and their associated basis.

$$\begin{array}{ccc} B(t_1) & \longleftrightarrow & B(t_2) \\ |b_1\rangle, |b_2\rangle, \dots & & |b_1, t_2\rangle, |b_2, t_2\rangle, \dots \end{array}$$

(Forget about what time actually means for a second and just think of 2 separate new operators. For that reason imagine for now we used "s" to label as our parameter not t)

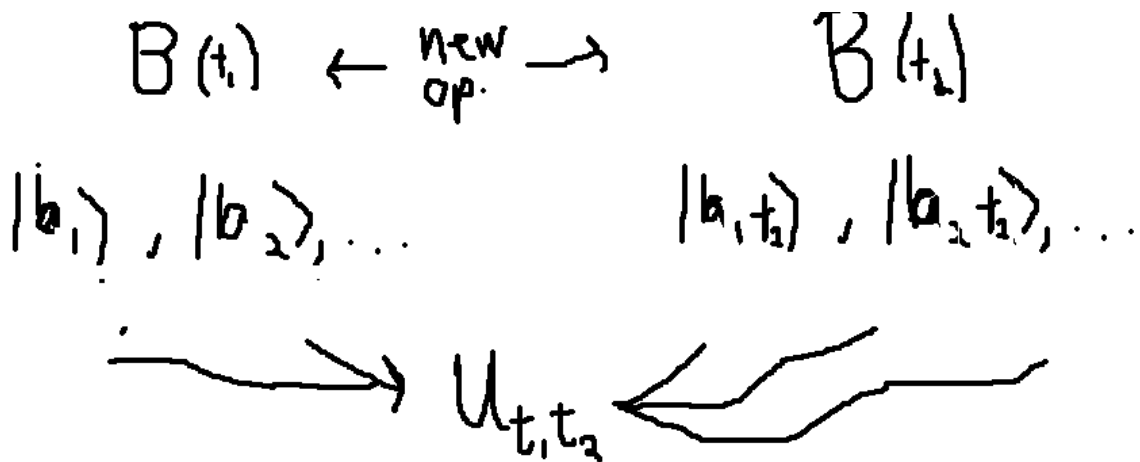
To be concrete we could think example: two incompatible operators C and D and simply consider

$$B = C \cos(t) + D \sin(t)$$

(concrete example: @  $t_1=0$   $|b_n\rangle = |c_n\rangle$ , while at  $t_2=\pi/2$ ,  $|b_n\rangle = |d_n\rangle$ )

**Postulate 0.1) Changes in the Parameter Should not Change the Hilbert Space:** The only thing we will want for this parameter at this stage is that we still have the same space for any value of the label.

This is equivalent to saying that ANY ket specified by a linear combination of  $|b_{t_1}\rangle$ 's can also be alternatively expanded in the  $|b_{t_2}\rangle$  basis.



THIS in turn means there is a unitary transformation operator that "connects" the two sets of basis states.

$$U_{t_1,t_2}$$

So far everything is like when we first introduced Unitary operators, it just that we've introduced a generalization of  $A \rightarrow B$  operators pairs to an arbitrary set of pairs  $B_{t_1} \rightarrow B_{t_2}$ .

**POSULATE 0.2)** Even though Hilbert Space is the same, **for 2 different values of the parameter, the system should change.**

Otherwise, there is no point to introduce time dependence. We can consider operators or states that are constant with time, but these will be considered special cases, and even then, there will still ALWAYS

be something about the system (some other state and/or some other operator) that is changing with time. Note that it does not have to be a physically observable change.

**Review: Two applications of Transformation Operators so far in this class:**

1) Diagonalization. Here we said we said all states should remain the same, and we use U mainly for **passive or temporary ket space rotations** of the coordinate system through it's matrix elements:

$$\langle b_n | \alpha \rangle = \sum_n (U_{mn})^* \langle a_m | \alpha \rangle$$

mainly for more convenient work in matrix rep. Active Rotate → work → but inversely Actively rotate (transform back) at the end.

2) Space Translation → Momentum Basis: Here we considered **active ket space rotations** translations, but we :

Didn't USE those rotated states for much.

Didn't assign much importance to them.

They were just a means for understanding the existence of the p operator

We can think of Time Evolution as our 3<sup>rd</sup> Application of Transformation operators **There is a MAJOR CONCEPTUAL DIFFERENCE here though:**

**Here we POSTULATE that ACTIVE ROTATIONS must continuously occur as time progresses,**

**So we will want our Transformation Operators  $U_{t_1 \rightarrow t_2}$  to define rotations that will actively change the system in the Hilbert space, but WHAT active rotation it is will be continually changing.**

What this DOESN'T mean for example:

Suppose state at t1 is measured so in eigenstate  $|b, t_1\rangle$

$|b, t_1\rangle$  = regardless of time, we could always expand  $|b, t_1\rangle$  in other basis.

ie write  $|\alpha, t_1\rangle = |b_n, t_1\rangle = \sum_n \langle b_n, t_1 | b, t_2 \rangle$  (example  $t_1 = 0, t_2 = \pi/2$ )  $|c\rangle = \sum \langle c | d \rangle |d\rangle$  (Eq 1)

We are POSTULATING  $|\alpha, t_2\rangle \neq |\alpha, t_1\rangle$  thus the expansion coeff's of  $|\alpha, t_2\rangle$  are not the same.

(Eq 1) is **not** what we want (nothing happened)!

What we want is more like the ACTIVE transformation: Transformation Operator like the following:

$$|b, t_2\rangle = U_{t_1 t_2} |b, t_1\rangle$$

E.g. if start in  $|b_1\rangle$  the system changes at t2 into some other eigenket  $|b, t_2\rangle$

In our example for  $t_1 = 0$ ,  $t_2 = \pi/2$  this would just be  $U = \sum |d\rangle\langle c|$ .

Is this how quantum states evolve? No! Not always!

If we experimental observation a physical system, we do NOT find that this exact kind of translation (1 to 1 mapping of basis states at different times) always works this way.

Only in very special case for our example (properties of C, and D) would the TIME EVOLUTION work properly using the  $U = \sum |d\rangle\langle c|$  form—ie directly connecting eigenstates

INSTEAD we will POSTULATE SEVERAL MORE SPECIFIC REQUIREMENTS of the time translation operators  $U$  so that will work how we want them to and correspond to physical experimental evidence:

→ This we will call the TIME EVOLUTION OPERATOR:  $U_t$

---

**To summarize:**

**1) Think of two different sets of operators/basis kets/states → different parameter  $t$  values**

**2) SAME ket space at different values though!**

**Time Evolution will correspond to some unitary operator  $U_t$  that we still need to establish the properties of. But so far we did establish one thing:**

**3) These transformations are ACTIVE ket transformations different from diagonalization transformation operators. : because we postulate CHANGE to the system.**

**B) Big picture (s):**

**It will turn out there are many ways to view this “active change” of the system:**

When we find the right  $U_t$  which does the transformations the way we want, we will think of two “big” pictures, based on how  $U_t$  is applied.

**1) Shrodinger:** The state will change—Thurs’s examples  $|\alpha, t_2\rangle = U_t |\alpha, t_1\rangle \rightarrow |\beta, t_2\rangle = U_t |\beta, t_1\rangle$

Expansion coefficients of  $|\alpha\rangle$  change, always stay in old ( $t_1$ ) basis → Shrodinger pictures

State vector being actively moved around.

**2) Heisenberg:** The observables will change  $U_t^\dagger B U_t$  while expansion coeff’s stay the same

State vector remaining in the same place: coordinate frame moving around—but state of the system still changed!

Comment example  $B = C \cos t + D \sin t$  from Th. Picture 2) only? Maybe but even if you're working in Shro: you can still have explicit time dependent operators—we can make them. They just won't be the basis we want to choose to expand in: choose C or D alone to expand in.

Either picture will work because we will describe the change to expectation values (more generally non-diagonal matrix elements) – ie things that carry PHYSICALLY OBSERVABLE CONSEQUENCES:

$$\langle A \rangle = \langle \psi | A | \psi \rangle \rightarrow \langle \psi | U_t^\dagger A U_t | \psi \rangle$$

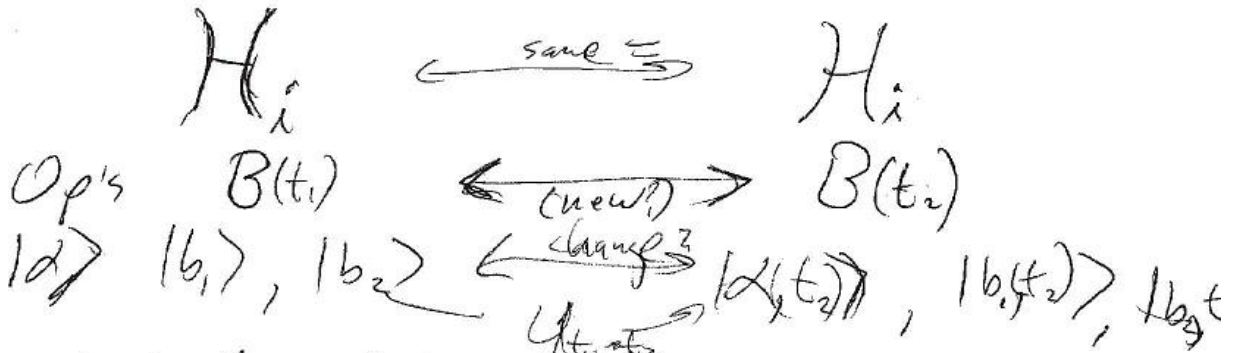
(doesn't matter how you "associate" the change.)

Scanned notes from actual class (the short version of the above) below:

# VI Time Dependence

A) Conceptual Intro: (Really Big Pic)

~~Q~~ ~~M~~ ~~is~~ Time is parameter  
 (Imagine  $s$  instead of  $t$ ) not observable (like  $\hat{x}$ )



Main ideas: 1) Something changes

2) First order: not  $H_{eff}$  Hilbert space

So what changes? Some combo: (bottom stuff: ops/basis/states)

- Entire combo depends on "picture"  
 = several mathematically equiv. views  
 (coord frame or vectors? (with?) changes?)

⇒ Implies a  $U_{t_1 \rightarrow t_2}$  Trans. Op. ⇒ Rotations in  $H_{eff}$   
 (update fig)



Uses of U's so far

- 1) Diagonalization: "Passive or Temporary"  $\rightarrow$  No change
- 2) Space Translation:  $U = T(a)$  Active Rotation/Mod.  
 Use: derive  $\hat{p}$  (did not connect to motion)

New 3) Time Translation:  $U = U(t_2, t_1) = U_t$

- Active Rotations Systems! Changes!
- occurring continuously!

(Back to picture)

What Properties for  $U_t$ ?

First pick  
Depends on picture

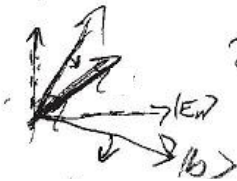
(Big Pic of Pictures)



1) Schrödinger

$|a(t_2)\rangle = U_{t_1, t_2} |a(t_1)\rangle$   
 (Active in all senses)

State Vector Rotates



2) Heisenberg

Op's / Basis Rotates  
 Passive? ~~Not~~ but No!  
 Because Absolute coordinate frame  
 $H \Rightarrow |E_n\rangle$  stays fixed  
 [Ham. determines  $H_i$  space]

3) Other Pictures: Interaction Picture

- Both change (Ops-Basis vectors)

## Time Evolution in the Shrodinger picture:

put all time dependence in expansion coeffs

$$\text{initial quantum state } |\alpha, t_0\rangle = \sum_a c_a(t_0) |a\rangle$$

$$\begin{array}{c} \downarrow \text{time evolution} \\ \text{state at time } t \quad |\alpha, t\rangle = \sum_a c_a(t) |a\rangle \end{array}$$

time evolution operator

$$|\alpha, t\rangle = U(t, t_0) |\alpha, t_0\rangle$$

Requirements for  $U_t$ :

postulates:  $\Delta U$  is linear

$$U(t, t_0) (|\alpha\rangle + |\beta\rangle) = U(t, t_0) |\alpha\rangle + U(t, t_0) |\beta\rangle$$

$$U(t, t_0) (\lambda |\alpha\rangle) = \lambda U(t, t_0) |\alpha\rangle$$

$\Rightarrow U(t, t_0)$  is determined by its action on base kets and does not depend on the  $c_a$

So it does not technically act ON the  $c(t)$  however: this is kind of a deep point: even in the Shro picture we technically do say the  $U$  is actually *acting on the base kets*, but apparently that action will be to make them remain fixed with respect to the greater Hamiltonian basis.

Other requirements making this choice of the "picture"...

The unitary requirement of  $U_t$  is now just a statement of the requirement of

$\Delta$  probability conservation

$$\sum_a |c_a(t)|^2 = \sum_a |c_a(t_0)|^2$$

$$\Rightarrow \langle \alpha, t | \alpha, t \rangle = \langle \alpha, t | \alpha, t \rangle = \langle \alpha, t_0 | U^\dagger U | \alpha, t_0 \rangle$$

$$\text{true for all } |\alpha\rangle \Rightarrow U^\dagger U = I$$

As with space translation we want successive translations to

add up....

$$U(t_2, t_1) U(t_1, t_0) = U(t_2, t_0) \dots$$

$$\Rightarrow U(t_0, t_0) = U(t_0, t_0) \Rightarrow U(t_0, t_0) = 1$$

As with space translation we might be tempted to choose a form of  $U$  since it will have these properties again as

$$U_i(\Delta t) = \exp(iX\Delta t) \text{ (????)}$$

with any hermitian operator  $X$  since it will have these properties, however we want to allow for  $X$  to also be time dependent, so this time we must start by defining only the infinitesimal case where we translate over some infinitesimal time  $\delta t$ .

$$U_i(\delta t)$$

(Switch to Sakurai's notation  $U_i(\Delta t) \rightarrow U_t(t, t_0) = U_t(t_0 + \Delta t, t_0)$  since  $\Delta t = t - t_0$ )

Then over such a small time we should reasonably be able to treat  $H$  as constant

$$U(t_0 + \delta t, t_0) \approx 1 - \frac{i}{\hbar} H \delta t$$

↑  
we use this operator the Hamiltonian

**it works: (ONLY FOR SUCCESSIVE INFINITESIMAL TRANS**

$$U^\dagger U = 1 \Rightarrow \left(1 + \frac{i}{\hbar} H^\dagger \delta t\right) \left(1 - \frac{i}{\hbar} H \delta t\right) = 1$$

$$\Rightarrow 1 + \frac{i}{\hbar} \delta t (H^\dagger - H) = 1$$

$$\Rightarrow H^\dagger = H$$

$\Rightarrow H$  can be an observable  
dim  $H$  = energy

Now this  $H$  is the same as  $H$  already defined and  $\hbar$  same as  $\hbar$  before.

Why? First  $H \rightarrow$  **classical mech.:**  $H = p^2/2m + V(x)$  is what **determines** speed of evolution / "oscillations" rates.

Think  $\rightarrow$  free particle. propagates through space faster for faster  $H = p^2/2m$

→ SHO  $H = p^2/2m + 1/2kx^2$  → Numerical value of  $H$  for isolated system always remains constant (Energy Conservation!). But oscillation rate independent of whatever that constant  $H$  value =  $E$  might be - > wait doesn't work? I guess not.

Still if we want to fix  $x$  and  $p$ , if value  $H$  goes up,  $\omega$  must go up so then  $H \propto \omega$

OK through some possibly very loose, unspecified comparison to classical mechanics → we expect our choice of operator  $\Omega$  in  $1-i\Omega dt$  to be related to  $H$ .

So try  $\Omega = kH$  → then we will find that  $k$  must be  $1/\hbar$  from matching to wave mechanics results and this also answers why  $\hbar$  here is the same as  $\hbar$  for the  $p$  operator.

### Lecture 2/17/2010

**New Pset will be posted tonight: Due Wed 2/25.**

**Reading: Sak Chapt 2.1-2.2 (~today!)**

#### Review:

Time Dependence: Think Hilbert Space  $\mathcal{H}_i$  ~constant, some combo of States/Op's/Basis's evolve by operator  $U(t)$  (Time Translation operator → rotations)

Which combo of these things will change? Depends on Formal "Picture":

So review also "Big Picture of Pictures" from yesterday:

(notes below)

**Notes combined below w/ 2/19/2010 lecture: Note 2/19/2010: Read Sak 2.1-2.3 by ~monday**

Big Pic of Pictures:  $U_t^*$



Also: State Vector  
Rotates



Heisenberg: Op's Basis  
Rotates

Both Active Rotations (change)  
Because Fixed Coordinate Frame

$$H \rightarrow |E_n\rangle$$

$H \rightarrow$  "Structure" of ket space  
(like GR)  $\rightarrow$  "mass"

$$U(t, t_0) = \mathbb{I} - \frac{iH dt}{\hbar}$$

(This is why  $H$  is so important?)

can't start  $e^{-iHt/\hbar}$  b.c.  $H \rightarrow H(t)$   
in general

P.3)  $U(t_2, t_1) U(t_1, t_0) = U(t_2, t_0)$

$$U(t+\delta t, t_0) = (U(t+\delta t, t) U(t, t_0))$$

$$= \left(1 - \frac{H \Delta t}{\hbar}\right) U(t, t_0)$$

$$\Rightarrow U(t + \delta t, t_0) - U(t, t_0) = -\frac{i}{\hbar} H U$$

$\hbar \frac{\partial U}{\partial t} = H U$  ← Schrödinger Equation for  $U$

So solutions:

1)  $H$  constant w/  $t$   $U(t) = e^{-\frac{iH}{\hbar} \Delta t}$

2)  $H = H(t)$  but  $[H(t_1), H(t_2)] = 0$   
 (Absolute coord frame remains same)

$$U_t = \exp\left[-\frac{i}{\hbar} \int_{t_0}^t dt' H(t')\right]$$

3) IF  $[H(t_1), H(t_2)] \neq 0$

UGLY: Dyson Series  
 (H coord. space changing not just rotation)

- IF  $\frac{dH}{dt}$  small enough  $\rightarrow$  Adiabatic Approx  
 Easier.

Case 1 — Most of this course.

# C) Other Schrödinger Eq's

For states

$$i\hbar \frac{d}{dt} |\alpha, t\rangle = H |\alpha, t\rangle$$

↑  
insert on both sides

$$i\hbar \frac{d}{dt} |\alpha, t\rangle = H |\alpha, t\rangle$$

For Wave Functions: (connect to W. Mech)

$$\langle x' | i\hbar \frac{d}{dt} |\alpha, t\rangle = \langle x' | H |\alpha, t\rangle$$

assume ↓

$$= \langle x' | \frac{\hat{p}^2}{2m} + V(\hat{x}) |\alpha, t\rangle$$

$$i\hbar \frac{\partial}{\partial t} \psi(x', t)$$

$$= \frac{1}{2m} \langle x' | \hat{p}^2 |\alpha, t\rangle + \langle x' | V(\hat{x}) |\alpha, t\rangle$$

by  $\langle x | \hat{p}^2 | \alpha \rangle$  expression

$$i\hbar \frac{\partial}{\partial t} \psi(x', t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x'^2} \psi(x', t) + V(x') \psi(x', t)$$

V) Expansion in ~~H~~ Eigenkets:

Suppose  $U$  act on  $|E_n\rangle$ ?

$\hat{=}$

$$U|E_n\rangle = ? = e^{-iE_n t/\hbar} |E_n\rangle$$

Means can derive alternative forms:

$$\begin{aligned} \|U\| &= \sum_{n'} \sum_n \langle n' | e^{-iHt/\hbar} |n\rangle \langle n| n'\rangle \\ &= \sum_n e^{-iE_n t/\hbar} \langle n | n \rangle \end{aligned}$$

Extremely Important Form

insights  $\rightarrow$   
consider

$$|\alpha, t\rangle = U |\alpha, t_0\rangle$$

$$= \sum_n c_n(t) |n\rangle \langle n | \alpha, t_0\rangle$$

compare to

$$|\alpha, t_0\rangle = \sum_n c_n(t_0) |n\rangle$$

i.e.

$$c_n(t) = c_n(t_0) e^{-iE_n t/\hbar}$$



operationally means

$$|\alpha\rangle = c_1 |E_1\rangle + c_2 |E_2\rangle + \dots$$

$$U(t) |\alpha\rangle = c_1 e^{iE_1 t / \hbar} |E_1\rangle + c_2 e^{iE_2 t / \hbar} |E_2\rangle + \dots$$

MOST IMPORTANT THING: - Defines evolution  
- This is why H basis  
most important

# Illustrative examples:

- 1) Suppose  $|\alpha, t=0\rangle = |\lambda^A\rangle$   
 where  $[A, H] = 0$

so  $|\lambda_n^A\rangle \propto |E_n\rangle$

$|\alpha, t_0\rangle = |\lambda_n^A\rangle = |E_n\rangle$

$|\alpha, t\rangle = e^{\frac{iE_n t}{\hbar}} |E_n\rangle$

meaningless b.c.  $|\alpha\rangle \Rightarrow |$

$|\alpha, t\rangle$  still  $\propto$   $|\lambda_n^A\rangle$   
 (prop to)

Stationary

- 2) Now suppose  $|\alpha, t=0\rangle = |\lambda^D\rangle$   
 where  $[D, H] \neq 0$

Now  $|\lambda^D\rangle = \sum_m c_m |E_m\rangle$

$|\lambda^D, t\rangle = c_1 e^{iE_1 t/\hbar} |E_1\rangle + c_2 e^{iE_2 t/\hbar} |E_2\rangle + \dots$

no longer prop. to !

$|\lambda^D\rangle \left[ \equiv |\lambda^D, t=0\rangle \right]$

rotates  $\Rightarrow$  non-stationary  
 in ket space

Review 2 Main Points Wed:

$$\psi(t, 0) = \sum_n |E_n\rangle \langle E_n| e^{-iE_n t / \hbar} \rightarrow$$

$$|\alpha, t\rangle = \sum_n c_n e^{-iE_n t / \hbar} |E_n\rangle$$

(inserted)

- If  $|\alpha, 0\rangle = |\lambda_n^0\rangle$  for  $[H, D] \neq 0$   
(D eigen)

$|\alpha, t\rangle$  not  $\propto |\lambda_n^0\rangle$

Why? Consider

$$\langle \alpha, t | \alpha, t \rangle = \sum_n \sum_m \langle E_n | c_n^* e^{+iE_n t / \hbar} (c_m e^{-iE_m t / \hbar} |E_m\rangle)$$

$$= \sum_n |c_n|^2 = \text{const} = 1$$



Norm const  $\rightarrow$  Rotation

## E) Expectation Values

$$\langle B \rangle = \langle \alpha, t | B | \alpha, t \rangle$$

$$= \sum_n \sum_m \langle E_n | c_n^* e^{+iE_n t / \hbar} B (c_m e^{-iE_m t / \hbar} |E_m\rangle)$$

~~Expect~~  $\langle u, 0 \rangle$

2 cases:

If  $[H, B] = 0$  (non-degenerate)  $\langle E_m | B | E_n \rangle = \lambda_n \delta_{mn}$

$\langle B \rangle = \sum_n c_n^* c_n \lambda_n$

$\sum_n |c_n|^2 \lambda_n = \text{const w/ time!}$

" Stationary state:  $|H, 0\rangle = |E_n\rangle$   
 (mentioned wed, but forgot to emphasize)  $\langle B \rangle = \lambda_n$   
 (constant!)

If  $[H, B] \neq 0$

no  $\delta_{mn}$ :  $\langle B \rangle = \dots e^{i\omega_{mn}t}$

Introduce notation  $\omega_{mn} = (E_m - E_n)/\hbar$

Actually generally  $\hbar \omega_n = E_n$

Also Previous Notation:  $B_{mn} = \langle E_m | B | E_n \rangle$

$\langle B \rangle = \sum_m \sum_n c_m^* c_n e^{-i\omega_{mn}t} B_{mn}$

Can we gain any more insight?  
 (or do anything more?)

Sort of, Yes:

First notice diagonal terms  
 $\sim B_{nn}$  have no time dependence

Second, If  $\text{Dim}(H) = N$

then sum has  $N^2$  terms,  
 $N$  of which are diagonal ( $\sim B_{nn}$ )

So rewrite:

$$\langle B \rangle = \sum_m \sum_{n \neq m} B_{mn} c_m^* c_n e^{-i\omega_m t} + \sum_n B_{nn} c_n^2$$

removes diagonal terms  
 $N^2 - N$  terms

constant  $\equiv C$  = somewhat like Trace B

But every term in this sum has  
 an  $m \leftrightarrow n$  symmetric pair so rewrite

$$= \sum_m \sum_{n < m} B_{mn} c_m^* c_n e^{-i\omega_m t} + B_{nm} c_n^* c_m e^{+i\omega_m t} + C$$

only  $(N^2 - N)/2$  "terms"  
 each "term" is 2 terms  
 $(nm + mn)$

If realize  
 that  $B_{mn} = B_{nm}^*$   
 then we can use  
 $w + w^* = 2 \text{Re}\{w\}$

in class  
 $\Rightarrow$  ERROR!  $B_{mn} \neq B_{nm}$   
 in general!  
 But it was  $B^\dagger = B$   
 that allowed us to  
 say  $B_{mn} = B_{nm}^*$

$$\langle B \rangle = \sum_m \sum_{n \neq m} 2 \operatorname{Re} \{ B_{mn} c_m^* c_n e^{-i\omega_{mn} t} \} + C$$

like Trace B

we've reduced # terms to  
consider substantially from  $N^2$   
to  $(N^2 - N)/2 + 1$  (grouping)

More insight: notice 1st  
part: If  $B_{mn} + c_{n/m}$  are always real!

$$\langle B \rangle = \sum_m \sum_{n \neq m} 2 B_{mn} c_m c_n \cos(\omega_{mn} t) + C$$

b.e.  $e^{i\theta} = \cos\theta + i \sin\theta$

In fact we can always write  
any complex num  $w = u + iv$   
in the form  $w = r e^{i\phi}$  (think of complex plane)  
 $r = |w|$  &  $\phi = \arctan(\frac{v}{u}) = \text{real number}$

Thus indeed can write (always)

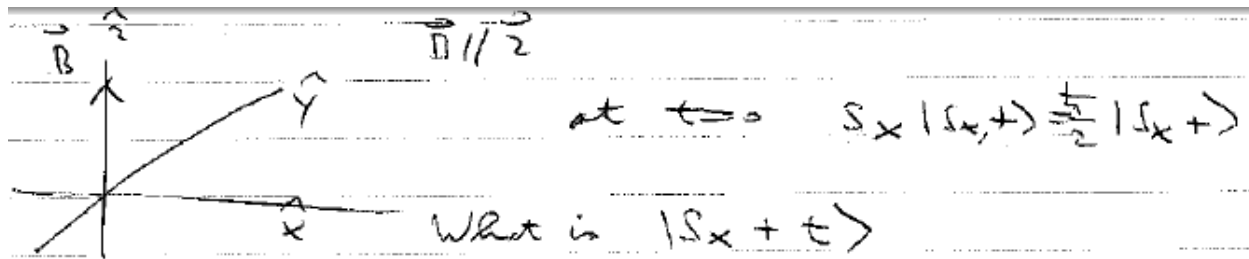
$$\langle B \rangle = \sum_m \sum_{n \neq m} 2 |B_{mn} c_m c_n| \cos(\omega_{mn} t + \phi) + C$$

oscillating term

constant  
 $\downarrow$   
 $\rightarrow \text{Tr}(B)$

Lecture 2/19/2010 continued

F) Application 1): Spin Precession



Hamiltonian  $H = -\frac{e}{mc} \vec{S} \cdot \vec{B} = -\frac{eB}{mc} \frac{\hbar}{2} \sigma_z$

Eigenstates eigenvalue  $-\frac{eB}{mc} \frac{\hbar}{2}$

$|+\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}$   $|-\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}$   $\frac{eB}{mc} \frac{\hbar}{2}$

$|S_x, +\rangle = \frac{1}{\sqrt{2}} |+\rangle + \frac{1}{\sqrt{2}} |-\rangle$  at  $t=0$

$|S_x, +\rangle = \frac{1}{\sqrt{2}} e^{\frac{1}{\hbar} i \frac{eB}{mc} \frac{\hbar}{2} t} |+\rangle + \frac{1}{\sqrt{2}} e^{-\frac{1}{\hbar} i \frac{eB}{mc} \frac{\hbar}{2} t} |-\rangle$

$\Rightarrow |S_x, +\rangle = \frac{1}{\sqrt{2}} e^{\frac{1}{\hbar} i \frac{eB}{mc} \frac{\hbar}{2} t} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}} e^{-\frac{1}{\hbar} i \frac{eB}{mc} \frac{\hbar}{2} t} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix}$   $\omega = \frac{eB}{mc}$

Therefore to calculate Expectation Value we bracket any operator with this state: for example: (I prefer to use matrix rep to calculate this—just preference—but it also allows us to visually see interesting connection to previous statements)

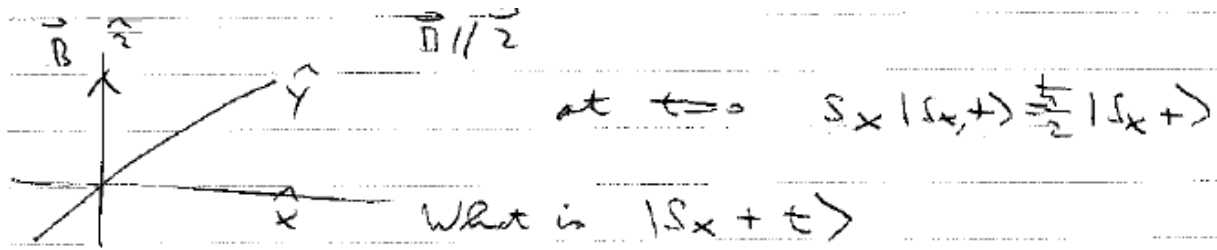
Expectation value of  $S_x$

$\langle S_x, +t | S_x | S_x, +t \rangle =$

$\frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix}^* \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix}$

$= \frac{\hbar}{4} (e^{i\omega t} + e^{-i\omega t}) = \frac{\hbar}{2} \cos \omega t$

So:



Hamiltonian  $H = -\frac{e}{mc} \vec{S} \cdot \vec{B} = -\frac{eB}{mc} \frac{\hbar}{2} \sigma_z$

Eigenstates:  $|+\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}$      $|-\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}$     eigenvalue  $-\frac{eB}{mc} \frac{\hbar}{2}$

$\frac{eB}{mc} \frac{\hbar}{2}$

$|S_x + t\rangle = \frac{1}{\sqrt{2}} |+\rangle + \frac{1}{\sqrt{2}} |-\rangle$  at  $t=0$

$|S_x + t\rangle = \frac{1}{\sqrt{2}} e^{i\frac{eB}{mc} \frac{\hbar}{2} t} |+\rangle + \frac{1}{\sqrt{2}} e^{-i\frac{eB}{mc} \frac{\hbar}{2} t} |-\rangle$

$\Rightarrow |S_x + t\rangle = \frac{1}{\sqrt{2}} e^{i\frac{eB}{mc} \frac{\hbar}{2} t} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}} e^{-i\frac{eB}{mc} \frac{\hbar}{2} t} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$= \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega t} \\ e^{i\omega t} \end{pmatrix}$      $\omega = \frac{eB}{mc}$

Indeed we see a nice connection to our previous general relation for  $\langle B \rangle$ !

First notice in this case ( $B = S_x$ ) the Trace of  $S_x$  (sum of diagonal terms) is 0: that's why there's no constant term!

Second, in this case indeed all the matrix elements of  $B=S_x$  were real, so we got the  $\cos \omega t$ !

Compare that to if we take the (still traceless)  $S_y$  (and remember that  $\sin x = \cos(x-\pi/2)$ )



$$\begin{aligned}
& \langle S_{x+t} | S_y | S_{x+t} \rangle \\
&= \frac{\hbar}{4} \begin{pmatrix} e^{-i\omega t/2} \\ e^{i\omega t/2} \end{pmatrix}^\dagger \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} e^{-i\omega t/2} \\ e^{i\omega t/2} \end{pmatrix} \\
&= \frac{\hbar}{4} i (-e^{+i\omega t} + e^{-i\omega t}) = \frac{\hbar}{2} \sin \omega t
\end{aligned}$$

the spin precesses about the z-axis with frequency  $\omega$

### G) Heisenberg Picture

Let's start out the way Sakurai does: If we consider both inner products and matrix elements between states for any case (not just time-dependence) where we want to impose these type of ACTIVE rotations, we are free to view the rotation/modification occurring on the operator itself instead of the states. This is generally true not just for time dependence, but for example as Sak shows at the beginning of Chapt 2, the momentum/space translation operation also has this ability for dual interpretation. Specifically what we mean is for any set of rotations, that is transformations that preserve the inner product

$$\langle \alpha | \beta \rangle = \langle \alpha | U^\dagger U | \beta \rangle \quad (\text{remembering that } \langle \alpha | U^\dagger \text{ is the bra of } U | \alpha \rangle)$$

Then consider  $\langle \alpha | B | \beta \rangle$

If we want to perform active rotations on the states, we change the matrix element:

$$\rightarrow \langle \alpha | U^\dagger B U | \beta \rangle$$

but we are also free to view this as a modified (diagonal/Unitary Equivalent like) version of the operator being bracketed by unchanged states

$$\langle \alpha | U^\dagger B U | \beta \rangle \rightarrow \text{ie } B \rightarrow U^\dagger B U$$

The latter interpretation for the time U operator, is what we call the Heisenberg Picture

Consider matrix element  $X_{\alpha\beta}(t) = \langle \alpha | X | \beta \rangle$

time evolution  $|\beta(t)\rangle = U(t) |\beta_0\rangle$   
 $U(t) = e^{-iHt/\hbar}$

$$\Rightarrow X_{\alpha\beta}(t) = \langle U\alpha | X | U\beta \rangle = \langle \alpha | U^\dagger X U | \beta \rangle$$

two alternatives

a) state kets change with time and operators

stay stationary

Schrödinger picture  $|\alpha\rangle_t = e^{-iHt/\hbar} |\alpha\rangle_0$

b) state kets are stationary but operators

change with time

$$X \rightarrow e^{iHt/\hbar} X e^{-iHt/\hbar}$$

This interpretation is more satisfying for comparing QM to classical mechanics, because there we like to think of the observables changing with time. In fact one of the first things we can derive that is important for using the Heisenberg picture is a relation that can be nicely compared to a corresponding classical relation for the change in an observable with time:

If we choose the Heisenberg picture we can always assume at some point in time what we call the Heisenberg operator which changes with time, and the Schro which doesn't, are the same for that starting moment: (we will call that  $t = 0$  usually, so often (and in Sakurai) we will use (w/ notation  $A_{\text{Heisenberg}} \equiv A_H$ ) that  $A_H(t=0) = A_{\text{Shro}} = A(0)$ ).

## Heisenberg equation of motion

$$\frac{dA^{\dagger}}{dt} = \frac{d}{dt} u^{\dagger} A_S u = \frac{d}{dt} u^{\dagger} A_S u + u^{\dagger} A_S \frac{du}{dt}$$

$$= -u^{-1} \frac{du}{dt} u^{\dagger} A_S u + u^{\dagger} A_S \frac{du}{dt}$$

$$\frac{du}{dt} = \frac{1}{\hbar i} H u$$

$$H_H = \int \frac{\hbar}{2} \frac{\delta H}{\delta \psi} \frac{\delta \psi}{\delta \psi} = H$$

if  $[H_H], [H_H] = 0$

$$= \frac{1}{\hbar i} \left( u^{\dagger} H_A_S u + u^{\dagger} A_S H u \right)$$

$$= + \frac{1}{\hbar i} \left( -H_H A_H + A_H H_H \right)$$

$$= \frac{1}{\hbar i} [A_H, H]$$

Heisenberg eqs. of motion  $\frac{dA}{dt} = \frac{1}{\hbar i} [A, H]$

This represents a differential equation for the operator  $A_H$  which we can solve using normal calculus methods, except now for expressions involving operators. This will form the main idea of using the Heisenberg pic: instead of finding the time dep of the states and then calculating things with that, we first find the time dependence of the operator with the Heis EOM and operate with that on constant states to find things like expectation values  $\rightarrow \langle A(t) \rangle$  which equals  $\langle A \rangle(t)$

This is best to see in an example. But first it is neat to note the close resemblance of the Heis EOM to a classical expression for the change in observables with time. First note:

### Consequence

$$\text{if } [A, H] = 0 \Rightarrow \frac{d}{dt} \langle A \rangle = 0$$

and  $\langle A \rangle$  is a constant of motion

here we can just replace the  $1/\hbar i$  into the classical commutator  $[A, H]_{\text{class}}$  ie: in classical mechanics we have

$$dA/dt = [A, H]_{\text{classical}} = dA/dq dH/dp - dH/dq dA/dp$$

Why? let's take the first term: if we assume  $q \rightarrow x$  then  $dH/dp$  is  $d(p^2/2m)/dp = p/m$  and thus we have  $p/m = v = dx/dt$  times  $dA/dx \rightarrow (dA/dx)(dx/dt)$  which is just the calculus chain rule for  $dA/dt$ . And obviously if  $dA/dt$  we called that a constant of motion in classical mechanics

OK now for the example of using and solving the Heisen EOM:

### Ehrenfest theorem

Simplest case  $V=0 \Rightarrow H = \frac{p^2}{2m}$

then  $\frac{d\langle x \rangle}{dt} = \frac{i}{\hbar} [x, \frac{p^2}{2m}]$

$$[x, p^2] = [x, p]p + p[x, p] = 2i\hbar p$$

$$\Rightarrow \frac{d\langle x \rangle}{dt} = \frac{p}{m} \Rightarrow \frac{d\langle x \rangle}{dt} = \frac{\langle p \rangle}{m}$$

(state do not depend on time)

~End of Lecture 2/23/2010

Atb → Heisen. EOM:  $\frac{\partial \hat{A}^H}{\partial t} = [A^H, H] / i\hbar$

# Ehrenfest Theorem (cont)

$$\frac{d\hat{x}^H}{dt} = \frac{[x^H, H]}{i\hbar} = \frac{\hat{p}}{m} \quad \frac{d\hat{p}}{dt} = [p, H] = [p, \frac{1}{2}mv^2] = 0$$

Free particle: solution by integration  
( $\hat{p}$  is constant - why?)  
 $\hat{x} = x(0) + \hat{p}(0)t$

If not free:

$$\frac{d\hat{p}}{dt} = [p, H] = [p, U(x)] = i\hbar \frac{\partial U}{\partial x}$$

- Ehrenfest:  $\frac{d\langle \hat{p} \rangle}{dt} = \langle \frac{\partial U}{\partial x} \rangle$  "Force"  
using  $\hat{x}$   $m \frac{d^2 \langle \hat{x} \rangle}{dt^2} = \langle \frac{\partial U}{\partial x} \rangle$

Again, major point of Heisen:

Find time dep  $A^H(t)$  ~~Ex~~ generally true!  
→  $x^H = x(0) + \frac{p(0)t}{m}$

Calc expectation val  $\langle \hat{x} \rangle$  Example Tomorrow  
by brackets (this expression) for SHO

Goal: trick: Relation for  $\langle \hat{x} \rangle$ 's (no brackets) from only  $[ ]$ 's!

$$[x(t), x(0)] = \frac{i\hbar t}{m} \Rightarrow \langle \Delta x^2 \rangle \langle \Delta x \rangle > \frac{\hbar^2 t^2}{4m^2}$$

## G.2) Application 2): SHO (Time dependent) --Both Pictures and the Baker Hausdorff Lemma

Note about Heisenberg /S pictures in SHO:

Time Evolution of basis states in Heisenberg pic doesn't apply to basis of Hamiltonian.

Question: Why? Because H always commutes w/ itself

Any problem like this-→ either picture H/S is ~equally easy to work in!

### 1) SHO in Shrodinger Picture

Like in wave mech: just assign a factor  $\exp(-iE_k t/\hbar)$  to any Hamiltonian basis state  $|k\rangle$ .

Midterm problem 4) gives us a very typical example: go over that solution:

In shrodinger: just assign  $\exp(-iE_n t/\hbar)$  to each basis state  $|n\rangle$

(a):  $\langle x \rangle = \langle \alpha | x | \alpha \rangle = (a^* \langle 0 | + b^* \langle 1 |) x (a | 0 \rangle + b | 1 \rangle) = a^* a \langle 0 | x | 0 \rangle + a^* b \langle 0 | x | 1 \rangle + b^* a \langle 1 | x | 0 \rangle + b^* b \langle 1 | x | 1 \rangle$ . Using  $x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$  and  $a|n\rangle = \sqrt{n}|n-1\rangle$ ,  $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$  one obtains  $\langle x \rangle = \sqrt{\frac{\hbar}{2m\omega}}(a^*b + b^*a) = \sqrt{\frac{2\hbar}{m\omega}}a\sqrt{1-a^2}$ , where in the last step the normalisation condition  $|a|^2 + |b|^2 = 1$  has been used together with  $a, b$  real since a complex phase does not affect the following. Maximum of  $\langle x \rangle$  is then obtained by  $d\langle x \rangle/da = 0$  giving  $a = 1/\sqrt{2}$  (maximum since  $d^2\langle x \rangle/da^2 < 0$  for  $a = 1/\sqrt{2}$ ), and then  $b = 1/\sqrt{2}$ . Hence  $\langle x \rangle_{max} = \sqrt{\hbar/2m\omega}$  for  $|\alpha\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$  (up to an overall phase factor).

(b): Applying the time evolution operator  $e^{-iHt/\hbar}$ , and using  $e^{-iHt/\hbar}|n\rangle = e^{-i\omega(n+1/2)t}|n\rangle$ , one gets  $|\alpha, t\rangle = e^{-iHt/\hbar}|\alpha, t=0\rangle = e^{-iHt/\hbar}(|0\rangle + |1\rangle)/\sqrt{2} = (e^{-i\omega t/2}|0\rangle + e^{-3i\omega t/2}|1\rangle)/\sqrt{2}$

as the state vector for  $t > 0$  in the Schrödinger picture. The expectation value is then  $\langle \alpha, t | x | \alpha, t \rangle = 1/\sqrt{2}(e^{i\omega t/2}\langle 0 | + e^{3i\omega t/2}\langle 1 |) x (e^{-i\omega t/2}|0\rangle + e^{-3i\omega t/2}|1\rangle)/\sqrt{2} = (\langle 0 | x | 0 \rangle + e^{-i\omega t}\langle 0 | x | 1 \rangle + e^{i\omega t}\langle 1 | x | 0 \rangle + \langle 1 | x | 1 \rangle)/2 = \dots$  (again using  $x \sim a + a^\dagger$  as in (a))  $\dots = \sqrt{\hbar/2m\omega} \cos \omega t$ .

Thanks to <http://www.isv.uu.se/thep/courses/QM/051028-solutions.pdf>

My version  $a = \sin s, b = \cos s \rightarrow$  Use

$$\sin(2u) = 2 \sin u \cos u$$

### 2) SHO in H picture

Sakurai: time evolution of operator in Heisenberg picture

Schrodinger picture is nice because we can use the  $a/a^\dagger$  operators in place of  $x/p$  and not worry about their time evolution.

It turns out same is true for H picture—see why:

General method: Solve for  $x(t)$  and  $p(t)$  operators in terms of  $x(t=0)$  and  $p(t=0)$  operators (only those operators and some functions of  $t$ .)  $t=0$  operators  $\rightarrow a, a^\dagger$

Most direct method—form  $A_H = U^\dagger A(0)U = U^\dagger A_S U$ . Book also uses method of :

a) evaluating  $d(a, a^\dagger)/dt$  w/ Heisenberg EOM b)  $\rightarrow$  Ehrenfest theorem  $dp_H/dt = -m\omega^2 x$ ,  $dx_H/dt = p/m$  solve for  $x(t)$  given initial conditions  $x(0)/p(0)$

e.g.  $da_H/dt = [a_H, H]/i\hbar = i\omega a \rightarrow a = a(0)e(i\omega t)$

This was demonstrated in class one gets similar equation for  $a^\dagger$  and the only subtle part is that you should expand the exponential in time to get the solution in Sakurai:

$\exp(i\omega t) = \cos\omega t + i \sin\omega t$ . Then add the expressions for  $a(t)$  and  $a^\dagger(t)$  collecting the terms equal to  $\cos$  and  $\sin$ : you get

$$x_H(t) = x(0)\cos\omega t + p(0)/m\omega \sin\omega t$$

### Alternative Method

As Sakurai explains another method within the Heisenberg picture besides solving the Heisen EOM, is to directly evaluate the operator product  $U^\dagger A(0)U$ . E.g. let's evaluate  $x_H = U^\dagger x(0)U = U^\dagger x_S U$  directly using Baker Hausdorf Lemma (also performed in Sak):

$$e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \frac{1}{3!}[X, [X, [X, Y]]] + \dots$$

Actually Wikipedia calls this the **Hadamard lemma** (special case of the more general Baker-Hausdorf)

We will always call it the Baker-Hausdorf lemma:

Baker Hausdorf lemma will be used several times in this course/book so useful to study it.

DIGRESSION:

PS:  $e^A e^B = e^{A+B}$  only when A,B commute.

**Did Prakash Go over this? Yes**

Third term in expansion see Prakash's notes. Solved by visual inspection. but to prove it's true for all terms:

General formula if A,B don't commute (Wikipedia: Baker-Campbell-Hausdorff Lemma):

### The Zassenhaus formula

[\[edit\]](#)

A related combinatoric expansion, useful in dual applications is

$$e^{t(X+Y)} = e^{tX} e^{tY} e^{-\frac{t^2}{2}[X,Y]} e^{\frac{t^3}{6}(2[Y,[X,Y]]+[X,[X,Y]])} e^{-\frac{t^4}{24}(\dots)}$$

where all exponents of order larger than  $t$  are likewise nested commutators.

Apparently  $e^A e^B = e^{A+B} e^{1/2[A,B]}$  is generally as far as one usually has to go because typically

$$[[A,B],A] = [[A,B],B] = 0$$

END DIGRESSION:

(obviously the Baker Hausdorff is related to the Zassenhaus)

Setting this theorem up for our relation we see

Sakurai 2.3.48

Then we note from Sak 1.9 relations (obviously very important)

$$[x, G(p)] = i\hbar dG/dp \quad [p, F(x)] = -i\hbar dF/dx \quad (\text{on board already})$$

$$\text{SHO A) } [H, x(0)] = -i\hbar p(0)/m \quad \text{B) } [H, p(0)] = i\hbar m\omega^2$$

We can evaluate each of these commutators.

First apply B for every appearance of  $[H, x(0)]$

...

Now for all remaining commutators apply  $[H, p(0)]$

Now repeat infinity times..

You see what happens Even powers end up as  $\propto x(0)$  odd powers end up  $\propto p(0)$

So we get

Sak. 2.3.50

Remembering trig relations (put on board before lecture)



$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots \quad -\infty < x < \infty$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \dots \quad -\infty < x < \infty$$

$$x_H(t) = x(0)\cos\omega t + p(0)/m\omega \sin\omega t$$

OK great—we have the operator from 2 methods both in the H picture.

What do we do with this solutions?

Well now we can e.g. calculate expectation values.

First it is obvious that  $\langle n | x, p | n \rangle =$  equals 0. TIME INDEPENDENT (symmetry argument.)

The only states which oscillate are linear combinations of the  $|n\rangle$  states.

**Example** reapply to Midterm problem:

$$1/\sqrt{2} (\langle 0 | + \langle 1 | (x_H(t)) | 0 \rangle + | 1 \rangle)$$

diagonal terms obviously cancel because for above reason

$$\frac{1}{2} (\langle 0 | x \cos \omega t + p/m\omega \sin \omega t | 1 \rangle + \langle 1 | x \cos \omega t + p/m\omega \sin \omega t | 0 \rangle)$$

$$1/2 \cos \omega t [\langle 0 | x | 1 \rangle + \langle 1 | x | 0 \rangle] + 1/2 m \omega \sin \omega t [\langle 1 | p | 0 \rangle + \langle 0 | p | 1 \rangle]$$

$$\text{Use } x = x_0 (a + a^\dagger / 2) \rightarrow p = a - a^\dagger / 2 i x_0$$

also, now one of either a or a<sup>†</sup> terms always vanish from inner product orthog when we expand each x,p operator

$$1/2 \cos \omega t [\langle 0 | x_0 a / 2 | 1 \rangle + \langle 1 | x_0 a^\dagger / 2 | 0 \rangle] + 1/2 m \omega \sin \omega t [\langle 1 | a^\dagger / 2 i x_0 | 0 \rangle + \langle 0 | -a / 2 i x_0 | 1 \rangle]$$

$$1/2 \cos \omega t [\langle 0 | x_0 a / 2 | 1 \rangle + \langle 1 | x_0 a^\dagger / 2 | 0 \rangle] + 1/2 m \omega \sin \omega t [1/2 i x_0 \langle 1 | 1 \rangle - 1/2 i x_0 \langle 0 | 0 \rangle]$$

ie the second term goes to 0

$$\frac{1}{2} \cos \omega t [ \langle 0 | x_0 a / 2 | 1 \rangle + \langle 1 | x_0 a^\dagger / 2 | 0 \rangle ] + \frac{1}{2} m \omega \sin \omega t [ \frac{1}{2} i x_0 \langle 1 | 1 \rangle - \frac{1}{2} i x_0 \langle 0 | 0 \rangle ]$$

-- forgetting constants  $\propto \cos \omega t$  !

We can see elements of our general expression here again: remember the matrix representations (in the  $n$  basis) of  $x$ ,  $a$  and  $a^\dagger$  from the problem set problem:

$$X = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & \cdot & \cdot \\ 1 & 0 & \sqrt{2} & 0 & 0 & \cdot & \cdot \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdot & \cdot \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \cdot & \cdot \\ 0 & 0 & 0 & \sqrt{4} & 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

this is  $x$  (it was also easy to guess that the  $a$ ,  $a^\dagger$  operator's MR should be the elements of  $X$  just above ( $a$ ) and below ( $a^\dagger$ ) the diagonal) with all other elements 0. Thus  $x \propto a + a^\dagger$ . But the point again is notice all fo these operators have 0's along the diagonal. And again we end up with a plain  $\cos \omega t$  where  $\hbar \omega = E_1 - E_0$

# 4) Amplitudes, Base kets, + Summary

## 4.1) Correlation Amplitudes

2/24/10

$$\langle \alpha, t | \alpha, t_0 = 0 \rangle$$

Energy Expansion  
like  $\langle \alpha | \alpha \rangle = \sum_n |c_n|^2 e^{-iE_n t/\hbar}$  → defines relation  
only Schrödinger Picture?

## 4.2) Transition Amplitudes

$$c_n(t) = \langle a_n | \alpha, t \rangle \Rightarrow c_n(0) e^{-iE_n t/\hbar} \quad [A, H] = 0$$

If  $[A, H] \neq 0$ ?

Consider Expansion Coeff  $c_a(t) \Rightarrow \text{Prob}(a, t) = |c_a|^2$   
(Notes online)

Schrödinger Picture

$$\begin{aligned} \langle a_n | U(t, t_0) | a_m \rangle &= \langle a_n | \sum_n c_n^a U(t, t_0) | a_m \rangle = \langle a_n | U(t, t_0) | a_m \rangle \\ &= \sum_n c_n^a \langle a_n | U(t, t_0) | a_m \rangle \end{aligned}$$

no  $E_a \Rightarrow e^{-iE_a t/\hbar}$

General Trans. Amp: "transition amplitude"

$$\langle a_n | U | b_m \rangle \Rightarrow \text{Prob}(B \rightarrow A)$$

Useful terminology: Scattering, Approximation Method

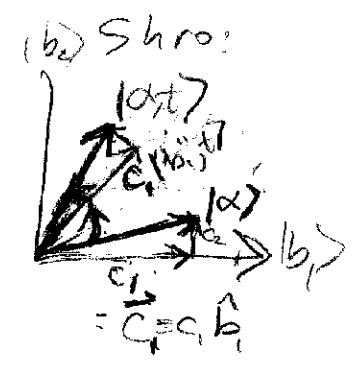
(In Schro,  $B$  is const  $\Rightarrow |b\rangle$  is const.  $U$  IS  $|b\rangle$  changing here

Note Conceptual difference in Schro:

**IMPORTANT**

$|\alpha, t=0\rangle = |b_n\rangle \neq \text{the } |b_n\rangle$

Think  $|\alpha(t)\rangle = |\alpha_{b_1}(t)\rangle + |\alpha_{b_2}(t)\rangle$  State starting as basis ket (changes always) different than basis ket itself



$B|b_n\rangle = b_n|b_n\rangle$   
 (re-start)  
 the  $|b_n\rangle \Rightarrow B|b_n\rangle = b_n|b_n\rangle$   
 (later notice constant w/ time)

True for even  
 $|\alpha, t=0\rangle = |E_n\rangle$  too!  
 $U|E_n\rangle = e^{iE_n t/\hbar} |E_n\rangle$

End of Lecture 2/24

1.3) Trans. Amp in Heisenberg Pic?

$B \Rightarrow B(t) = U^\dagger B U$

$|b_n\rangle(t) = |b_n\rangle ? \Rightarrow$  Base Ket Evolution

2 ways:

(T.A. physical  $\rightarrow$  same both pics)  
 (physical quantity should be same)  
 $\langle b_n | U | a_m \rangle$   
 $\langle b_n, t | \Rightarrow U^\dagger | b_n, t \rangle = |b_n, t\rangle$

More important: Eigen values Remain constant

( $|b_n\rangle$  rotate w/  $B(t)$ )  $(U^\dagger B U)(U | b_n \rangle) = b_n (U^\dagger | b_n \rangle)$

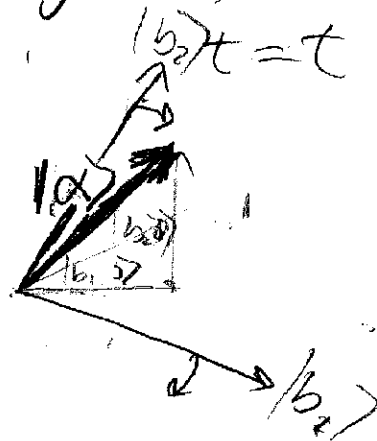
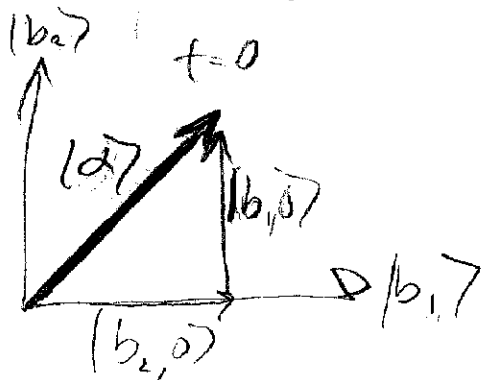
THUS Base kets rotate "backwards"  
 in Heis. Pic  $|b(t)\rangle = U^\dagger |b\rangle$

table from notes online

Note: similar subtlety as for Schro: " $|\alpha, 0\rangle = |b_n\rangle \neq$  the  $|b_n\rangle$ "

Heis Pic:  $|\alpha\rangle_H = \text{const}$  but  $|\alpha\rangle = c_1 |b_1\rangle + c_2 |b_2\rangle + \dots$   
 Why  $|\alpha\rangle_H = \text{const}$ ? rotating bkws?  
 No! incorrect  $\uparrow$

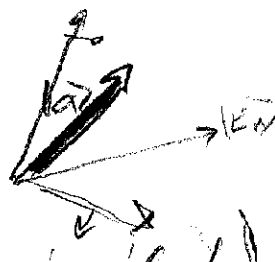
Because  $|\alpha\rangle_H$  defined w/ constant  $|b_n\rangle_s$ : at one instant (e.g.  $t=0$ )



Thus really like

Passive Rotation

(but "active" because  $|b_n\rangle$  can actively rotate w/ respect to  $|E_n\rangle$ ...)



(... If  $[B, H] \neq 0!$ )

H.4) Base kets of  $H$  (Ham) in Heis

But  $U^\dagger H U = H$  i.e.  $H_{\text{shro}} = H_{\text{Heis}}$

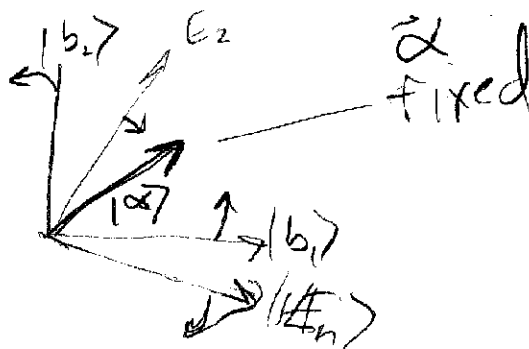
-  $H$  const. :  $\overset{\text{should}}{|E_n\rangle} \Rightarrow U^\dagger |E_n\rangle?$

Yes  $\Rightarrow$  "conceptual" difficulty for Heisen?   
  $\Downarrow$

Best to truly view as passive rot of  $H$  basis (of  $[A, H] = 0$   $A$  basis)



But  $[B, H] \neq 0$   $B$  basis defines  
yet "another" rotation  $\rightarrow$  "active"



Thus I am now  
 modifying what I previously  
 stated for "Big Pics" of Pictures:

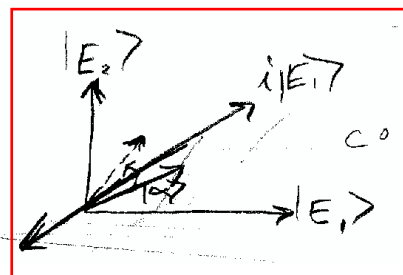
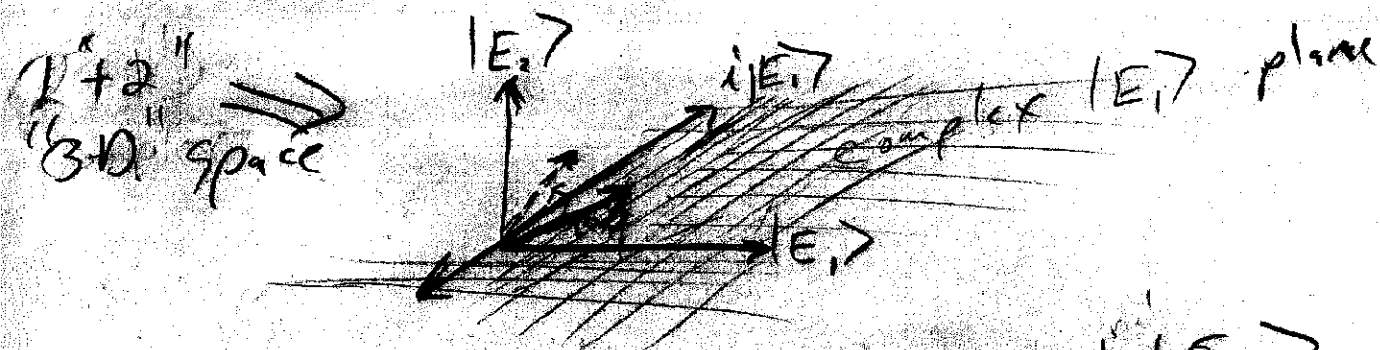
In Heis. pic, the  $H(\mathbb{R}^n)$   
 basis is (passively) rotating  
 too. But other basis's (for  $[H] \neq 0$  B's)  
 will still rotate w.r.t. this  
 passive rotation.

- The situation is  
 just a little more  
 complicated than my original  
 intro: it is still a  
 good Mnemonic!  
 (ie not a pneumonic)

Reason for this: (final thought)

Rotations are taking place in complex space  $\rightarrow$  weird

Visualization:



Thus for  $|\alpha, t\rangle = a|E_1\rangle + b|E_2\rangle$

$$|\langle E_1 | \alpha, t \rangle| = |\langle E_1 | \alpha, 0 \rangle| \quad (\text{const w/ } t)$$

$$+ |\langle E_2 | \alpha, t \rangle| = |\langle E_2 | \alpha, 0 \rangle| \quad (\text{const w/ } t)$$

[if  $a, b$  real  $\Rightarrow a^2, b^2$  respectively]  
b.c.  $|ae^{i\omega t}|^2 = a^2$

but  $|\langle \alpha, 0 | \alpha, t \rangle| \sim N + M \cos \omega_1 t$   
not constant!  
oscillating!

This is the sense by which we mean  $|\alpha, t\rangle$  is not stationary (ie rotating)



END OF TIME DEPENDENCE  
 Debt: Go for Baker's Method on slide  
 + Cos, Sin relations

$$x(t) = x(0) \cos \omega t + \frac{p(0)}{m\omega} \sin \omega t$$

Promised Direct Eval of  $U^t x(0) U^0$

$$e^{iHt/\hbar} x(0) e^{-iHt/\hbar}$$

$$= x(0) + \frac{i t}{\hbar} [H, x] + \frac{i^2 t^2}{2! \hbar^2} [H, [H, x]] + \frac{i^3 t^3}{3! \hbar^3} [H, [H, [H, x]]] + \dots$$

$$= -i t \frac{p}{m} \Rightarrow -[H, \frac{p}{m}] = i \hbar \omega^2 x$$

$$= x(0) \left[ 1 + \frac{(i^2 t^2 (\hbar^2 \omega^2))}{2! \hbar^2} + \dots \right] + \frac{p(0) + \dots}{m\omega} \left[ \frac{i t (-i \hbar)}{\hbar} + \frac{i^3 t^3}{3! \hbar^3} + \dots \right]$$

cos  $\omega t$

$\frac{1}{m\omega}$  sin  $\omega t$



Finishing up Heisenberg Picture (H. Picture) implications

Heisenberg Picture:

- 1) Operators change with time.
- 2) States remain constant

What does 2) mean?

Heisenberg Picture:

- 1) Operators change with time.
- 2) States remain constant (**expansion coefficients remain constant**)
- 3) **Eigenvalues remain constant**

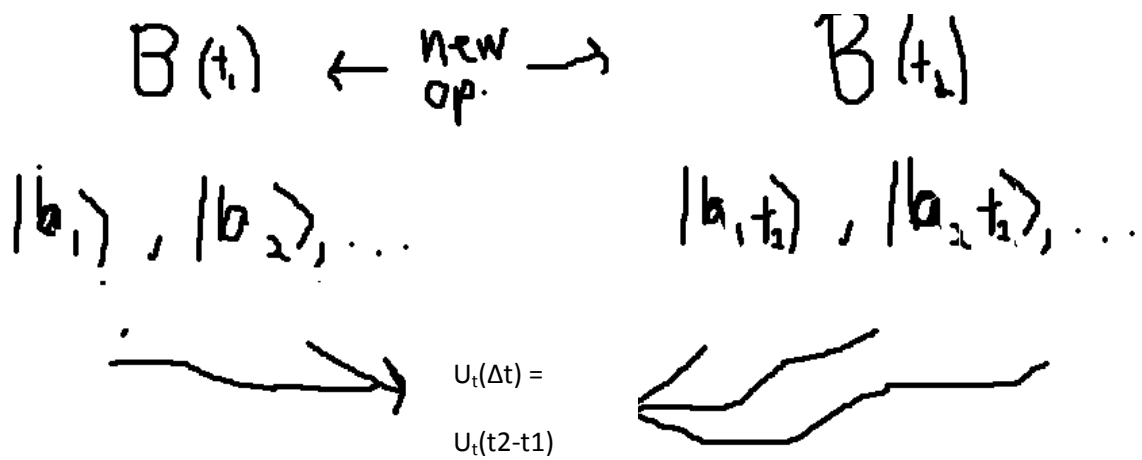
$|a, t\rangle = U^\dagger |a\rangle$  related to deeper property of BOTH pictures: What is it?

Property (postulate?) for BOTH pictures  $\rightarrow$  Related to Measurement Postulates

**Eigenvalues Remain Constant!!!**

This was obviously true in the Schro picture

But may not have been obvious thinking of very general picture before for cases like the Heisenberg picture where we want the operator to change



Thus even in Heisenberg picture we want transformations such that

$$B(t_2) |b_1, t_2\rangle = b_1 |b_1, t_2\rangle \text{ where eigenvalue } b_1(t_2) = b_1(t_1)$$

Implications for H picture:

Thus state kets in H picture evolve oppositely – Prakash notes

General explicit outer product rep. of any operator should look like this:

see separate handout:

Summary of Pictures from H/S pictures

Schrodinger picture		Heisenberg picture		Interaction Picture
				(mixture of the two)
State ket	<p>Moving</p> $ a, b; t\rangle = U(t, t_0)  a, b\rangle$ $i\hbar \frac{\partial}{\partial t}  a, b; t\rangle = H  a, b; t\rangle$	<p>Stationary</p> $ a, b; t\rangle =  a, b\rangle$	<p>Moving</p> $A^{(H)}(t) = U^\dagger(t) A^{(S)} U(t)$ $\frac{dA^{(H)}(t)}{dt} = \frac{1}{i\hbar} [A^{(H)}, H]$	moving (time dependence determined by $V(x)$ )
Observable (operator)	Stationary	Stationary	Moving	moving (time dependence determined by $V(x)$ )
Base ket	Stationary	Stationary	Moving oppositely	moving (time dependence determined by $p^2/2m$ )
			$ a', b\rangle_H = U^\dagger  a'\rangle$ $i\hbar \frac{\partial}{\partial t}  a', b\rangle_H = -H  a', b\rangle_H$	

Question: is there another "picture" that doesn't shove all the time dependence one way or the other?

Answer: Yes: Interaction Picture is Mixture of the two.

RESTATEMENT of SOME THOUGHTS expressed in slides already:

in Heisenberg Picture base kets evolve "backwards" to S picture state ket evolution

$$|a, t\rangle = U^\dagger |a\rangle$$

Motivated yesterday by requiring that matrix elements  $\langle a|\alpha\rangle(t>0)$  in H picture  $\rightarrow$  **matches** (= to)  $\langle a|\alpha\rangle$  in S picture.

Because Shro pic:  $\langle a|\alpha\rangle(t>0) = \langle a|U(t)|\alpha\rangle$  in H picture  $\rightarrow = \langle a, t=0|U(t)|\alpha\rangle$ , so convenient solution if we say in H picture

$$\langle a|\alpha\rangle = \langle a, t|\alpha\rangle \rightarrow \langle a, t=0|U|\alpha\rangle \text{ Thus } \langle a, t| = \langle a|U \rightarrow |a, t\rangle = U^\dagger |a\rangle$$

Now why would we want this quantity to match?

Because it is indeed related to something physical:

The **Transition Amplitude**  $\rightarrow$  Probability to be in new eigenket. **PHYSICALLY OBSERVABLE!**

It should automatically independent of picture  $\rightarrow$  **GOOD!!!!**

More general form for Transition Amp.:

Take  $\langle a, t=0| = \langle b|$  some general eigenket, doesn't need to be from same basis  $|a\rangle$

In either picture:  $\langle b|U(t)|a\rangle$  **Transition Amplitude is time dependent**

**(in H picture it means  $\langle b, t=t_x|$  == some fixed time  $t_x$ )**

**Very Important Side Point:** Now there conceptual difference between

$|\alpha\rangle = |a\rangle$  @  $t=0$  and the base ket itself  $|a\rangle$ .

In Shrodinger  $|a\rangle$  does not evolve, but in both pictures  $|\alpha\rangle$  can (in general) even when it starts as  $|\alpha\rangle = |a\rangle$ . That is even when  $|\alpha, t=0\rangle = |a\rangle$  in Shro picture,  $d|\alpha\rangle/dt \neq 0$ .

Original measurement postulate not met? No it's not!—remember “immediately afterwards” was specified for measurement postulate.

In general “Quantum Decoherence” can cause original  $|\alpha\rangle = |a\rangle$  to change in to other states

Only remains constant (“stationary”)

- 1) if A commutes with Hamiltonian
- 2) AND if Hamiltonian remains constant!!!

Thus important point: **things change**, even when the situation is seemingly static with time (H is constant.)



## I) Further points about the SHO: Coherent States

The SHO ground state is also Gaussian: this is easy to derive using our requirement that the annihilation operator annihilates the  $|0\rangle$  state.

$$\begin{aligned} \langle x | a | 0 \rangle &= 0 \\ \Rightarrow \sqrt{\frac{m\omega}{2\hbar}} \left( x + \frac{i\hbar}{m\omega} \frac{d}{dx} \right) \langle x | 0 \rangle &= 0 \\ \Rightarrow \left( x + \frac{\hbar}{m\omega} \frac{d}{dx} \right) \langle x | 0 \rangle &= 0 \\ \Rightarrow \langle x | 0 \rangle &= e^{-\frac{m\omega}{2\hbar} x^2} \frac{1}{\sqrt{\frac{\pi 2\hbar}{m\omega}}} \end{aligned}$$

Incidentally we can use this wave function to derive all the others' states...

we have to calculate  $\langle x | n \rangle$

$$\begin{aligned} \langle x | n \rangle &= \langle x | a^\dagger | n-1 \rangle \frac{1}{\sqrt{n}} \\ &= \frac{1}{\sqrt{n}} \sqrt{\frac{m\omega}{2\hbar}} \left( x - \frac{\hbar}{m\omega} \frac{d}{dx} \right) \langle x | n-1 \rangle \end{aligned}$$

Interesting : Min Uncert. Relation easier to derive for this case: purely work in ket operators.

e.g. integrals not necessary:

$$\text{operator } x^2 = \hbar/2m\omega(a^2 + a^\dagger^2 + N + aa^\dagger)$$

$\langle 0 | x^2 | 0 \rangle$  only last term doesn't vanish  $\rightarrow x^2 = \hbar/2m\omega$

Solve Heisenberg EOM for  $a$ ,  $a^\dagger$  obtained solutions.

$$a(t) = a(0) \exp(-i\omega t) \quad , \quad a^\dagger(t) = a^\dagger(0) \exp(i\omega t)$$

We discussed the Baker Hausdorf Lemma

$$e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!} [X, [X, Y]] + \frac{1}{3!} [X, [X, [X, Y]]] + \dots$$

for evaluating  $U^\dagger A U = \exp(iHt/\hbar) A \exp(-iHt/\hbar)$  directly.

Another good application is related to the Coherent states discussed in Sakurai.

Should have familiarity of these after this course...

For midterm/ prob set you solved Sak. 2.18a: Follow Solutions handed out--:

Main crux: one can derive the following relation, just as for  $x, p$  simply because of the commutation relations.

$$[a, f(a^\dagger)] = \frac{df(a)}{da^\dagger}$$

Thus proof is just like on midterm—other problem set

Thus the coherent state

$$e^{-|\lambda|^2/2} e^{\lambda a^\dagger} |0\rangle$$

is an eigenstate of the  $a$  operator.

Note some of the remarkable properties of coherent states elucidated on the following slides:



a) Completeness

$$\sum_{\lambda} |\langle \lambda | \langle \lambda | = \int d^2 \lambda \sum_{\lambda \text{ complex}} |\lambda\rangle \langle \lambda|$$

In h.o. basis

$$\sum_{\lambda} \langle n | \lambda \rangle \langle \lambda | m \rangle = \sum_{\lambda} \langle n | e^{\lambda a^\dagger} | 0 \rangle \langle m | e^{\lambda a^\dagger} | 0 \rangle \cdot e^{-|\lambda|^2}$$

$$|n\rangle = \frac{1}{\sqrt{n!}} a^{\dagger n} |0\rangle \quad \langle n| = \frac{1}{\sqrt{n!}} \langle 0| a^n$$

$$\Rightarrow \langle n | e^{\lambda a^\dagger} | 0 \rangle = \frac{1}{\sqrt{n!}} \langle 0 | a^n e^{\lambda a^\dagger} | 0 \rangle$$

$$= \frac{1}{\sqrt{n!}} \lambda^n$$

$$\Rightarrow \sum_{\lambda} \langle n | \lambda \rangle \langle \lambda | m \rangle = \sum_{\lambda} \frac{\lambda^n \lambda^{*m}}{\sqrt{n!} \sqrt{m!}} e^{-|\lambda|^2}$$

$$\lambda = r e^{i\varphi}$$
$$= \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} d\varphi$$

$$\int_0^\infty r^{n+m+1} dr \int_0^{2\pi} d\varphi e^{-r^2} e^{in\varphi - im\varphi} = \int_0^\infty r^{n+m+1} dr \int_0^{2\pi} d\varphi e^{-r^2} = \int_0^\infty r^{n+m+1} dr \cdot 2\pi = \pi \int_0^\infty r^{n+m+1} dr = \pi \int_{-\infty}^{\infty} dx \delta(x) = \pi$$

$$= \frac{2\pi \int_0^\infty r^{n+m+1} dr}{n! m!} = \pi \int_{-\infty}^{\infty} dx \delta(x) = \pi$$

$$= \pi \int_{-\infty}^{\infty} dx \delta(x) = \pi$$

$$\Rightarrow \mathbb{1} = \frac{1}{\pi} \int d^2 \lambda |\lambda\rangle \langle \lambda|$$

2) Interpretation

$$e^{-\omega^2/2 + \lambda a^\dagger} |0\rangle = \sum_n \frac{1}{n!} (\lambda a^\dagger)^n |0\rangle e^{-\omega^2/2}$$

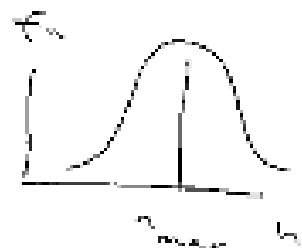
$$= \sum_n \frac{1}{n!} \lambda^n \sqrt{n!} |n\rangle e^{-\frac{1}{2}\omega^2}$$

$$= \sum_n f_n |n\rangle$$

$$f_n = \frac{\lambda^n}{\sqrt{n!}} e^{-\omega^2/2}$$

For  $n_{max} \gg 1$

$$f_{n_{max}+1} \approx f_{n_{max}}$$



$$\Rightarrow \frac{\lambda^{n_{max}+1}}{\sqrt{(n_{max}+1)!}} = \frac{\lambda^{n_{max}}}{\sqrt{n_{max}!}} \Rightarrow \lambda = \sqrt{n_{max}+1} \approx \sqrt{n_{max}}$$

By increasing  $\lambda$  we increase the number of oscillator quanta in  $|n\rangle$

g) Time evolution of a coherent state

$$\begin{aligned}
 S-29 \quad |\lambda, t\rangle &= e^{-iHt/\hbar} |\lambda_0\rangle \\
 &= e^{-i\hbar\omega(N+\frac{1}{2})t/\hbar} |\lambda_0\rangle \\
 &= e^{-i\omega t(N+\frac{1}{2})} e^{\lambda a^\dagger} |\lambda_0\rangle \\
 &= e^{-i\omega t(N+\frac{1}{2})} e^{-\lambda e^{-i\omega t} a^\dagger} |0\rangle \\
 &= \sum_k \frac{1}{\sqrt{k!}} \lambda^k e^{-i\omega t(k+\frac{1}{2})} |k\rangle \\
 &= e^{-\frac{1}{2}i\omega t} \sum_k \frac{1}{\sqrt{k!}} (\lambda e^{-i\omega t})^k |k\rangle \\
 &= e^{-\frac{1}{2}i\omega t} |\lambda e^{-i\omega t}\rangle
 \end{aligned}$$

⇒ coherent state remains a coherent state under time evolution and also a minimum uncertainty state.

Above time evolution of Coherent State

Use the last property listed in book without proof: (also problem 2.18e):

**Sakurai Problem 2.11: Other use of Baker Hausdorff Lemma**

Coherent states: Sakurai Problem 2.11 Important: it also turns out that we can write the coherent state as a spacial translation of the SHO ground state: ie apply the operator  $e^{ika}$  from our discussion of momentum: You will show this on your problem set. But assuming it is true

Sak 2.11: Find time dependence of  $\langle x \rangle$  for the state  $|\alpha\rangle = \exp(-ipa/\hbar)|0\rangle$  where  $p = p_s$  is the (constant) momentum operator in the Shrodinger picture

$$\begin{aligned} \langle x \rangle &\equiv \langle \psi_S(t) | \hat{x}_S | \psi_S(t) \rangle = \langle \psi_S(0) | \hat{x}_H | \psi_S(0) \rangle = \dots \\ &= \langle 0 | e^{\frac{i p_s a}{\hbar}} \left( (\hat{a} + \hat{a}^\dagger) \frac{x_0}{\sqrt{2}} \right)_H e^{-\frac{i p_s a}{\hbar}} | 0 \rangle = \\ &= \frac{x_0}{\sqrt{2}} \langle 0 | e^{i p_s a / \hbar} (\hat{a}_H + \hat{a}_H^\dagger) e^{-i p_s a / \hbar} | 0 \rangle = \\ &= \frac{x_0}{\sqrt{2}} \langle 0 | e^{i p_s a / \hbar} (\hat{a}_S e^{-i \omega t} + \hat{a}_S^\dagger e^{i \omega t}) e^{-i p_s a / \hbar} | 0 \rangle = (*) \end{aligned}$$

Using the Baker-Hausdorff Lemma (see proof at the end of this solution set):

$$\begin{aligned} e^{i p_s a / \hbar} \hat{a}_S e^{-i p_s a / \hbar} &= \left[ e^{i p_s a / \hbar} \hat{a}_S e^{-i p_s a / \hbar} \right] = \left[ \hat{a}_S + \frac{i p_s a}{\hbar} [\hat{a}_S, \hat{a}_S] + \frac{1}{2} \left( \frac{i p_s a}{\hbar} \right)^2 [\hat{a}_S, [\hat{a}_S, \hat{a}_S]] + \dots \right] = \\ &= \hat{a}_S + \frac{i p_s a}{\hbar} \cdot \frac{\hbar}{x_0 \sqrt{2}} + 0 + 0 + \dots = \hat{a}_S + \frac{a}{x_0 \sqrt{2}} \end{aligned}$$

$$e^{i p_s a / \hbar} \hat{a}_S^\dagger e^{-i p_s a / \hbar} = \left( e^{i p_s a / \hbar} \hat{a}_S e^{-i p_s a / \hbar} \right)^\dagger = \hat{a}_S^\dagger + \frac{a}{x_0 \sqrt{2}}$$

Plugging these into (\*):

$$\begin{aligned} \langle x \rangle &= \frac{x_0}{\sqrt{2}} \langle 0 | e^{-i \omega t} \left( \hat{a}_S + \frac{a}{x_0 \sqrt{2}} \right) + e^{i \omega t} \left( \hat{a}_S^\dagger + \frac{a}{x_0 \sqrt{2}} \right) | 0 \rangle = \\ &= \frac{e^{-i \omega t} + e^{i \omega t}}{2} a \cdot \langle 0 | 0 \rangle = \underline{a \cos \omega t} \end{aligned}$$

Lecture 3/1/2010-3/3/2010

SLIGHTLY DIFFERENT IN-CLASS VERSION afterwards

2-12 ... Time independent:  $S$ -eq

Substitution  $\Psi(x,t) = \Psi_E(x) e^{-iEt/\hbar}$

$$\Rightarrow E \Psi_E = \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi_E$$

general solution  $\Psi(x,t) = \sum_E C_E \Psi_E(x) e^{-iEt/\hbar}$

$C_E$  are fixed by the initial condition

time independent equation

$$\left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi = E \Psi \quad \begin{array}{l} 2^{\text{nd}} \text{ order linear} \\ \text{diff. eq.} \end{array}$$

It has 2 independent solutions,  $\psi_1, \psi_2$

general solution  $\Psi = A \psi_1 + B \psi_2$

boundary conditions

bound states:  $|\Psi(x)|^2 \rightarrow 0$  for  $x \rightarrow \pm\infty$   
probability to find a particle

In general, we find that this is only possible for a discrete set of  $E$ -values

## 2.13 Probability Current and density

probability density  $\rho(\vec{x}, t) = |\psi(\vec{x}, t)|^2$

time change of  $\rho$

$$\begin{aligned} \partial_t \rho &= \partial_t \psi^* \psi = (\partial_t \psi^*) \psi + \psi^* \partial_t \psi \\ &= -\frac{i}{\hbar} \left[ \left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi^* \right] \psi + \psi^* \frac{i}{\hbar} \left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi \\ &= \frac{1}{2\pi i \hbar} (\psi \nabla^2 \psi^* - \psi^* \nabla^2 \psi) \\ &= \frac{1}{2\pi i \hbar} \nabla \cdot (\psi \nabla \psi^* - \psi^* \nabla \psi) \\ &= -\nabla \cdot \vec{j} \end{aligned}$$

terms dropped only if  $V$  is real

$$+ (V - V^*) \rho \propto \text{Im}\{V\}$$

$$\Rightarrow \vec{j} = \frac{\hbar}{2im} (\psi^* \nabla \psi - \psi \nabla \psi^*)$$

↑ probability current

Continuity eq.  $\partial_t \rho + \nabla \cdot \vec{j} = 0$

interpretation



$$\begin{aligned} \partial_t \int_V \rho(\vec{x}, t) d^3x &= \int_V -\nabla \cdot \vec{j} d^3x \\ &\stackrel{\text{Gauss' Theorem}}{=} -\int_{\partial V} \vec{j} \cdot d\vec{A} \end{aligned}$$

total probability decreases by the outgoing current

Interpretation if  $\text{Im } V$  is non-zero

$$\int \rho dV = N, \quad dN/dt - \text{Im} V dV = \text{Integral } J \cdot dA$$

Cross section  $\sim dN/dt$  missing

$$\sigma \propto \text{Im } V$$

## 2 Classes of Problems to Review/Introduce from Wave Mech

### 1) Review: Simple 1-D Constant Potentials

Comments: a) you won't be expected to do problems like this, but if you don't remember you should refresh your memory look at Liboff. b) We will discuss qualitative features only and quote results only:

### 2) Delta Fn Potential Problems.

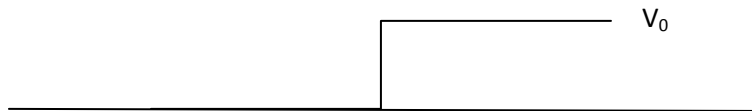
-----

Free Particle:  $V = 0, H = p^2/2m$

Solution:  $\psi = A \exp(\pm ikx - \omega t)$   $E_k = \hbar^2 k^2/2m$

Half free particle on a constant potential "step" (region of constant potential  $V_0$ )

Remembering our  $\theta(x)$  definition  $\rightarrow V(x) = V_0 \theta(x)$



Solution in the right hand region is

$$\psi = A \exp(-\kappa x) \text{ with } E_\kappa = V_0 - \hbar^2 \kappa^2/2m$$

when  $E < V_0$

Scattering: Typically we set this up as a scattering problem of waves entering ("incident") from the left, "reflecting" back to the left and choose a single direction for the Right Hand Region, as being "transmitted" to the right:

$$A \rightarrow I, \quad B/A \rightarrow R, \quad C/A \rightarrow T$$

This comes from the idea that we will think of some current density  $j$  as being associated with these three, incident, reflected, and transmitted, parts:

E.g. we can calculate some  $J_{inc}$ , for  $\psi_{inc}(x) = e^{ikx}$

$$= \frac{\hbar}{2mi} (\psi^* d\psi/dx - \psi d\psi^*/dx) \rightarrow \frac{\hbar}{2mi} (\exp[-ikx])(ik \exp[ikx]) = \hbar k/m$$

Thus the current density  $j$  is  $\propto k$  and if this was more than 1-D, the direction of  $j$  = direction of  $k$  (nothing would really change – except the  $d/dx \rightarrow \nabla$ ) In 1-D direction is same as sign.

Rest of problem is just solving for T or R by imposing the “matching conditions”. This is the key.

See Liboff 7.6 Remembering that  $\sinh x = (e^x - e^{-x})/2$

Note that we often are interested in something called the transmission coefficient

$$T_{coeff} = \frac{|j_{trans}|}{|j_{inc}|}$$

which is simply the ratio of the probability that gets transmitted: this is directly interpretable as the probability for a single particle approaching from the left to be transmitted to right. Typically we are imagining a case where the potential is such that the large positive  $x$  behavior of the potential is constant (often 0—ie we end up with a free particle again, and we are describing the transmission through some “barrier” region).

Thus as above we would typically want a wave function in the large  $x+$  region of the form  $\psi = T \exp(+ikx)$  following the convention described above for the letter used for the amplitudes of the wave functions.

In this case thus  $T_{coeff} \propto |T|^2$

HOWEVER: note that  $T_{coeff} \neq |T|^2$  in fact evaluating the  $j$ 's for the free particle solutions (w/  $\psi_{inc}$  amplitude convention  $A = 1$ )

$$T_{coeff} = |T|^2 k_{trans}/k_{inc}$$

### Other points

This matching of solutions is important for demonstrating the bound state solutions: they are the reason the bound state solution has discrete energies in the simple potential well problem:

Bound State Example: Liboff: Finite Potential Well Chapter 8.

Talked about Bound State example: horribly complicated solutions but yet still demonstrative.

-----



The basics of these type of Wave Mech problems: bound state and scattering type problems should be remembered. Application of them now to 1 special kind of potential:

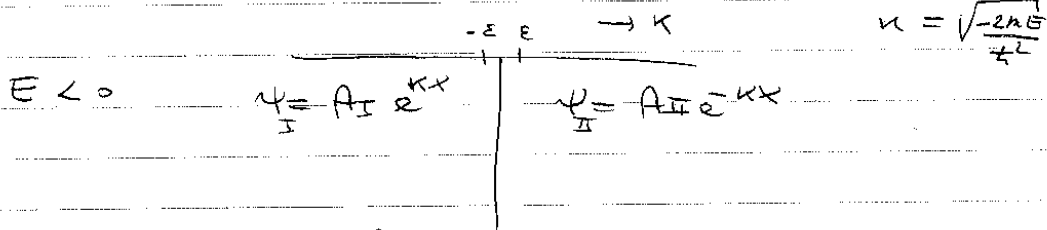
-----

Wave Mechanics:  $\delta$  fn Potential Problems (often explored in 611 type courses)

(59)

d)  $\delta$ -Function Potential

$$\left(-\frac{\hbar^2}{2m} \partial_x^2 + A \delta(x)\right) \psi = E \psi$$



Integrate  $\delta$ -eq between  $x = -\epsilon$  and  $x = \epsilon$

$$\Rightarrow \int_{-\epsilon}^{\epsilon} -\frac{\hbar^2}{2m} \partial_x^2 \psi + \int_{-\epsilon}^{\epsilon} A \delta(x) \psi = E \int_{-\epsilon}^{\epsilon} \psi dx$$

$$\Rightarrow \left( \partial_x \psi \Big|_{x=\epsilon} - \partial_x \psi \Big|_{x=-\epsilon} \right) \left( -\frac{\hbar^2}{2m} \right) + A \psi(0) = E \psi(0) \epsilon \epsilon + O(\epsilon^2)$$

$\psi$  continuous at  $x \rightarrow 0 \Rightarrow A_I = A_{II}$

$$\left( -\kappa A_{II} - \kappa A_I \right) \left( -\frac{\hbar^2}{2m} \right) + A A_I = 0$$

$$\Rightarrow -2\kappa A_I \left( -\frac{\hbar^2}{2m} \right) = -A A_I$$

$$A_I \neq 0 \Rightarrow \frac{\hbar^2 \kappa}{m} = -A$$

Note that  $A$  is negative for an attractive  $\delta$ -function

$$\Rightarrow \frac{-2mE}{\hbar^2} \frac{\hbar^2}{m} = A^2$$

$$\Rightarrow E = -\frac{mA^2}{2\hbar^2}$$

We find exactly one bound state no matter how weak the potential

Solving  $\delta$  fn potential problems always is similar:

Same problem as a scattering example:  $\delta$  fn

Only difference is if we want to treat this as a scattering problem, we consider  $E > 0$ , then on either side,  $0$  we want plane wave solutions.

End review: Now Discuss  $S(x)$  WKB Approximation

---

### Intro of $S(x)$

Remember from complex analysis we can represent any complex number  $z$  in 2 ways

$$z = x + iy = re^{i\phi} \quad (r = \sqrt{x^2 + y^2})$$

where  $x, y, r, \phi$  are real

This can also be done for any complex function  $w(z) = w(x, y) = u(x, y) + i v(x, y)$

$$r(x, y)e^{i\phi(x, y)}$$

$$\rightarrow \psi(x, t) = \sqrt{\rho(x, t)} e^{iS(x, t)} \quad \sqrt{\rho} = \sqrt{\text{Re}^2(\psi) - \text{Im}^2(\psi)}$$

**Prakash's notes** Reminder of Classical Mech: see supplemental notes...

Derivation of the Hamilton Jacobi Equation

$$\frac{1}{2m} |\nabla S(x, t)|^2 + V(x) + \frac{\partial S(x, t)}{\partial t} = 0$$

Point no one remembers Hamilton Jacobi Eq. from classical mechanics. Just remember that there is another relation to classical mechanics here.

Reminder: Hamiltonian's Principle Function :

Not equal to the Hamiltonian: --- Related to the action  $S = \int L dt = \int (T - V) dt$

Hamilton-Jacobi Equation Non-linear Differential Equation: not very easy to solve. So is it really useful? Not likely often—Lagrangian Mechanics is obviously preferred (that is what you learn). However, it provides this link for Wave Optics and also link for QM.

**WKB or Semi Classical Approximation:**

# Point out Coherent states 3/1/2010

Coherent: fixed phase relationship betw  
components,

Announcement →

Lilias F. Reading  
+ Sak. Ch. 7  
- 246 (selected sections)

Informal: any effect which depends on multiple "components" acting together interdependently in some regular way

- Time evolution (first:  $\exp(-i\hat{H}t)\psi$ )
- Hint: how work → Zassenhaus →  $e^{-i\hat{p}l} = e^{-i\hat{K}(a-t)l} e^{i\hat{K}a-l\hat{K}}$
- ~~Lasers~~ Laser → Poisson statistics for each component important → important for "particle" interpretation.

## VII Advanced Topics in Wave Mechanics (WM)

(Applications will use formalism only sometimes)  
(Better Applications of formalism in 612)

~~A~~ WM Schrödinger Eq  
Derived from formalism (already)

~~TDSE~~ TDSE (TDSE)

# Wave Mech Review

$$-i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi$$

$$= -\frac{\hbar^2}{2m} \nabla^2 \psi + V(x) \psi$$

WM: Assume Separable  $\psi = \psi(x) f(t)$

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

What next? = constant  $\Rightarrow E$  (already from formalism)

$$i\hbar \frac{df(t)}{dt} = E f(t) \Rightarrow f(t) = e^{-iEt/\hbar}$$

$$U|p\rangle = e^{i(E_p t/\hbar - px/\hbar)}$$

$\downarrow A(p) = \langle p | \psi \rangle$  solution  $|p\rangle$

2) TISE:  $-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x)$

two independent

2nd order ODE  $\rightarrow$  2 solutions

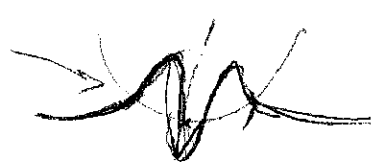
$V(x)$  has min  $\Rightarrow$  bound solutions

consider  $E < V(\pm\infty)$

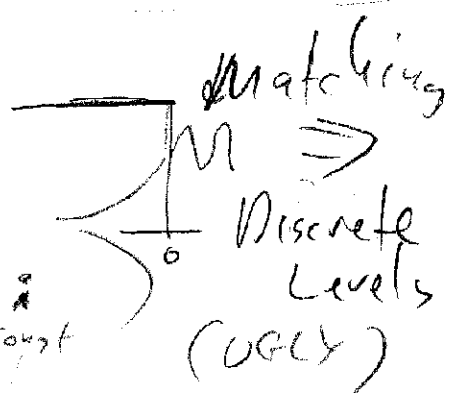
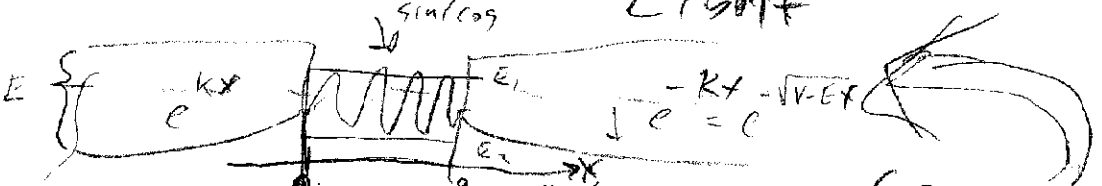
## 1-D Examples:

1-D Box (Infinite)

SHO



1-D Finite Box (Chapter 8.1 Liboff)



General Method:  $V(x) = V_{const}$  (or piecewise const's  $V_{const}$ )

$$\psi(x) = e^{\pm ikx} \quad \frac{\hbar^2 k^2}{2m} = \pm |E - V_{const}|$$

$k = ik$  or  $e^{\pm Kx}$   $\Rightarrow$  by inspection

## A.2) TISE 1D Examples (cont)

 $\delta$ -fn Potentials  $V(x) = -D\delta(x)$ 

$$\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - D\delta(x) \right) \psi(x) = E\psi$$

Seek Negative  $E$  (Formalism:  $H=H^\dagger \Rightarrow$  real solution) (see for well via Lippoff (Chapt 8, 25) not necessary)

Method for  $\delta$ -fn: Integrate TISE btw  $[\epsilon, -\epsilon]$

$$-\frac{\hbar^2}{2m} \int_{-\epsilon}^{\epsilon} \frac{d^2 \psi}{dx^2} - \int_{-\epsilon}^{\epsilon} D\delta(x) \psi(x) = E \int_{-\epsilon}^{\epsilon} \psi dx$$

$$-\frac{\hbar^2}{2m} \left( \frac{d\psi}{dx} \Big|_{\epsilon} - \frac{d\psi}{dx} \Big|_{-\epsilon} \right) - D\psi(0) = 2\epsilon E \psi(0)$$

$\xrightarrow{\epsilon \rightarrow 0}$   $\lim_{\epsilon \rightarrow 0}$

$$= \frac{\hbar^2}{2m} (KA - KA) = \pm DA$$

$(A_{II} = A_I = A \text{ continuity})$

$$D = \frac{\hbar^2 K}{m} \Rightarrow D^2 = \frac{2mE}{\hbar^2} \frac{\hbar^4}{m^2}$$

$$E = -\frac{m D^2}{2\hbar^2}$$

One bound state!

# VII Advanced Topics in Wave Mechanics

- (Applications I will use formalism sometimes)  
(Better applications (6/2))

~~B) Probability Current~~

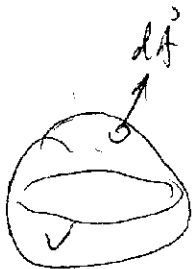
use  $\frac{1}{2} \psi^* \psi \rightarrow \psi^* \psi$  usually obvious ..

$$\langle \psi | \psi \rangle = \psi^*(x) \psi(x) = \rho(x) \Rightarrow \begin{matrix} \text{Prob} \\ \text{density} \\ \equiv \text{Prob/unit volume} \end{matrix}$$

$$\begin{aligned} \partial_t \rho &= \partial_t (\psi^* \psi) = (\partial_t \psi^*) \psi + \psi^* (\partial_t \psi) \\ &= \frac{1}{\hbar^2} \left[ \left( \frac{\nabla^2 \psi^*}{2m} + V \psi^* \right) \psi + \psi^* \left( -\frac{\nabla^2 \psi}{2m} + V \psi \right) \right] \\ &= \frac{\hbar^2}{2mi} [\psi \nabla^2 \psi^* - \psi^* \nabla^2 \psi] \\ &= -\nabla \cdot \vec{j} \Rightarrow \vec{j} = \frac{\hbar}{2mi} (\psi^* \nabla \psi - \psi \nabla \psi^*) \end{aligned}$$

for  $V(x) = \text{real} \Rightarrow 0$

$\frac{\hbar}{2m} \text{Im} \{ \psi^* \nabla \psi \}$



$\partial_t \rho + \nabla \cdot \vec{j} = 0$  continuity eq.

$\int_{\text{Prob}} \partial_t \rho dV = \int_{\text{Prob}} -\nabla \cdot \vec{j} dV = \int_{\text{Prob}} \vec{j} \cdot d\vec{A}$  Probability flux  $\vec{j}$

Like Incompressible Fluid  
(Fluid Mech)

For Brf:  $e^{+ikx}$  /  $e^{-ikx}$

$\delta$ -fn potential

Scattering Setup  $\psi_j$

Use  $\vec{j}$  as particle flux:  $\frac{N_{particles}}{unit\ dA\ /s}$

$\rho = |\psi|^2 \Rightarrow$  particle number density

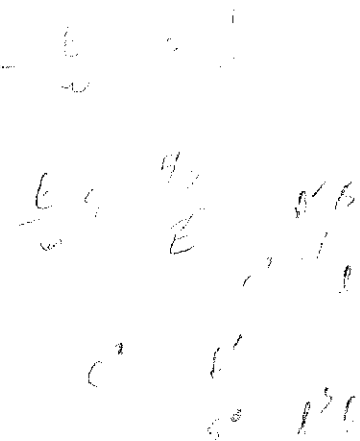
$\int \rho dV \Rightarrow N_{particles}$

TISE: Choose Unbound Solutions  
 oscillating  $(in \vec{x})$  only,  $E \geq V(x)$  (consider)

1-D Example (Libble / deep well) (Step)  
 Region I      Region II

$E \uparrow$

Scattering "from left"





Choose  $\psi_I$  to make  $\vec{j}$  "incident from left"

$$\psi_I(x) = A e^{ikx} + B e^{-ikx}$$

$$\vec{j} = \frac{\hbar}{2mi} (\psi^* \nabla \psi - \psi \nabla \psi^*) = \vec{j} = \vec{k} = +k$$

Reflected component  
 $\vec{j} = \vec{k} = -k$

Region II:

$$C e^{ikx} + \cancel{D e^{-ikx}} \Rightarrow \text{throw out for scattering setup}$$

Transmission Coeff =  $T_{\text{coeff}} = \frac{|\vec{j}_{\text{trans}}|}{|\vec{j}_{\text{inc}}|}$

Reflection Coeff =  $R_{\text{coeff}} = \frac{|\vec{j}_{\text{refl}}|}{|\vec{j}_{\text{inc}}|}$

Chapter 7 Additional One-Dimensional Problems. Bound and Unbound States

The kinetic energy decreases by  $V$  and is given by

$$\frac{\hbar^2 k_2^2}{2m} = E - V \quad (7.119)$$

In terms of  $k_2$ , (7.118) appears as

$$\varphi_{xx} = -k_2^2 \varphi \quad \text{in region II} \quad (7.120)$$

Writing  $\varphi_I$  for the solution to (7.117) and  $\varphi_{II}$  for the solution to (7.120), one obtains

$$\begin{aligned} \varphi_I &= A e^{ik_1 x} + B e^{-ik_1 x} \\ \varphi_{II} &= C e^{ik_2 x} + D e^{-ik_2 x} \end{aligned} \quad (7.121)$$

Since the term  $D e^{-ik_2 x}$  (together with the time-dependent factor  $e^{-i\omega_2 t}$ ) represents a wave emanating from the right ( $x = +\infty$  in Fig. 7.18), and there is no such wave, we may conclude that  $D = 0$ . The interpretation of the remaining  $A$ ,  $B$ , and  $C$  terms is given in (7.112). To repeat,  $A \exp(ik_1 x)$  represents the incident wave;  $B \exp(-ik_1 x)$ , the reflected wave; and  $C \exp(ik_2 x)$ , the transmitted wave.

It is important at this time to realize that  $\varphi_I$  and  $\varphi_{II}$  (with  $D \equiv 0$ ) represent a single solution to the Schrödinger equation for all  $x$ , for the potential curve depicted in Fig. 7.18. Since any wavefunction and its first derivative are continuous (see Section 3.3), at the point  $x = 0$  where  $\varphi_I$  and  $\varphi_{II}$  join it is required that

$$\begin{aligned} \varphi_I(0) &= \varphi_{II}(0) \\ \frac{\partial}{\partial x} \varphi_I(0) &= \frac{\partial}{\partial x} \varphi_{II}(0) \end{aligned} \quad (7.122)$$

These equalities give the relations

$$\begin{aligned} A + B &= C \\ A - B &= \frac{k_2}{k_1} C \end{aligned} \quad (7.123)$$

Solving for  $C/A$  and  $B/A$ , one obtains

$$\frac{C}{A} = \frac{2}{1 + k_2/k_1}, \quad \frac{B}{A} = \frac{1 - k_2/k_1}{1 + k_2/k_1} \quad (7.124)$$

Substituting these values into (7.114) gives

$$T = \frac{4k_2/k_1}{[1 + (k_2/k_1)]^2}, \quad R = \left| \frac{1 - k_2/k_1}{1 + k_2/k_1} \right|^2 \quad (7.125)$$

Liboff  
7.6

# C) 1D Scattering Setup (cont) $\vec{j} = \frac{\hbar}{m} \text{Im} \{ \psi^* \nabla \psi \}$

Key Elements: 1)  $E > V(x \rightarrow \pm\infty)$   $\in$  continuous  $\rightarrow k/2m$

Theme for scatt  
plus wk / next  
choosing solution forms

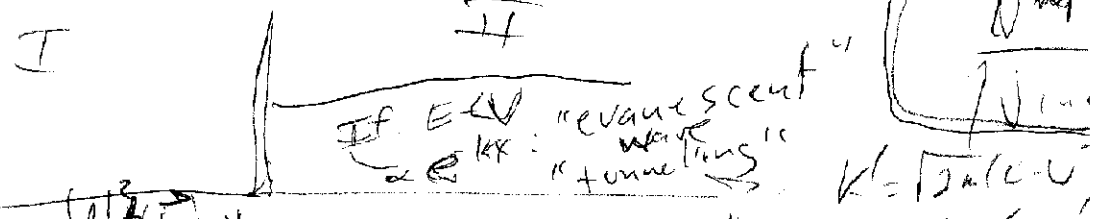
2) Choose Unbound Solutions  
- "Normalize"  $\vec{j} = \frac{N_{part}}{S_{area}}$  not  $\psi$

3) Choose  $\psi_{inc}$  components based on  $\vec{j}_i$   
- "From left"  $\vec{j}_{inc} \rightarrow$   
- @  $x = +\infty \Rightarrow \vec{j}_{trans} \rightarrow$  only!

4) Enforce continuity etc  
as usual  $\Rightarrow$  solve for Tcoeff & Rcoeff  
"fraction of flux"  $\Rightarrow$

## Example 2)

$V(x) = V_0 \delta(x) + G \delta(x)$



$k = \frac{\sqrt{2mE}}{\hbar}$

$\psi_I = A e^{+ikx} + B e^{-ikx}$

$\psi_{II} = C e^{+ikx} + D e^{-ikx}$   
scattering

note  
common convention:  
 $A \rightarrow I$

$B \rightarrow R$   
(Because Tcoeff  $\propto \frac{|C|^2}{|A|^2}$ )

$C = T$   
Note  $T \neq$  Tcoeff  
"R" =  $R \neq$  Rcoeff

No  $\delta$ -fn liboff

same  $\psi_I(0) = \psi_{II}(0)$   
w/  $\delta$ -fn  $\psi_I'(0) = \psi_{II}'(0)$

$A + D = C$   
 $1 + R = T$

$\Downarrow$   
for  $\delta$ -fn  
instead Integrate TISE

$\delta$ -fn Integrate TISE  $\int \psi^* \psi dx$

$\frac{\hbar^2}{2m} (\psi|_{x=0} - d\psi|_{x=0}) + \int_{-\epsilon}^{\epsilon} V_0 \delta(x) \psi dx + \int_{-\epsilon}^{\epsilon} G \delta(x) \psi dx = \int_{-\epsilon}^{\epsilon} E \psi dx$   
 $\frac{\hbar^2}{2m} (C i k - ik(1 + R)) - G \psi(0) = 0$   
 $\frac{\hbar^2}{2m} (k(1 - R) - k' - G \psi) = 0$

Get Result

$$T_{\text{coeff}} = \left| \frac{1}{\tau} \right|^2 \frac{k'}{k}$$

$$= \frac{2 \left| \left( \frac{i\hbar^2}{2m} \right) \right|^2}{\left| \frac{i\hbar^2}{2m} k - k - G \right|^2} \left( \frac{k'}{k} \right)$$

D)

WKB Approx.

Phase Function  $S(x)$ Remember  $x + iy \Rightarrow r e^{i\theta}$   
 $\psi(x)$  is complex.

$$r = \sqrt{x^2 + y^2}$$

$$\theta = ?$$

$$\text{Rewrite } \psi = \frac{\psi(x)}{\sqrt{\psi(x)}} e^{+i \frac{S(x)}{\hbar}} = \sqrt{\rho} e^{+i \frac{S(x)}{\hbar}}$$

Real Fun

 $S(x)$  : Phase FunctionQM Insight: Study Properties of  $S(x)$ 

$$\text{consider } \vec{j} = \frac{\hbar}{m} \text{Im} \{ \psi^* \nabla \psi \}$$

$$= \frac{\hbar}{m} \text{Im} \left\{ \left( \sqrt{\rho} e^{-i \frac{S}{\hbar}} \right) \left( \sqrt{\rho} e^{+i \frac{S}{\hbar}} + i \sqrt{\rho} e^{+i \frac{S}{\hbar}} \right) \right\}$$

$$= \frac{\hbar}{m} \text{Im} \left\{ \rho \left( \frac{1}{\hbar} + i \frac{\rho \nabla S}{\hbar} \right) \right\} = \frac{\rho \nabla S}{m}$$

Stronger  $\nabla S \rightarrow$  Stronger  $\vec{j}$

In fluid mech  $\vec{j} = \rho \vec{v}$

$$\text{so } \vec{v} = \frac{\nabla S}{m}$$

~~Plane~~ Plane wave:  $\vec{k} \cdot \vec{x} = \omega t$

$$S = \vec{p} \cdot \vec{x}$$

$$\nabla S = \frac{\vec{p}}{m} = \vec{v}$$

Derivation of Hamilton-Jacobi  
see Prakash notes

Expect you to be able to do  
Another Connection to classical mech  
but not important for final

WKB Approx:

Solutions to ANY 1-D  $V(x)$

Derivation: Sak - tomorrow details

## Lecture 3/5/2010

The WKB approximation finds a set of approximate solutions to ANY potential problem based on the above starting point, proportional to  $1/\sqrt{k(x)} \exp(\pm i \int k(x) dx)$  where  $k(x) = \sqrt{2m(E-V(x))}/\hbar$

Two methods of deriving: Note we will not derive in detail: NO ONE EVER REMEMBERS THIS

in particular the “connection process” is always cloudy: so ignore if so! It’s OK if you can’t derive why—people just use the formulas:

### Main Points I expect you to learn / remember

-1) Using the WKB approx: (most important)

how to construct WKB Wave Fn.

how to use formulas

above for both Bound State and Scattering problems.

2) When the WKB Wave Fn should be accurate (almost as important)

condition for applicability

3) How the matching procedure works (less important)

What it means to match. e.g. What is matched?

What function for what region : why Airy Functions ( $\equiv$  Bessel Functions order 1/3) ?

How matching affects “Main” WKB Wave Functions?

How this leads to E formula for Bound States.

4) Details of Derivation? (Not very important)

You don’t need to be able to reproduce derivation

---

**Main Points of WKB Approx:**

**1) Wave Fn's themselves:** For any shape of potential, (scattering / or bound state situation) above form approximates the wave function.

Like plane wave solution If  $E > V$

Constant Potential Solution:  $\sim A \exp i(\pm kx) \quad \hbar^2 k^2 / 2m = E - V$

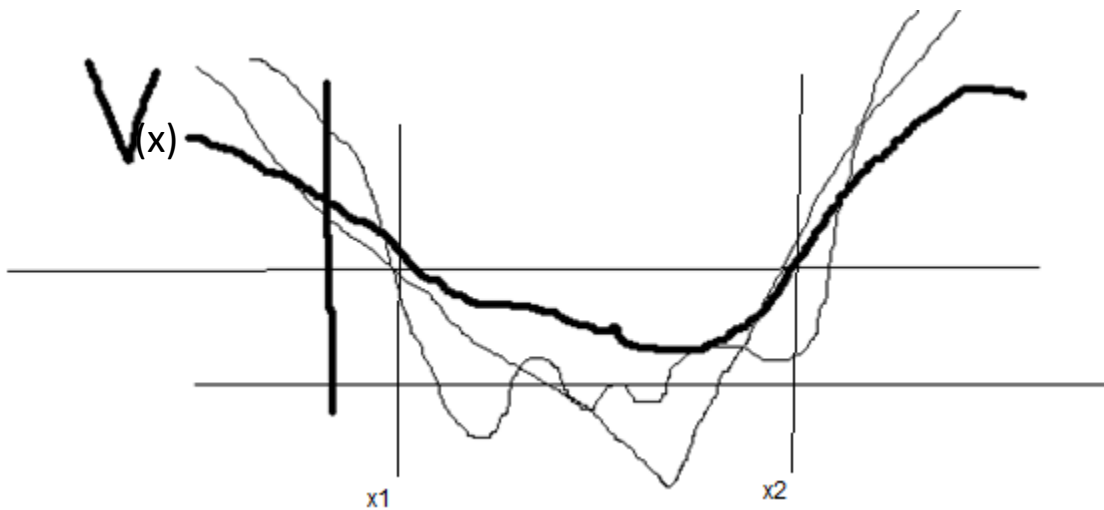
$\rightarrow$  WKB:  $1/\sqrt{k(x)} \exp \pm i \int k(x) dx \quad k = \sqrt{2m(E - V(x))}/\hbar$

And if  $V < E$

Constant Potential Solution:  $\sim A \exp i(\pm kx) \quad \hbar^2 \kappa^2 / 2m = V - E \rightarrow 1/\sqrt{\kappa(x)} \exp \pm \int \kappa(x) dx \quad \kappa = \sqrt{2m(V(x) - E)}/\hbar$

Just like for plane wave solutions... except for the factor of  $1/\sqrt{k}$

**2) Arbitrary Bound State Potential Problems:** Most importantly, for any problem like this:

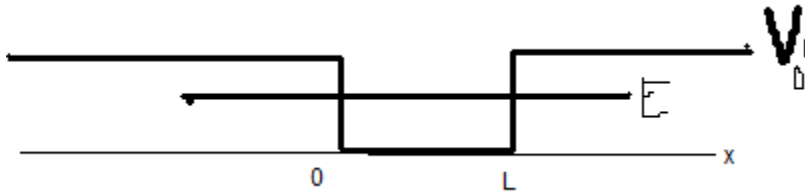


It yields a formula for the discreteness of the energy spectrum of bound states:

$$\int_{x_1}^{x_2} \sqrt{2m(E - V)} dx = (n + \frac{1}{2}) \pi \hbar$$

$x_1$  and  $x_2$  are called the “turning points” ‘

Examples: See Liboff



Finite potential well -- remember how ugly finding the energy spectrum looked? Transcendental equations to find the energy spectrum.

Now it's really easy:

For WKB  $x_1 = 0$ ,  $x_2 = L$  (turning points),  $V(x) = 0!$  (between the turning points)

$$\text{Now } \int_0^L \sqrt{2m(E - V(x))} dx = \int_0^L \sqrt{2mE} dx = \sqrt{2mE}L$$

This is the left hand side of the prescription:

$$\int_{x_1}^{x_2} \sqrt{2m(E - V)} dx = (n + \frac{1}{2})\pi \hbar$$

To get the energies just set this equal to  $(n+1/2)\pi\hbar$  and solve for E

$$E = (n+1/2)^2 \pi^2 \hbar^2 / 2mL^2$$

Particle in a box the same!!!

Book gives another example.

$$V(x) = mg|x| \quad \sqrt{2m(E - mgx)} \text{ Easy integral!!!! } (\sim u^{1/2} du)$$

Performance of the calculation is shown in Sakurai for the odd solutions. Great—even for lowest energy values...

We shall see that it's performance for low values of the energy in these cases is seemingly a lucky accident, however usually works! Always yields accuracy for higher values of n.



SHO:  $V(x) = 1/2\omega^2x^2$

$\int \sqrt{2m(E - m\omega^2x^2)} = a \int \sqrt{1 - x^2/a^2}$

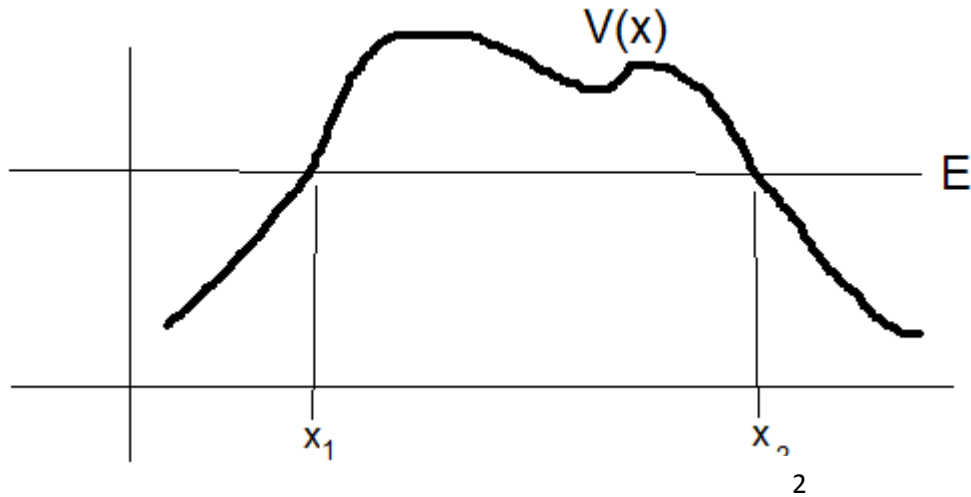
$a = \sqrt{2mE}$

introduce variable  $u \rightarrow \cos u = x/a$

Exact result!

$E_{wkb} = \hbar \omega (n+1/2) = E_{SHO \text{ exact}}$

**3) Arbitrary Scattering barriers**—of the type:



For such problems, use scattering set –up :: Solutions:

For  $x < x_1$  :  $1/\sqrt{k(x)} \exp(i\int k(x) dx) + R/\sqrt{k(x)} \exp(-i\int k(x) dx)$

For  $x > x_2$  :  $T/\sqrt{k(x)} \exp(i\int k(x) dx)$  (don't allow leftward moving solution in this region)

Then, probability to tunnel through such barrier from left: assuming T is amplitude of the transmission wave function coefficient to the right, WKB leads to another universal formula (independent of actual form of V(x))

$$T_{\text{coeff}} = \exp -2 \int_{x_1}^{x_2} \kappa(x) dx$$

where  $\kappa(x) = 1/\hbar \sqrt{V(x) - E}$ . Again, exact same type of integral, different use...this is the probability for the wave function to tunnel through the barrier.

One of the most important applications: nuclear decay – see Liboff (we will do a problem with this on last pset).

-----

---

**Method 1)** In Sakurai : Ignore terms in the differential equation of order  $\hbar$  and higher.

Then assume

1) separable solution.  $\Psi = f(x)g(t) = e^{i(St)} = v\rho(x) e^{iW(x)} e^{iEt}$

2) Borrow from constant potential solutions  $\exp(ikx)$   $k^2 = 2m(E-V_0)/\hbar$

$$W(x) = k(x)/\hbar = \int \sqrt{2mE-V(x)} / \hbar$$

(book: above 2 steps: Guess these because of H-J-E method: but who remembers that!)

Details: because of continuity equation there must be  $1/\sqrt{k}$  factor

$$\psi \sim 1/\sqrt{k} \exp(\pm i \int \sqrt{2mE-V(x)} / \hbar)$$

**Method 2)** More common derivation Again assume separable solutions of form

First we assume the basic form  $\psi = A \exp(iS(x)/\hbar)$

$$-i\hbar \frac{d^2 S}{dx^2} + \left(\frac{dS}{dx}\right)^2 = 4m^2 \sqrt{E - V(x)} \quad (0.1)$$

The crux is to expand the solution around  $\hbar$  itself.

[Taylor series expansion:  $f(x-x_0) = f(x_0) + (x-x_0)f'(x_0) + (x-x_0)^2/2 (f''(x_0)) + \dots$  ]

$$S = S_0(x) + \hbar S_1(x) + \hbar^2/2 S_2(x) + \dots$$

Simple substitution of expansion into (0.1) and grouping all terms to the LHS we get an equation

$$F_0 + \hbar F_1(x) + \hbar^2 F_2(x) \dots = 0$$

where  $F_0 = (dS_0/dx)^2 - 4m^2 (E-V(x)) = 0$  for example.

The key is that every term in this series must vanish independently. Thus we can set each term = 0;

$$F_0 = 0 \rightarrow dS_0/dx = k(x) \quad (w/ k(x) \text{ given above.})$$

If we collect the terms propto  $\hbar$ , examining the next equation  $F_1(x) = 0$ , we find we get a solution for  $S_1(x) \propto \ln(1/\sqrt{k(x)})$  which means our total solution ignoring all higher terms will have also a  $1/\sqrt{k(x)}$  factor.

-----  
This gives better motivation for trying the solutions of this type.

Lot's of equations:

Very Easy to get lost in all the math – lose sight of the usefulness of the WKB

because it's easy to lose sight of the main result e.g. which equation is the useful one

**Strategy:**

Point out main result: **forget about derivation!** Then we can go back and point out in a very high level discuss where the derivation comes from:

**Details:**

-----

**1) Review: where does the wave fn come from?**

$1/2m (dS/dx)^2 + V = dS/dt \rightarrow$  assumed form  $S(x,t) = W(x) - Et$  ( $\rightarrow$  from separable  $\Psi$  assumption)

$$1/2m(dS/dx)^2 + V(x) = E \rightarrow dS/dx = \sqrt{2m(E - V(x))} : S(x_{(only)}) \equiv W(x) = \hbar \int^x k(x) dx$$

(Sakurai's  $W(x)$  is just my  $\int k(x) dx * \hbar$ )

**2) Where does the  $1/vk$  come from?**

This comes 1 of 2 sources: -- see above "more common derivation": look at the next higher order term (in  $\hbar$ ) in the equation, those proportional to  $\hbar$  (now careful also to expand our exponential solution  $\exp(iS(x)/\hbar$  in terms of  $\hbar$  as well) we find a second order term needed for  $S(x) = \ln(1/v(k))$  which when exponentiated yields the  $1/v(k)$ .

Sakurai also derives it from the continuity equation, defining the **first requirement** to use: we want a **stationary state** solution --- means time evolution has "settled down" and we will only treat time independent potentials  $V(x) \neq V(x,t)$

Since this is the case  $d\rho/dt = 0$ , and thus from the continuity eq:

$$d\rho/dt + \nabla \cdot \mathbf{j} = 0 \rightarrow \nabla \cdot (\rho \nabla S/m) = 0 \rightarrow 1-D \rightarrow d(\rho dS/dx)/dx = 0$$

thus

$$\rho dS/dx = \text{constant}$$

$$\text{if } S(x) = \hbar \int k(x) dx \text{ then } dS/dx = \hbar k(x) \rightarrow \rho \hbar k(x) = \text{constant}$$

so

$$\rho \propto \text{const}/k(x) \rightarrow \psi = \sqrt{\rho} e^{iS(x,t)/\hbar} \rightarrow \psi \propto 1/\sqrt{k}$$

### 3) Validity:

We ignored terms of  $\hbar$  and higher to get the above Hamilton-Jacobi version of the Shro equation:  
Actually we ignored the term

$$\propto \hbar \nabla^2 S \ll |\nabla S|^2$$

this is what allowed us to derive the solution in the first case. Under our solution choice this equates to

$$\text{or } \hbar d^2W/dx^2 \ll (dW/dx)^2 \rightarrow d^2k(x)/dx^2 \ll (dk(x)/dx)^2$$

So what this translates to, given the following derivatives:

$$dS/dx = k(x) / \hbar$$

$$d^2S/dx^2 = dk(x)/dx = \sqrt{2m} d(\sqrt{E-V(x)})/dx = 1/\hbar \cdot \frac{1}{2} \frac{1}{\sqrt{E-V(x)}} dV/dx$$

is the following:

$$\begin{aligned} & |\partial_x^2 S| \ll (\partial_x S)^2 \\ & \Rightarrow \frac{dV}{dx} \frac{\hbar}{\sqrt{2m(E-V)}} \ll |E-V| \end{aligned}$$

What does this condition mean physically?

Remember de Broglie relation:  $\lambda = h/p \rightarrow \lambda/2\pi = \hbar/p =$

Regroup

$$dV/dx * \text{wavelength} = \Delta V_{\text{over 1 wave}} = \Delta (E-V)_{\text{over 1 wave}} \ll |E-V| \text{ value of function } E-V(x)$$

$$\text{or } \Delta (E-V) / (E-V) \ll 1 \text{ (small number)}$$

So it just says what one might have guessed: we want the relative change of the function  $E-V(x)$  to be small over 1 wavelength. This implies a slowly varying  $V(x)$  in order for this approximation to work. Slowly varying with respect to the wavelength of the wave function—that is over one wavelength, the relative change in the potential (actually the difference function  $E-V(x)$ ) should be small.

Note: breaks down at turning points!!

And it's not just the validity statement that breaks down: you can see that the wave function also becomes infinite... (except maybe for  $\sin()$  linear combination).

Solution?...this is where the matching procedure comes in.

**Matching procedure:**

Make linear approximation to potential in turning point region. Then differential equation (Shro  $\rightarrow$  H-J-E) becomes exactly solvable. Solutions are Airy Functions ( $Ai(x)$ )

These are explained in a page from Liboff. Key points:  $Ai(\text{turning point}) \neq 0$  !!!!

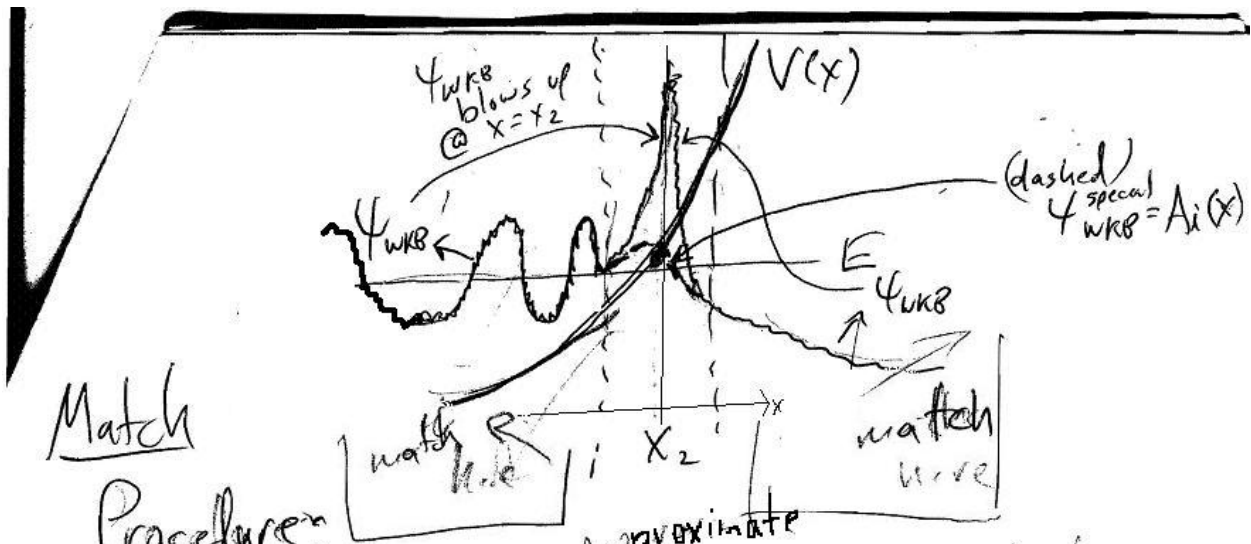
See scanned notes below:

Just explain graphically

See Liboff Section on Airy fn's.

Method: see drawing.

tips 1) memorize picture qualitatively....



Match

Procedure:

1) Find Another  $\Lambda$  function for bad region. This is achieved by

Steps 1 + 2 in Sec 2.4.40

Note  
no one really  
does this  
themselves

- 1) Make linear approx of  $V$
- 2) Solution is a known ("horrible" fn: an Airy function  $Ai(x)$ )

see Liboff

2) Match: the three solutions not @  $x_2$  (so not like continuity matching) but rather at  $x \gg x_2$  &  $x \ll x_2$

**Points:**

1) Asymptotic behavior of the Airy function explains for the  $\cos(\pi/4)$  the  $\pi/4$  and the two and the  $A = B$

**This type of matching is what is meant by the “ $\rightarrow$ ” ‘s in Sak. (eq.2.4.41-42).** Different than 1-D exact solution matching between regions (continuity, etc...)

Seemingly **amazing agreement (?)** in form of special functions to WKB forms. --- has roots in doing the problem as a complex integral –no reference to Airy functions necessary. (footnote in Sak).

**Review :** Matching procedure: finding yet another approximate form for the wave fn in the turning point vicinity (approximation to the approximation!) Points about these airy fn solutions:

1) one could use it as the wave fn instead of the WKB forms in this region (but our main uses haven't really involved using the wave fn's themselves.)

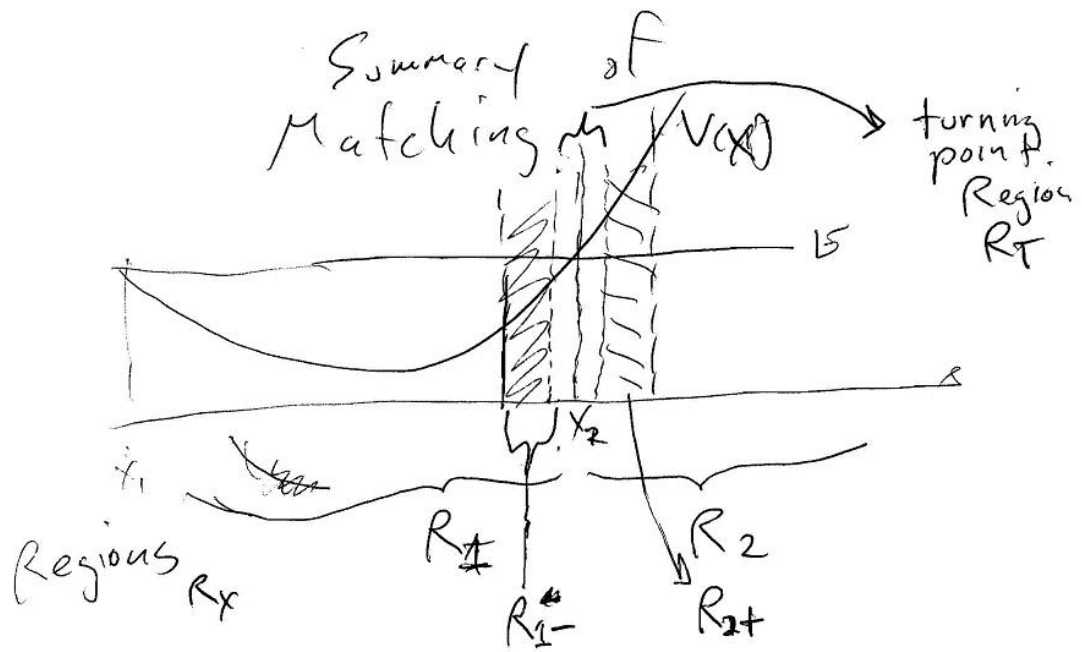
2) Q: why not use it everywhere instead of the WKB solutions? : because linear approx doesn't hold every where. See plot in Liboff—very far away from turning point, phase of oscillation messed up for the Special Airy Function solution.

3) Primary use is just using it's asymptotic behavior to constrain the relations between the WKB solution amplitudes, phase factor. (the match)

Turning points also imply constraints on validity of (when to trust) the wave fn's themselves: you want to have many wavelengths away from the turning points ideally to trust it.

Note in below scans, I reverted to not including the  $\hbar$  in the definition of  $k(x) \rightarrow$  so  $k(x) = \sqrt{2m(E-V(x))}$  in below





For  $R_1$  our solutions are  $\psi_{WKB}$

$$= \frac{A e^{\frac{i}{\hbar} \int k(x) dx}}{\sqrt{k(x)}} + \frac{B e^{-\frac{i}{\hbar} \int k(x) dx}}{\sqrt{k(x)}} \rightarrow (G)$$

$$= \frac{C \sin\left(\frac{1}{\hbar} \int k(x) dx\right)}{\sqrt{k(x)}} + \frac{D \cos\left(\frac{1}{\hbar} \int k(x) dx\right)}{\sqrt{k(x)}} = \frac{G \cos\left(\int k(x) dx + \delta\right)}{\sqrt{k(x)}}$$

For  $R_T$ : Solution is  $\psi_{WKB}^{special} = A_i(y)$

For  $R_{1-}$

$A_i(y) \Rightarrow y \neq 0$  :

$$\frac{2}{\sqrt{E - (E - E_2(x - x_2))}} \cos\left(\frac{1}{\hbar} \int \sqrt{E - (E - E_2(x - x_2))} dx + \frac{\pi}{4}\right)$$

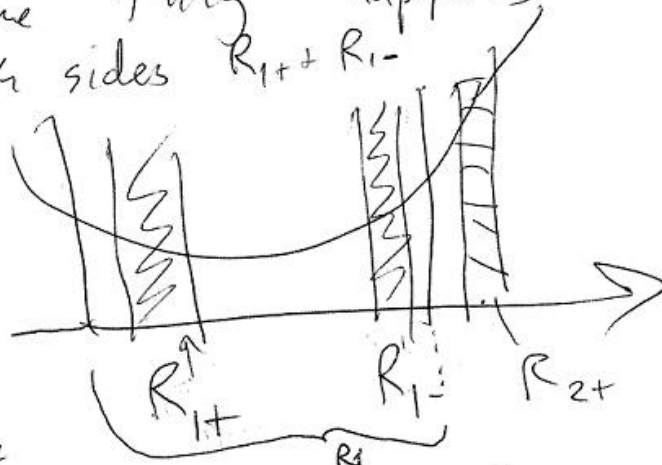
$\psi_{WKB}$  :

$$\frac{G}{\sqrt{E - V(x)}} \cos\left(\frac{1}{\hbar} \int \sqrt{E - V(x)} dx + \delta\right)$$

match parameters:  $G \rightarrow 2$      $\delta \rightarrow \frac{\pi}{4}$

This is what it means to match  $[V(x) \approx E - E_2(x - x_2)]$

Same thing happens  
on both sides  $R_{1+}$  &  $R_{1-}$



except at  $R_{1+}$

$$R_{1+} : \psi_{wkB} = \frac{2}{\sqrt{k(x)}} \cos\left(\frac{1}{\hbar} \int k(x) dx - \frac{\pi}{4}\right)$$

+ remember

$$R_{1-} : \psi_{wkB} = \frac{2}{\sqrt{k(x)}} \cos\left(\frac{1}{\hbar} \int k(x) dx + \frac{\pi}{4}\right)$$

Formula comes from

$\psi_{wkB} = \psi_{wkB}$  requirements can be met

$$\frac{1}{\hbar} \int_{x_1}^{x_2} k(x) dx = (n + \frac{1}{2})\pi$$

$$\cos x = \sin(x + \frac{\pi}{2})$$

Propagator

Definition  $K(x'|t', x|t) = \langle x'|t' | x|t \rangle$   $t' > 0$   
 $= 0, t' < 0$   $\swarrow \nearrow$   
 base states, depend on time in Heisenberg picture

$K(x'|t, x|t)$  is the transition amplitude to go from  $x|t$  to  $x'|t'$

Interpretation

$$\langle x'|t' | \alpha \rangle = \int d^3x \langle x'|t' | x|t \rangle \langle x|t | \alpha \rangle$$

$\uparrow$  completeness at time  $t$

$$\Rightarrow \psi_\alpha(x', t') = \int d^3x K(x'|t', x|t) \psi_\alpha(x, t)$$

$\uparrow$  kernel

$K$  propagate the wave function in space time

$K$  depends on the Hamiltonian (or alternatively we will see, the Lagrangian) really means it depends on  $V(x)$

As with WKB concentrate on the following aspect  $\rightarrow$  it's use!!!!

Go directly to a result which we can derive later:

For  $V(x) = 0$ , the free particle propagator  $K_{free}$  has the following nasty form:

$$K(x'|t', x|t) = \frac{1}{(2\pi i \hbar)^3} \left( \frac{\pi 2m \hbar}{i(t'-t)} \right)^{3/2} e^{i \frac{(x'-x)^2 m}{2(t'-t) \hbar}}$$

This is derived in Sak.

So let's look at Sak. Problem 2.23

$V(x) = \lambda \delta(x)$  suddenly turned off.  $\rightarrow \lambda = 0 @ t = 0 \rightarrow$  find wave function for  $t > 0$ .

Free particle after  $t = 0$  so can use  $K_{free}$  given above.

From last week we know what  $t=0$  wave function looks like: ( $\delta(x)$ ) solution:  $\sim Ae^{-k'x}$  ( $k' \sim \sqrt{2m E}/\hbar$  for  $x > 0$ ;  $Ae^{k'x}$  for  $x < 0$ .)

So to get the wave function for  $t > 0$  (and let's restrict ourselves to the contribution from  $x > 0$ )

$$\begin{aligned}\psi(x, t) &= \int_{-\infty}^{\infty} dx' \psi(x', t=0) K_{free}(x, t, x', 0) \\ &= \int_0^{\infty} dx' Ae^{-k'x'} K_{free}(x, t, x', 0) + \int_{-\infty}^0 dx' Ae^{k'x'} K_{free}(x, t, x', 0) \\ &= 2 \int_0^{\infty} dx' Ae^{-k'x'} K_{free}(x, t, x', 0)\end{aligned}$$

Insert into our nasty form we get -  $\psi(x, t) =$

$$\int \frac{1}{(2\pi\hbar)^3} \left( \frac{\pi 2m\hbar}{i(t-t')} \right)^{3/2} e^{i \left( \frac{x(x-x')^2 m}{2(t-t')\hbar} - k'x' \right)} dx$$

(note now I've reversed  $x, x' \rightarrow$  replace every  $x$  with  $x'$  and vice versa (we are integrating over  $x'$ ))

OK we got back a nasty integral. It is probably doable by "completing the square" (see later when we actually derive nasty propagator form). When I was in grad school, no one I knew was successful in doing it (or motivated to anyway), and in the problem it says: "you need not evaluate the integral that comes up": so no one did. **Point:** Even Sakurai implies: this propagator method may not be a particularly nice way of handling things analytically, but still it is functional/usable. I may not be able to do this integral analytically, but numerically it would be quite straightforward to evaluate. (just separate real and imaginary parts).

I would always need to go look up propagator for free particle from Sak. though.

### Properties of Propagator K:

$$\begin{aligned}a) \quad K(x', t', x, t) &= \langle x' | U | x \rangle = \delta^3(x' - x) \\ b) \quad K(x', t', x, t) &= 0 \text{ for } t' < 0 \\ &\text{Causality; only propagation} \\ &\text{forward in time}\end{aligned}$$

Implies often unstated  $\theta(t-t')$  function. (Unstated in Sakurai)  $K \rightarrow K \times \theta(t-t')$

Remember  $\theta(t) = \int_{-\infty}^t \delta(x) dx$

We discussed it before when we said  $\delta(x) = d\theta(x)/dx$

### c) Representation in terms of energy eigenstates.

$$|\alpha, t\rangle = U(t) |\alpha, t=0\rangle$$

$$|\alpha, t\rangle = \sum_{a'} |a'\rangle \langle a' | \alpha \rangle \exp(iE_{a'}(t-t_0)/\hbar)$$

bra-ing both sides w/  $\langle x'' |$

$$\langle x'' | \alpha, t \rangle = \sum_{a'} \langle x'' | a' \rangle \langle a' | \alpha \rangle \exp(iE_{a'}(t-t_0)/\hbar)$$

insert  $\int |x'\rangle \langle x' |$  here

we get

$$\langle x'' | \alpha, t \rangle = \int dx \sum_{a'} \langle x'' | a' \rangle \langle a' | x' \rangle \langle x' | \alpha \rangle \exp(iE_{a'}(t-t_0)/\hbar)$$

$$= \int dx \sum_{a'} \langle x'' | a' \rangle \langle a' | x' \rangle \exp(iE_{a'}(t-t_0)/\hbar) \langle x' | \alpha \rangle$$

$$\psi(x'', t) = \int dx \underbrace{\sum_{a'} \langle x'' | a' \rangle \langle a' | x' \rangle \exp(iE_{a'}(t-t_0)/\hbar)}_{\equiv K(x'', t, x', t_0)} \psi(x', t_0)$$

$$= \text{Sak 2.5.8} = \sum_{a'} \langle x'' | a' \rangle \langle a' | x' \rangle \exp(iE_{a'}(t-t_0)/\hbar) \text{ slightly different way}$$

-----

example:

Propagator for a free system

$$H = \frac{p^2}{2m}$$

$$H|p\rangle = \frac{p^2}{2m}|p\rangle$$

$$\Rightarrow K(x', t'; x, t) = \int d^3p \langle x'|p\rangle \langle p|x\rangle e^{-i\frac{p^2}{2m}(t-t')} \theta(t-t')$$

$$= \int \frac{d^3p}{(2\pi\hbar)^3} e^{-i\frac{(t-t'-i\epsilon)}{2m\hbar} \left( p - \frac{m(x-x')}{t-t-i\epsilon} \right)^2} \theta(t-t')$$

$\downarrow$   $\frac{e^{i\pi x^2}}{\sqrt{2\pi\hbar}}$        $\uparrow$   $\frac{e^{-i\pi x^2}}{\sqrt{2\pi\hbar}}$   
 $\downarrow$   $\frac{e^{i\pi x^2}}{\sqrt{2\pi\hbar}}$        $\uparrow$   $\frac{e^{-i\pi x^2}}{\sqrt{2\pi\hbar}}$

put  $i\epsilon$  to make the integral convergent

shift integration variable  $p' = p - \frac{m(x-x')}{t-t-i\epsilon}$

Fourier Trans (gaus) = gaus—easy way to remember

$$K(x', t'; x, t) = \frac{1}{(2\pi\hbar)^3} \left( \frac{\pi m \hbar}{i(t-t-i\epsilon)} \right)^{3/2} e^{i\frac{m(x-x')^2}{2(t-t-i\epsilon)\hbar}} \theta(t-t')$$

**Exercise Finish Integral yourself.** Putting the  $i\epsilon$  in probably means evaluating it with a complex contour integration.

**d) Green's Fn:**

Note that we can write our relation from d) Sak 2.5.58

$$\sum_{a'} \langle x'' | a' \rangle \langle a' | x' \rangle \exp(iE_{a'}(t-t_0)/\hbar)$$

$$K(x'', t; x', t_0) = \sum_{\alpha} \psi_{\alpha}^*(x'', t) \psi_{\alpha}(x', t_0) e^{i\frac{E_{\alpha}}{\hbar}(t-t_0)}$$

$$= \sum_{\alpha} \psi^{\alpha}(x'', t) \psi_{\alpha}(x', t_0)$$

( $\alpha \rightarrow a, t' \rightarrow t_0$ )

Example where should put  $\theta$  fn in: really should be

$$= \underbrace{\sum_{\alpha} \psi^{\alpha}(x'', t) \psi_{\alpha}(x', t_0)}_{\text{call } K^*} \theta(t-t_0)$$

( $\alpha \rightarrow a, t' \rightarrow t_0$ )

call  $K^*$

Now consider the time derivative times-  $i\hbar$  (= the RHS of Time Dep Shro. Eq)

$$= -i\hbar \frac{d}{dt}(K)\theta(t-t_0) + i\hbar K \delta(t-t_0)$$

but from property a)  $K(x, t, x', t) = \delta(x-x')$  so second term becomes  $i\hbar \delta(x-x')\delta(t-t')$

This explains the appearance of the extra delta functions in eq. 2.5.12

$$(H - \hbar i \partial_t) K(x', t', x, t) = -\hbar i \delta(t'-t) \delta^3(x'-x)$$

which you guys know from your **Classical Electro Dynamics course: defines K as the Green's fn.** (e.g. plug this into Green's Theorem). This was already apparent from its use. Now we've defined it formally.

e) **Relation to Partition Function (not covered in lecture, so optional)**

$$G(t) = \int d^3x K(x, t, x_0) = \sum_{\alpha} e^{-iE_{\alpha} t / \hbar}$$

$$\begin{aligned} \text{Partition function } Z &= \sum_{\alpha} e^{-\beta E_{\alpha}} \\ &= \int d^3x K(x, \frac{\beta \hbar}{i}, x_0) \end{aligned}$$

Partition function is the trace of the propagator in imaginary time

Thus techniques for evaluating propagators in QM can be applicable to Statistical Mechanical calculations. I've seen this done in "Lattice QCD" calculations for Heavy Ion Physics. Remember  $\beta = 1/kT$  so  $t \propto 1/T$  is something one must remember when looking at results of these calculations.

This is easily seen as shown in Sakurai:

The key was that once we pull out a factor of  $\exp(-iEt)$  we have separated out all the time dependence of a heisenberge basis state:  $|x, t\rangle = |x\rangle \exp iEt$ .

Thus our expression for the propagator expressed as a sum over energy states,

$$K(x'', t', x', 0) = \sum_{\alpha} \langle x'' | \alpha \rangle \langle \alpha | x' \rangle \exp(-i(E_{\alpha} - E_0)t'/\hbar)$$

if integrated over  $x'$  and with values forced to satisfy  $x''=x'$  then

$$K(x, t=i\beta, x, 0)$$

Then we can easily write partition function version of the propagator

$$K(x, t = i\hbar/\beta, x, 0)$$

$$= \sum_a \langle a | \left( \int dx |x\rangle\langle x| \right) |a\rangle \exp(E\beta)$$

with middle completeness relation removed:

$$= \sum_a \langle a | a \rangle \exp(\beta E) \rightarrow \text{ortho normality: } \langle a | a \rangle = 1$$

$$= \sum_a \exp(\beta E) = \text{partition function}$$

### f) Composition

(starting definition of propagator  $\langle x, t | x', t' \rangle$ )

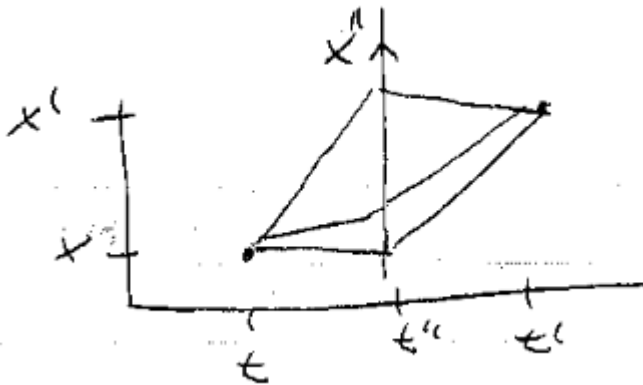
$$\begin{aligned} \langle x', t' | x, t \rangle &= \int d^3x'' \langle x', t' | x'', t'' \rangle \\ &\quad \langle x'', t'' | x, t \rangle \\ &= \int d^3x'' K(x', t'; x'', t'') K(x'', t''; x, t) \end{aligned}$$



## Lecture 3/9/2010

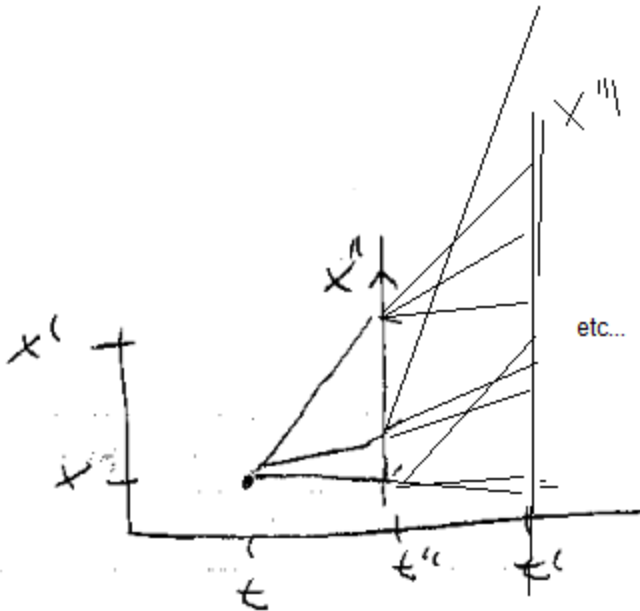
### I) Feynman Path Integral

This is another “formulation” of Quantum Mechanics based on this last idea of composition. Suppose we visualize the composition form of the propagator  $K$  given on the previous page as an integral over “paths” in “label space” – an  $x,t$  plane. Going from the point  $(x=x, t=t)$  to the final point  $(x=x', t=t')$ . Since we are integrating over all values of  $x''$  at  $t=t''$  we can think of this as the sum over a bunch of different paths as drawn. Note that here the lines themselves are artificial what we are really talking about is 3 points for each “path” with the 2 points on the end fixed, and the middle point varying.

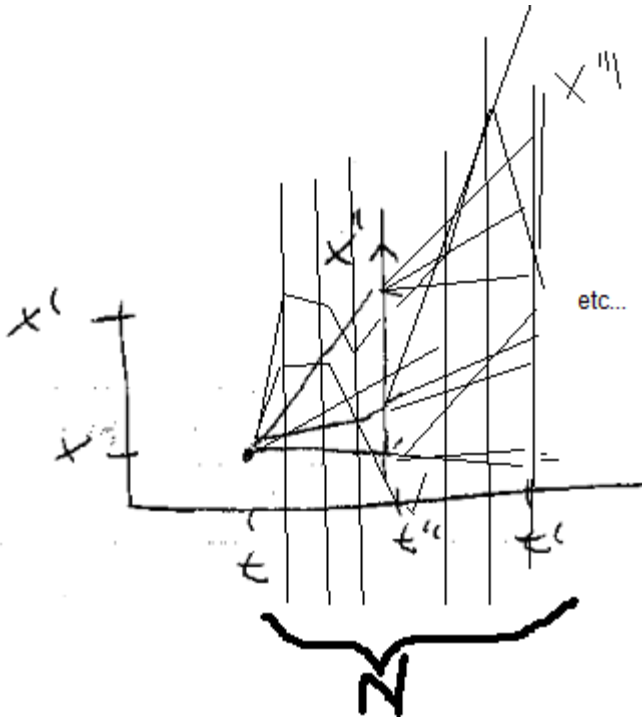


So = for  $K(x',t'; x,t)$  we can actually break up evolution / propagation in arbitrary number of steps.

Do last suggestion: Applying composition property arbitrary number of times: As we increase the number of intermediate steps, we start tracing out more and more possible paths between  $x,t$  and  $x',t'$ .



If we do it formally N times



Eventually If we take the limit of  $N \rightarrow \infty$  and each time interval infinitesimally small:  $(t_n - t_{n-1})/N \rightarrow 0$ . then each set of the actual lines that connect  $x, t$ , to  $x', t'$  become more and more “real” (include more and more points) such that at  $N = \infty$  we really are talking about all arbitrary paths (in the sense of a line integral) between  $x, t$  and  $x', t'$  that lie on the infinite swath of the  $x, t$  plane between  $t$  and  $t'$ .

Therefore in this case it should be clear that this represents:

### Sum Over All Paths

So instead of a single integration **always think of Quantum Propagation as Sum Over All Paths, which** In Quant Mech called “**path integral**”. (not the same as typical path/line integral, because it’s all paths).

**This expression for K would look like**

$$\lim N \rightarrow \infty ( K_{1-N} = \int dx_1 K_1, \int dx_2 K_2 \dots \int dx_N K_N )$$

Note that for each path we are still integrating over a propagator each integration:

$$K_n \equiv K(x_n, t_n, x_{n-1}, t_{n-1}) = \langle x_n, t_n | t_n, t_{n-1} \rangle$$

This is an infinitesimal propagator  $\langle x, t | x+dx, t+dt \rangle$

**Feynman Path Integral Method of Propagation:** Simply says that it turns out that the infinitesimal propagator is given by

$\exp(iS)/\hbar$  where now  $S$  is the classical action

$$\int_t^{t_1} dt L(t) = S \text{ is the action of a path}$$

where

a)  $L$  is the Lagrangian =  $T - V$ : different from the Hamiltonian  $H$  in two ways 1) the  $-$  sign in front of  $V$  and 2) because  $T = p^2/2m$ ,  $V(x)$  are now classical quantities, NOT functions of the operators  $p$  and  $x$ .

In fact this result can be derived from what we said so far: see this derivation on the next page (taken from Verbaarschot)

b) this integral IMPLIES A PATH taken through  $x-t$  space, though not explicit in notation. In classical mechanics there is only 1 path, (the one for which  $\delta S = 0$ ) so no need to make it explicit  
Review classical action integrals: See Sakurai p116-117 for example. In our case we must consider all paths.

The point is that we can use this form of the propagator to derive the time evolution of the wave function  $\psi(x,t)$  at any arbitrary point  $x$  given an initial starting wave function  $\psi(x_0, t_0)$  through the "propagation of source" integral defined before for the propagator, and this computationally can be done by integrating over all paths in  $x, t$  space through the Feynman Path Integral

(71)

Such integral is called a path integral

Can we calculate the propagator for  $t' \rightarrow t$

$$\begin{aligned}
K(x't', x, t) &= \langle x't' | x, t \rangle \\
&= \langle x't' | e^{-iH(t'-t)/\hbar} | x, t \rangle \\
&= \langle x't' | e^{-\frac{i(t'-t)}{\hbar} \left( \frac{p^2}{2m} + V \right)} | x, t \rangle
\end{aligned}$$

$$BC4 \quad e^{A+B} = e^{A+B - \frac{1}{2}[A, B]}$$

$$\begin{aligned}
A \psi(t-t) & \\
B \psi(t-t) & \Rightarrow [A, B] \sim \mathcal{O}((t-t)^2) \\
& \Rightarrow \text{we can neglect the}
\end{aligned}$$

commutator in the limit  $t' \rightarrow t$

$$\begin{aligned}
\Rightarrow K(x't', x, t) &= \langle x't' | e^{-\frac{i(t'-t)}{\hbar} \frac{p^2}{2m}} e^{-\frac{i(t'-t)}{\hbar} V} | x, t \rangle \\
&= \sum \langle x't' | e^{-\frac{i(t'-t)}{\hbar} \frac{p^2}{2m}} | x''t'' \rangle \langle x''t'' | e^{-\frac{i(t'-t)}{\hbar} V} | x, t \rangle
\end{aligned}$$

Ed. note: ie this is just the free particle propagator! (given by Sak)

↑ we cannot expand this in a Taylor series because  $t$  may be large.

However we already calculated this matrix element

$$\begin{aligned}
\Rightarrow K(x't', x, t) &= \sum_{x''} \left( \frac{m}{2\pi i \hbar (t'-t)} \right)^{\frac{1}{2}} e^{\frac{im(x'-x'')^2}{2\hbar(t'-t)}} e^{-\frac{iV(t'-t)}{\hbar}} \psi(x''-x) \\
&= \left( \frac{m}{2\pi i \hbar (t'-t)} \right)^{\frac{1}{2}} e^{\frac{im(x'-x)^2}{2\hbar(t'-t)} - \frac{iV(t'-t)}{\hbar}}
\end{aligned}$$

$$t' \rightarrow t \Rightarrow \frac{im}{2\hbar} \frac{(x'-x)^2}{(t'-t)} = \frac{im}{2\hbar} \frac{\Delta x^2}{\Delta t} = \frac{i\Delta p^2}{\hbar} = \frac{i\Delta p^2}{2m}$$

(72)

$$K(x't', x, t) = \left( \frac{m}{2\pi i \hbar \Delta t} \right)^{\frac{1}{2}} e^{\frac{i}{\hbar} \left( \frac{p^2}{2m} - V \right) \Delta t}$$

The sign of  $p^2$  has changed. What enters is the Lagrangian instead of the Hamiltonian

$$\mathcal{L} = \frac{p^2}{2m} - V$$

However,  $p$  is not anymore an operator. It is now the classical momentum

Back to the path integral

$$\begin{aligned} K(x't', x, t) &= \mathcal{N} \int dx_1 \dots dx_{N-1} e^{\frac{i}{\hbar} \sum_{k=1}^{N-1} (\frac{p_k^2}{2m} - V(x_k)) \Delta t} \\ &= \mathcal{N} \int dx_1 \dots dx_{N-1} e^{\frac{i}{\hbar} \Delta t \sum_{k=1}^{N-1} (\frac{p_k^2}{2m} - V(x_k))} \\ &= \mathcal{N} \int_{\mathcal{D}(x(t))} dx_1 \dots dx_{N-1} e^{\frac{i}{\hbar} \int_t^{t'} dt (\frac{p^2}{2m} - V(x))} \\ &= \int_{\mathcal{D}(x(t))} \mathcal{D}(x(t)) e^{\frac{i}{\hbar} \int_t^{t'} dt \mathcal{L}(t)} \end{aligned}$$

$$\mathcal{N} = \left( \frac{m}{2\pi i \hbar \Delta t} \right)^{\frac{N-1}{2}}$$

$\int_t^{t'} dt \mathcal{L}(t) \equiv S$  is the action of a path

Feynman: the propagator is given by the sum over all paths weighted by  $e^{iS/\hbar}$

## What was all this good for?

Q: OK what can **we** use this for?-- A: Sakurai: for us ~NOTHING analytic because in general this  $\int D[x]$  operation (infinite number of integrals) seems impossibly unwieldy. In more advanced treatments (quantum field theory, etc) where it will have a slightly different formulation, it can become useful.

### Exceptions (ie 3 uses/implications for us)

1) (Exact) In Quantum Field Theory you've no doubt noticed from talks you've seen that the Lagrangian seems to be what is focused on, instead of the Hamiltonian in advanced physics. This is the major if not the only reason why.

2) (Approx) **Numerical Integrations over small regions** If we limit the number of N to something finite, but still large, and also (where space which paths can go over is finite)

3) (More approx) **Semi-classical approximations:** However one point that Sakurai is trying to make but does not concentrate on (he hints at) is that it's good if we want to use it to make a certain **approximation** -- a "semi classical" approximation!!!! -- we don't have to deal with the sum over all paths. ---Only the classical path contributes.

(See handout from Liboff!)

Thus in this case

$$\text{propagator} : \int D[x] \exp i S(x)/\hbar \rightarrow \int_{1 \text{ class path}} \exp(iS(x)/\hbar)$$
$$\Psi \rightarrow \Psi_{\text{WKB}}$$

As the handout from Liboff explains, **this means we actually get the WKB solution back !** as we approach the classical limit. (explain details) This implies two things which are major points I hope you remember:

a) Feynman Path Integral justifies WKB and generalizes it (we could do it in 3-D too with Feynman)

b) Going backwards, Feynman Path Integral "formulation" automatically recovers classical mechanics, through the logic which we connected WKB→Hamilton Jacobi Equation

3) **Phase changes within semi-classical approximations:** Under this semiclassical approximation we are justified to calculate approximate expressions for phase changes gained or lost when traversing classical paths. QM amounts to phase changes added onto classical dynamics. This is what much of the next Sakurai section 2.6 is based on, although the path integral is only mentioned explicitly for the Aharonov-Bohm effect.

Why can we? Recall Liboff prescription

$$\text{propagator} : \int_{\text{all paths}} D[x] \exp i S(x)/\hbar \rightarrow \int_{\text{1 class path}} \exp(iS/\hbar)$$

$$\rightarrow \exp(i/\hbar \int_{\text{class path}} L dt) \rightarrow L = T - V \rightarrow 2T - E = mv^2 - E$$

class path  $\delta E = 0$ , so we can define a different action  $L+E$

$$\text{then } \rightarrow \exp(i/\hbar \int_{\text{class path}} (mv^2) dt) = \exp(i/\hbar \int mv v dt)$$

$$= \exp(i/\hbar \int p dx)$$

in other words  $\Psi \rightarrow \psi_{\text{WKB}}$

Review Feynman Path Integral: Not much use in elementary Quantum Mechanics

Exceptions: 1) calculating Quantum phase changes for semi-classical trajectories (today's topic)

## 2 Questions remaining in my mind about Feynman Path Integral after reading Sakurai:

1) How is this a complete formulation of QM? How could we use it to solve 1-D problems? Answer: Use the WKB approximation + other nearby paths systematically to progressively get better & better results (like a numerical solution).

2) Feynman: **Free particle** propagator for **infinitesimal** propagator  $K(\delta t) \rightarrow$  **form still works for finite  $\Delta t$  propagator  $K(\Delta t)$**  ? propagator (because we derived  $K(\Delta t)$  before talking about Feynman). Exactly, how does this work out?

**Answer:**  $\int D[x] K_{\text{free}}^n = K_{\text{free}}?$  **Product/Convolution of Gaussians = Gaussian?** This probably works

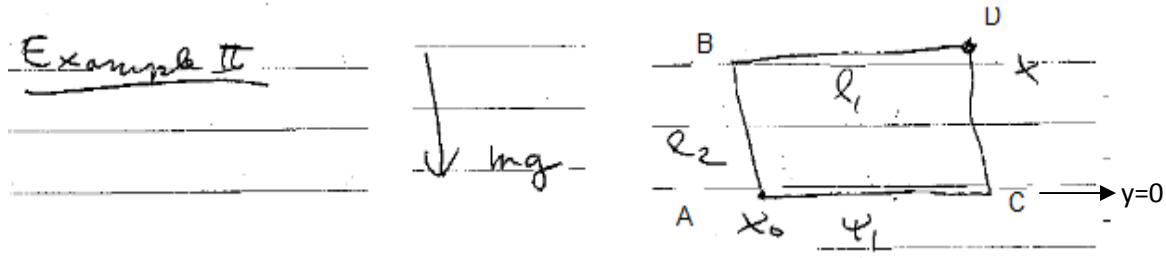
**J) Sakurai 2.6: Feynman Applications: phase changes in QM from Potentials**

1) Example: Gravity in QM.

Gravitational Potential:

$$H = p^2/2m + mgy$$

Consider quantum phase changes of  $\psi$  as particle propagates around square loop in this potential



Suppose propagation of identical particles to D along two paths different paths ACD, ABD, examine interference

This time REALLY USE Feynman Path Integral  $\rightarrow$  w/ classical approximation  $\rightarrow$  WKB like solutions

In other words, since we're on a 1 dimensional classical path, we can treat it like a 1-D problem. However the path integral goes over the path in 3-D space.

e.g. bottom leg AC:

$$\psi_+(x) \propto \frac{1}{\sqrt{p}} e^{-\frac{i}{\hbar} \int_{x_0}^x p_1 dx}$$

More importantly for this application, we can calculate the phase gain  $\phi$  of each leg from this term. This phase gain can lead to QM interference if superimpose two such wave functions, just as with the last example.

$$\phi_{AC} = \int_{x_0}^x p_1 dx$$

$$\phi_{BD} = \int_x^{x_0} p_2 dx$$

$$\phi_{CD} = \phi_{AB} = \int_0^y p_2(y) dy \equiv \phi_y$$

**Phase difference  $\Delta\phi = 1/\hbar \int (p_1 - p_2) dx = (p_1 - p_2) l_1 / \hbar$**



to get in form of Sakurai 2.6.17  $\rightarrow$  E is constant so  $p_2^2/2m + mgl_2 = p_1^2/2m$

$$p_2^2 - p_1^2 = (p_2 + p_1)(p_2 - p_1) = -2m^2 g l_1$$

$$\text{so } \Delta\phi = -\frac{2m^2 g l_1 l_2}{[\hbar (p_1 + p_2)]} \text{ if } p_1 \cong p_2 \text{ then } = 2p_1 \rightarrow \text{de Broglie} = 2\hbar/\lambda$$

$$= -\frac{2m^2 g l_1 l_2 \lambda}{\hbar^2}$$

same as Sakurai except Sakurai considered rotating loop such that  $l_2 \rightarrow l_2 \sin\delta$

ie if  $\delta = 0$ , flat table top no effect

**Physical Consequence of  $\Delta\Phi$  :** You already learned in Wave Mech (see Liboff Ch. 2.5/2.6) how phase differences cause interference effects in Quantum Mechanics. In any case where the wave function of a system is made up of a superposition (ie the sum) of two parts OR even has a part that is, the probability, which is the norm<sup>2</sup> of  $\psi$  will have an "interference" term if those 2 parts have any difference in phase:

$$\text{E.g. if } \psi_{\text{tot}} = \psi_0 + \psi_1 + \psi_2$$

$$+ \psi_1 = |\psi_1| e^{-i\Phi_1} + \psi_2 = |\psi_2| e^{-i\Phi_2}$$

then

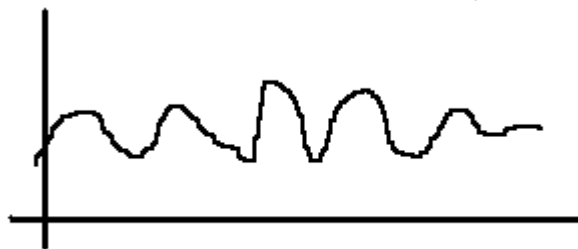
$$\text{Prob} \propto A + \underbrace{B \cos \Delta\Phi_{12}}_{\text{interference}}$$

where  $A$  and  $B$  are some other real numbers and  $\Delta\Phi = \Phi_1 - \Phi_2$ . The  $\cos \Delta\Phi$  term is called an interference term the probability represents the probability to find the particle whose wave function it is, and thus that probability oscillates—it has minima (“destructive” interference) and maxima (constructive interference).

In the gravity case above the interference could be observed at least two ways for example: 1) the way I explained in class was since the experiment described in Sakurai sent neutrons on these two trajectories, it turns out that neutrons have funny property: they are elementary particles which are “identical” meaning there is no way to distinguish one neutron from another. This means that a system of 2 neutrons will always need to have a “coupled” ie a single wave function if they are close enough in space—that single wave function will include two terms that each (more or less) have the phase of each individual neutron. In this case if we shoot two neutrons off from point A at exactly the same time over the two separate trajectories ACD and ABD, the probability to detect either will have this interference term. 2) even more simply than that, comparing with the double slit example of interference, one could just allow one neutron to take either path but not measure which path—then the wave function of the one neutron will still need to include components that are a superposition of going over both paths. Thus the interference will still result. (Note that whether one sees a minima/maxima also depends the exact lengths of  $l_1$  and  $l_2$ .)

**Corners of the loop:** By the way another approximation that was made in the gravity example was that whatever force/potential that caused the neutrons to bend at the corners of the square loop somehow cancels out or can otherwise be ignored. This is probably the hardest part of the experiment—ensuring that this happens.

Interference plotted vs  $\delta \rightarrow$  **experimental verification of gravitational effect. (Sak Fig 2.6)**



This result is especially important because it proves that gravity affects particles even on the quantum scale, which is a very small scale compared to usual scale of gravity effects. Further considering that Einstein's General Relativity describes gravity as just a modification to the geometry of space, it may even be surprising. In any case this result must constrain any quantum theory of gravity, something that is currently being searched for—string theory is one candidate.

## 2) Phases from Electromagnetic and Constant Potentials

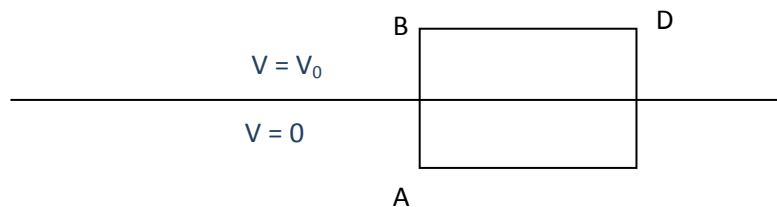
### a) Static Electric Potential and Constant Potentials

**Constant E field:** For the static Electric potential  $\phi(x)$  things work exactly the same as they did with gravity above in the case of a constant electric field, for example imagine in the y direction again. Then instead of a neutron we would want to consider a charged particle, but everything else would be exactly the same since the potential function would be  $\phi(x) = Ey$ . Same results w/  $mg$  replaced by  $E$ .

We can imagine more complicated potential functions  $\phi(x)$ , we would just need to integrate that function with a line integral along the trajectory.

**Constant Potential.** A special case of this would be  $\phi(x) = \text{constant}$ . This is just a specific example of any constant potential  $V(x) = V_0$  everywhere. Thinking of 2 trajectories within this potential, both trajectories will always have the same phase gain when we integrate, so there would be no phase difference.

But it is also quite easy to imagine two regions of space with different constant values e.g.



Then if we imagine the same loop of 2 trajectories ABD and ACD we will just indeed obtain the exact same phase difference did as for the gravity case again, but now just with  $V(y = BD) = mgl_2$  replaced by the value of the potential along the top leg BD in *this* case which is  $V_0$ . (We can assume the side legs still cancel in the difference of phase. )

**Sakurai** chooses to treat the case of constant potentials differently and only considers phase differences arising from the difference in time dependence due to the region of constant potential. Although we won't cover this in class, this is covered after this section in the notes below.

## b) Full Electromagnetism: Vector Potential A (adding Magnetic Fields)

First need to introduce some properties of A and convenient way of working with it:

First part of this section is kind of a digression from the phase changes part, in that I expect you to learn a little about the Full Electromagnetic treatment in our Quantum Formalism....

**Unfortunate:** 1) Electrodynamics First Semester : Hamiltonian/Lagrangian involving A not covered yet!!!

& 2) Undergrad EM courses won't cover Hamiltonians → ie this is first time you've seen classical H with A!

Sakurai states form of H—where did this come from? It's a little bit circular...

Summary of Sakurai 2.6: :

State form of H (from classical physics) → QM commutation → < Eq.'s O.Motion > → Erhenfest → Classical EOM

state  $p - eA/c$  is called it "kinematic" momentum

Then (surprise!) state Lagrangian (from classical physics) →  $L + e/c \mathbf{v} \cdot \mathbf{A}$  classically w/ no justification

My strategy, and also this is how H should be derived in classical mech

First derive form of Lagrangian L from classical EOM

$L \rightarrow$  generalized momentum Lagrange Eq  $p_{gen} = p + eA/c$

$L \rightarrow H$  Lagrange Definition of the Hamiltonian

### Lagrangian in Classical Mech

$$L = \frac{1}{2}m\mathbf{v}^2 - q\phi + q/c (\mathbf{v} \cdot \mathbf{A})$$

$\phi$  is electric potential A is the vector potential where the electric field  $\mathbf{E} = -\nabla \phi$  and magnetic Field  $\mathbf{B} = \nabla \times \mathbf{A}$

**Why does the Lagrangian have this form?**

Start w/ Lorentz Force eq replace q w/ e suppress c

$$\mathbf{F} = e\vec{E} + q\vec{v} \times \vec{B}$$

Remembering also (w/  $\partial_t \equiv \partial/\partial t$ ) that

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \partial_t \vec{A}$$

So rewriting the Lorentz Force, we have:

$$m \frac{d\vec{v}}{dt} = q[-\nabla\phi - \partial_t \vec{A} + \vec{v} \times (\nabla \times \vec{A})]$$

Remember Vector identity from e.g. Front Cover of Griffiths E&M: (or view Wikipedia)

$$\nabla(A \cdot B) = A \times \nabla \times B + B \times \nabla \times A + (A \cdot \nabla)B + (B \cdot \nabla)A$$

so our equation becomes (dropping space derivatives of velocity, like  $d\vec{v}/dx$ , because in the Lagrangian/Hamiltonian formulation of classical mechanics  $\dot{x} = v$  is treated as variable independent of  $x$ )

$$= q[-\nabla\phi - \partial_t \vec{A} - (\vec{v} \cdot \nabla) \vec{A} + \nabla(\vec{v} \cdot \vec{A})] = \nabla[-q\phi + q\vec{v} \cdot \vec{A}] - q \frac{d\vec{A}}{dt}$$

where **total derivative**:  $dA/dt = \partial A/\partial t + dA/dx \cdot dx/dt \rightarrow \partial A/\partial t + (\mathbf{v} \cdot \nabla) A$

So for x-component of this equation we get

$$\frac{d}{dt} \left( mv + \frac{e}{c} A \right) = \frac{d}{dx} (q\phi + qv \cdot A)$$

Recall Euler-Lagrange equation, which is the main equation of Lagrangian Mechanics—it defines what the Lagrangian is used for.:

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = \frac{\partial L}{\partial x}$$

looking at the equation it is clear that the choice  $L = 1/2mv^2 - (q\phi - qv \cdot A)$  will work

because

-V

We want  $L = T - V \quad V \rightarrow V(x) \quad dL/dx = -dV/dx$  takes care of RHS

Defining "generalized momentum":  $\tilde{p} = dL/d\dot{x} = dL/dv = mv + eA/c$  works for LHS

Now the form of H comes from E-L equation  $H = \sum x \tilde{p} - L = x\tilde{p} - L$

more on this later... in class we were confused by the fact that it appeared that putting this substitution in led to a Hamiltonian:

$$H = \frac{1}{2} m v^2 + e\phi \quad \text{which in terms of the plain old momentum } p = mv: \quad H = p^2/2m + e\phi$$

Confusing for 2 reasons: Where did the vector potential go? And does this disagree with what Sakurai defined as the Hamiltonian which was

$$H = 1/2m(p-qA)^2 + e\phi \quad ?$$

**Confusion about  $L \rightarrow H \rightarrow$  Is generalized momentum  $p+A/c$  or  $p- A/c$ ?**

Generalized Momentum is indeed  $p_{\text{gen}} = mv+A/c$  Also called canonical momentum in Sakurai

First see weblink on webpage: proves the following: Yes: since  $p_{\text{gen}} \equiv \tilde{p} = mv + qA/c = p_{\text{old}} + qA/c$

...copied from Wikipedia

## Charged particle in an electromagnetic field

[edit]

A good illustration of Hamiltonian mechanics is given by the Hamiltonian of a charged particle in an [electromagnetic field](#). In [Cartesian coordinates](#) (i.e.  $q_i = x_i$ ), the Lagrangian of a non-relativistic classical particle in an electromagnetic field is (in [SI Units](#)):

$$\mathcal{L} = \sum_i \frac{1}{2} m \dot{x}_i^2 + \sum_i e \dot{x}_i A_i - e\phi,$$

where  $e$  is the [electric charge](#) of the particle (not necessarily the electron charge),  $\phi$  is the [electric scalar potential](#), and the  $A_i$  are the components of the [magnetic vector potential](#) (these may be modified through a [gauge transformation](#)).

The generalized momenta may be derived by:

$$p_j = \frac{\partial \mathcal{L}}{\partial \dot{x}_j} = m \dot{x}_j + e A_j.$$

Rearranging, we may express the velocities in terms of the momenta, as:

$$\dot{x}_j = \frac{p_j - e A_j}{m}.$$

If we substitute the definition of the momenta, and the definitions of the velocities in terms of the momenta, into the definition of the Hamiltonian given above, and then simplify and rearrange, we get:

$$\mathcal{H} = \sum_i \dot{x}_i p_i - \mathcal{L} = \sum_i \frac{(p_i - e A_i)^2}{2m} + e\phi.$$

This equation is used frequently in [quantum mechanics](#).

# Points

- Indeed the generalized mom  $\tilde{p} = m\dot{x} + e\mathbf{A}/c$  (+ sign!) and thus it's true that  $H = 1/2m\dot{x}^2 + e\phi$  even w/  $\mathbf{A}$  present. That doesn't mean  $\mathbf{A}$  has no effect however, because now  $\dot{x}$  depends on  $\mathbf{A}$ . In fact writing it this way just hides the dependence on  $\mathbf{A}$ .
- Thus in Sakurai the "p" in his H is actually  $\tilde{p}$  !

$$H = \frac{1}{2m} \left( \tilde{p} - \frac{e}{c} \vec{A} \right)^2 + e\phi$$

*Canonical momentum*

- Two important points:
  - $\tilde{p}$  is still the operator that generates translation, when a magnetic potential is present: it is therefore the operator that has the commutation relation  $[x, \tilde{p}] = i\hbar$
  - The old momentum,  $m\dot{x}$ ,  $mv$ , which is what Sakurai calls  $m\dot{x} = \pi = \tilde{p} - eA/c$  now therefore has a different commutation relation

-----REPEAT

$\tilde{p} = m\dot{x} + eA/c$  and thus it's true that  $H = 1/2m\dot{x}^2 + e\phi$  even w/  $A$  present. That doesn't mean  $A$  has no effect however, because now  $\dot{x}$  depends on  $A$ . In fact writing it this way just hides the dependence on  $A$ .

Two important points:

$\tilde{p}$  is still the operator that generates translation, when a magnetic potential is present: it is therefore the operator that has the commutation relation  $[x, \tilde{p}] = i\hbar$

The old momentum,  $mv$ , which is what Sakurai calls  $m\dot{x} = \pi = \tilde{p} - eA/c$  now therefore has a different commutation relation

-----

Quick way to see  $[\tilde{p}, x] = i\hbar \rightarrow$  From the Euler Lagrange equation  $d/dt(dL/d\dot{x}) = dL/dx \rightarrow$  LHS

$d/dt(dL/d\dot{x}) \equiv d\tilde{p}/dt = 1/i\hbar [H, \tilde{p}] = 1/i\hbar [V, \tilde{p}] = dL/dx = -dV/dx \rightarrow$  ie satisfies same relation for any function  $V(x)$  as previous p did. (Relations in prob Sak 1.29)

OK now that we've established that note another interesting feature of the  $\Pi$  operators:

$$\begin{aligned}
 p_i &= \hbar \nabla_i \Rightarrow [p_i, p_j] = 0 \\
 \text{but } [\pi_i, \pi_j] &= [p_i - \frac{q}{c} A_i, p_j - \frac{q}{c} A_j] \\
 &= -\frac{q}{c} [p_i, A_j] - \frac{q}{c} [A_i, p_j] \\
 &= -\frac{q}{mc} \hbar \partial_{x_i} A_j + \frac{q}{c} \hbar \partial_{x_j} A_i \\
 B_k &= \epsilon_{kmn} \partial_n A_m = \frac{q \hbar}{c m} \epsilon_{ijk} B_k \\
 \epsilon_{ijk} \epsilon_{klm} &= \delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}
 \end{aligned}$$

Be comfortable with exploiting the commutation relations of the  $\tilde{p}$  and  $\Pi$  operators.

For example in class we went over the solution of Sak Problem 2.36: Constant B field  $B_z$  in the z direction implies that  $[\Pi_x, \Pi_y] = B_z$ . Since this is true, it should be easy to guess 2 different linear combinations of  $\Pi_x, \Pi_y$  we could call "a", and "a<sup>†</sup>" that will satisfy the real a and a<sup>†</sup> commutation relations of  $[a, a^\dagger] = 1$  AND at the same time can make up the part of the Ham that include  $\Pi_x, \Pi_y$ . Which is just

$$\Pi^2 = \Pi_x^2 + \Pi_y^2 + \Pi_z^2 \quad (\text{hint: think } A \Pi_x \pm i B \Pi_y)$$


---

For now, we've defined the Lagrangian, so let's finish up our last example of phase gains from the vector EM potential A—the Aharonov-Bohm effect:

However now that we've introduced the form of the Lagrangian we first must note that the velocity term causes a change to the form of the Semi-classical Feynman path integral Wave Function form ( $\Psi_{\text{WKB}}$ ).



If we call  $v \cdot \vec{A}$  term  
 in Lagrangian  $L_{\text{mag}}$   
 ie  $L_{\text{mag}} \equiv e \vec{v} \cdot \vec{A}$

then  $L_{\text{mag}}$  modifies semi-classical  
 Feynman from previous WKB  
 form

Why?

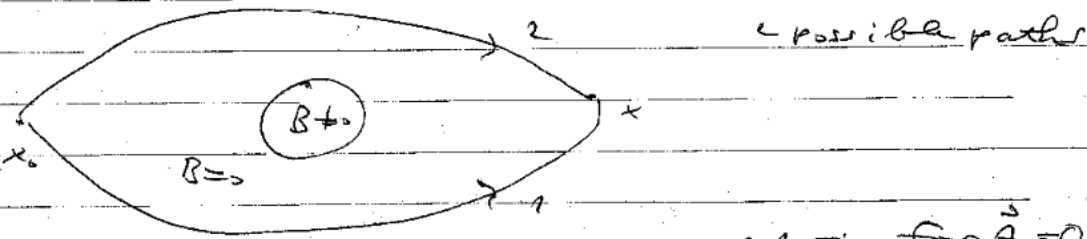
$$\int L_{\text{mag}} dt = \int \frac{e}{c} \vec{A} \cdot \underbrace{\vec{v}}_{\frac{d\vec{x}}{dt}} dt = \frac{e}{c} \int \vec{A} \cdot d\vec{x}$$

Thus

$$\Psi_{\text{in mag field}}^{\text{semi-class.}} = \Psi_{\text{WKB}} e^{-\frac{i}{\hbar} \frac{e}{c} \int \vec{A} \cdot d\vec{x}} \quad \text{Sak: } \vec{A} \cdot d\vec{s}$$

This is slightly inaccurate as the  $1/vk$  term should also be modified, but clearly the exponential/phase  
 function part "splits off" this way, and we are only concerned again where with the phase. This split off  
 follows simply from the fact that  $\exp(iS_{\text{action}}/\hbar) = \exp(i/\hbar \int L_0 + L_{\text{mag}} dt) = \exp i/\hbar \int L_0) \exp(i/\hbar \int L_{\text{mag}})$

## h) Aharonov-Bohm effect



$$\psi_1(x) = e^{i\frac{e}{\hbar c} \int_{x_0}^x A_1 ds} \psi_{10}$$

$$\psi_2(x) = e^{i\frac{e}{\hbar c} \int_{x_0}^x A_2 ds} \psi_{20}$$

solution for  $\vec{A} = 0$

interference term  $\psi_1^* \psi_2 + \psi_2^* \psi_1$

phase factor

$$e^{i\frac{e}{\hbar c} \int_{x_0}^x (A_2 - A_1) ds} = e^{i\frac{e}{\hbar c} \oint A ds}$$

$$= e^{i\frac{e}{\hbar c} \oint \vec{A} ds}$$

$$= e^{i\frac{e}{\hbar c} \oint \vec{\nabla} \times \vec{A} \cdot d\vec{a}}$$

total enclosed flux

where flux is the Magnetic field flux since  $\text{Curl } \vec{A} = \vec{B}$

Point : once again Quantum effect where in classical mechanics there would be no effect since there is no magnetic (or electric) field anywhere in the classical trajectory!

### Two other things

1) In class we mentioned that following Sakurai's example we don't necessarily have to make the semi-classical approximation to see this phase difference--- we can just consider the full Feynman Path Integral expression:

$\int_{\text{all paths}} D[x] \exp \int L dt$  because even though this is over all paths, the  $\int A ds$  that comes from  $\int L dt$  for

all paths will be the same for all paths because the conservative vector field path integrals are path independent.

This just means we can write the Feynman propagator

$K = \int_{\text{all paths}} D[x] \exp \int L dt = \int_{\text{all paths}} D[x] \exp \int A ds$  where the  $\int A ds$  can now be evaluated by choosing any single path above or below.

The phase difference  $\oint A ds = \Phi_B$  comes when we take the phase diff  $\int A_{\text{up}} - A_{\text{down}} ds$

### 3) Constant Potential in QM → weird:

Constant (in space) Electric/Gravitational Potential causes no observable forces in **classical mechanics**—no effect from value assigned to  $V$

However **but they do have observable effect in QM!**

Explore this idea: consider  $\Delta V = \text{constant}$

Such change of these fields called a **gauge change** → because in classical mech we are just redefining the strength of the potential, and in classical mech, we say observables are symmetric in --constant with respect to—the choice of this gauge.

Compare situation w/ and w/o a constant pot  $W$

$$V_0 \rightarrow V_0 + W \quad \Rightarrow \quad E \rightarrow E + W$$

and stationary state

$$\psi(x) e^{-iEt/\hbar} \rightarrow \psi(x) e^{-\frac{iWt}{\hbar} - \frac{iEt}{\hbar}} = e^{-iWt/\hbar} \psi(x, t)$$

OK—this is just a **phase factor**: when we look at the QM observable  $\rho = \psi^* \psi \rightarrow$  still no effect.

To see effect, we must look at the **phase difference btw 2 states in different regions of potential**, which means we need to have a change in potential between 2 regions:

To accomplish (Sakurai): have a constant potential which changes with time.

$$H \rightarrow H+W(t) \rightarrow H + V_0 t$$

oooh : We have so far been avoiding  $H$ 's w/ explicit time dependence.

Recall from beginning of Chap. 2) — Solutions for Time Evo Operator  $U(t)$  (on board)

- 1)  $U = \exp iHt/\hbar$  only for time independent  $H$
- 2)  $U = \exp i/\hbar \int dt H(t)/\hbar$  for slowly varying (and commuting)  $H$
- 3) otherwise (non-commuting)  $U = \text{messy} = \int dt_1 \int dt_2 H(t) \rightarrow$  Dyson series (like Feynman  $\int D[x]$ )

Use case 2 of our solutions here: applying to a wave function  $\rightarrow \langle x | U(t) | \alpha \rangle$

$$= \langle x | \exp i/\hbar \int dt (H_0(t)+W(t))/\hbar | \alpha \rangle$$

since  $W(t)$  and  $H_0(t)$  obviously commute (Q: why?)  $\rightarrow$  we can rewrite this

$$\langle x | \exp(i/\hbar \int dt W(t)) \exp(i/\hbar \int dt H_0(t)) | \alpha \rangle$$

$$\exp(i/\hbar \int dt W(t)) \langle x | \alpha, t \rangle$$

so NOW we have

---



---


$$E \rightarrow E + V(t) \Rightarrow \psi(x,t) e^{-i \int_0^t W(t') dt' / \hbar} \psi(x,t)$$


---

$\psi$  remains a solution

---



---

Before Continuing:

When applied to the Wave Functions like this, this is example of **Adiabatic Approximation**

## Adiabatic Approximation (A.A.) (Reminder from Wave Mech)

if  $H(t)$  changes slow enough  $\rightarrow$  even if  $[H(t_1), H(t_2)] \neq 0$  don't worry about "messy"

If in "nth" eigenstate stays in the "nth" eigenstate. e.g. ground state remains ground state, spin up remains spin up, even though it's really a new state defined by the new Hamiltonian

Another example: SHO time dependent  $\omega$   $H = p^2/2m + \frac{1}{2} \omega(t) x^2$

Ground state energy changes w/time  $E_0 = \hbar \omega(t) / 2$

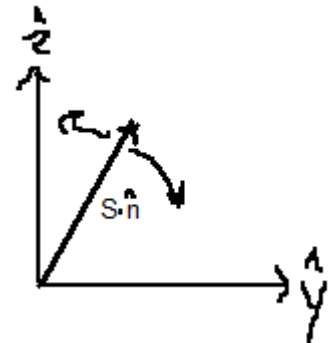
Phase gain by wave function from Time Dependence operator =  $\exp i/\hbar \int dt (H_0(t))$  so  $|0_{old}\rangle \rightarrow |0_{new}\rangle \exp i/\hbar \int \hbar \omega(t) / 2 dt$

**Our Example:** time dependent Stern Gerlach Hamiltonian :

$$H = e/m_e c \mathbf{S} \cdot \mathbf{B}$$

suppose oscillating  $\mathbf{B}$ :  $\mathbf{B} \rightarrow |\mathbf{B}| \hat{z} \cos(at) + \hat{y} \sin(at)$

$$H = \omega (S_z \cos(at) + S_y \sin(at)) = \omega \mathbf{S} \cdot \mathbf{n}(t)$$



Obviously  $\mathbf{H}$  at different  $t$ 's do not commute e.g.  $[S_z(t=0), S_y(t=\pi/2)] \propto S_x$

**Adiabatic Approx:** says that  $|\alpha\rangle =$  eigentate  $|\uparrow\rangle$  at  $t=0$  will stay as spin up eigenket  $|\mathbf{S} \cdot \mathbf{n}(t)\uparrow\rangle$  : as long as (if  $a$  is small enough.) ie the  $\rightarrow$  state moves slowly along with the  $\mathbf{H}$  operator

In this case the time dependence is the following: Energy doesn't change ( $E = e\hbar B/2mc$ ) only eigenket direction changes so we don't need to worry about  $\exp i/\hbar \int dt (H_0(t))$  integral  $\rightarrow \exp iE_{|\uparrow\rangle} t/\hbar$  (constant)

### Berry's Phase's

**Actually this is not quite true.** In fact because of the direction change, there is another factor that arises from consideration of the **Schrodinger eq itself**  $\mathbf{H} \Psi = \partial/\partial t \Psi$  (partial time derivative rhs?)

There must be a term related to the **total** time derivative of  $\mathbf{H}$ ,  $d\mathbf{H}/dt = d\mathbf{H}/d\mathbf{B} d\mathbf{B}/dt$ , that should arise.  $\mathbf{B}$  is a vector so this should be written as a gradient in "B-space" =  $\nabla_{\mathbf{B}} \mathbf{H} d\mathbf{B}/dt$

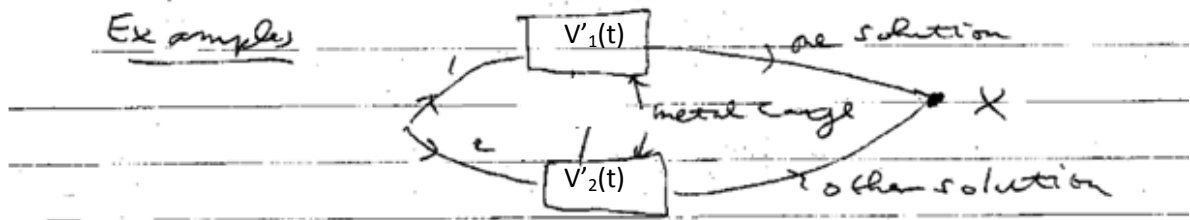
As described in Sakurai Appendix: this leads to an extra phase term, that is called a "**Berry's phase.**"

This phase depends on the geometry of the three components of  $\mathbf{B}$  being a vector. These components are parameters which  $\mathbf{H}$  depends on. So it depends on "**Geometry of the Parameter Space of  $\mathbf{B}$ .**"

If we generalize this situation to **any Hamiltonian** that which depends on **any set of parameters**: we can find that whether this extra phase arises depends the geometry of the parameter space: Hence the alternative name **Geometric Phase** (it refers to the geometry of the parameter space!)

OK back to our example:

Make simple set up to test



Note: it is the Feynman path integral / Semi classical approximation that tells us to think of the situation this way, with well defined classical trajectories

So we have within the cages

assuming identical particles  
wave fn interfere:

$$\psi_1 \rightarrow e^{-i \int V_1(t) dt} \psi_1$$

$$\psi_2 \rightarrow e^{-i \int V_2(t) dt} \psi_2$$

Probability at X

$$P = \left| e^{-i \int V_1(t) dt} \psi_1 + e^{-i \int V_2(t) dt} \psi_2 \right|^2$$

$$\psi_\alpha^* \psi_\alpha = |\psi_1| + |\psi_2| + \frac{\psi_1^* \psi_2 - \psi_2^* \psi_1}{2} e^{-i \int (V_1 - V_2) dt} + \frac{\psi_2^* \psi_1 - \psi_1^* \psi_2}{2} e^{i \int (V_1 - V_2) dt}$$

Imagine if  $\psi_1 \approx \psi_2$ . This should be the case at the interference region, since there  $V_1 = V_2$

$$= 2|\psi_1| \left( 1 + \frac{\psi_1^* \psi_2 - \psi_2^* \psi_1}{2} e^{-i \int (V_1 - V_2) dt} + \frac{\psi_2^* \psi_1 - \psi_1^* \psi_2}{2} e^{i \int (V_1 - V_2) dt} \right)$$

$$\propto 1 + 2 \cos(\int -V_2(t) - V_1(t) dt) \rightarrow \text{interference term}$$

Observable effect from potential !!!! contrast with classical situation !

First example of potential gauge

