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$$\frac{dA_H}{dt} = \frac{dU^+}{dt} A_S U + U^+ \frac{\partial A_S}{\partial t} U + U^+ A_S \frac{dU}{dt}.$$

Write $\frac{\partial A_S}{\partial t}$ for the explicit t -dep. of A_S , just as in the classical formula.

Now, $\frac{dU}{dt} = -\frac{i}{\hbar} HU = -\frac{i}{\hbar} UH$

$$\frac{dU^+}{dt} = \frac{i}{\hbar} U^+ H = \frac{i}{\hbar} HU^+,$$

so

$$\boxed{\frac{dA_H}{dt} = \frac{i}{\hbar} [H, A_H] + \left(\frac{\partial A}{\partial t}\right)_H}$$

where $\left(\frac{\partial A}{\partial t}\right)_H$ means compute $\frac{\partial A}{\partial t}$ in Sch. picture, then convert to

Heis. picture by sandwiching betw. U^+, U . Note similarity to classical eqn. One goes into the other if we make the formal replacement,

$$[A, B] \rightarrow i\hbar \{A, B\}$$

commutator P.B.

Evolution of density operator. Let

$$P = \sum_n f_n |\psi_n\rangle \langle \psi_n|, \quad |\psi_n\rangle \text{ states, } f_n \geq 0 \text{ probabilities, } \sum_n f_n = 1.$$

Then

$$i\hbar \frac{\partial P}{\partial t} = \sum_n f_n (H |\psi_n\rangle \langle \psi_n| - |\psi_n\rangle \langle \psi_n| H),$$

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or

$$\boxed{i\hbar \frac{\partial p}{\partial t} = [H, p]}$$

This may look like a Heisenberg eqn. of motion, but it is not; it is in the Schrödinger picture. It's analogous to the classical Liouville equation,

$$\frac{\partial \rho}{\partial t} = \{H, \rho\}$$

where $\rho(q, p, t)$ is the probability density on phase space.

Rules for Commutators

Let A, B, C, \dots = operators

a, b, \dots = complex numbers.

Def: $[A, B] = AB - BA$.

Rules:

$$\begin{aligned} 1. \quad [aA + bB, c] &= a[A, c] + b[B, c] \\ [A, bB + cC] &= b[A, B] + c[A, C] \end{aligned} \quad \left. \right\} \text{Linearity}$$

$$2. \quad [A, B] = -[B, A] \quad \text{Antisymmetry.}$$

$$\begin{aligned} 3. \quad [AB, C] &= A[B, C] + [A, C]B \\ [A, BC] &= [A, B]C + B[A, C] \end{aligned} \quad \left. \right\} \text{Leibnitz rule}$$

$$4. \quad [A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0 \quad \text{Jacobi identity.}$$

The classical Poisson bracket is defined by

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$$\{A, B\} = \sum_{k=1}^n \left(\frac{\partial A}{\partial q_k} \frac{\partial B}{\partial p_k} - \frac{\partial A}{\partial p_k} \frac{\partial B}{\partial q_k} \right).$$

($n = \#$ of deg. of freedom). It obeys exactly the same rules as the commutator, except that the order of the factors does not matter.

Charged particle in EM field; Classical Mechanics.

Let charge = q . Newton-Lorentz eqns,

$$m\vec{a} = q(\vec{E} + \frac{1}{c}\vec{v} \times \vec{B}).$$

To get a Lagrangian formulation, need potentials:

$$\begin{aligned} \vec{E} &= -\nabla\phi - \frac{1}{c} \frac{\partial \vec{A}}{\partial t} \\ \vec{B} &= \nabla \times \vec{A} \end{aligned} \quad \left. \begin{array}{l} \phi = \phi(\vec{x}, t) \\ \vec{A} = \vec{A}(\vec{x}, t) \end{array} \right\} \text{in general.}$$

Given \vec{E}, \vec{B} , \vec{A} and ϕ are not unique; can subject them to a gauge transformation,

$$\left. \begin{aligned} \vec{A}' &= \vec{A} + \nabla f \\ \phi' &= \phi - \frac{1}{c} \frac{\partial f}{\partial t} \end{aligned} \right\} \quad \text{where } f = f(\vec{x}, t) \text{ is the gauge scalar.}$$

Then

$$\left. \begin{aligned} \vec{E}' &= \vec{E} \\ \vec{B}' &= \vec{B} \end{aligned} \right\}. \quad \text{The physical fields don't depend on the gauge.}$$

The Lagrangian is

$$L(\vec{x}, \dot{\vec{x}}, t) = \frac{m}{2} |\dot{\vec{x}}|^2 - q\phi(\vec{x}, t) + \frac{q}{c} \dot{\vec{x}} \cdot \vec{A}(\vec{x}, t),$$

so

$$\vec{p} = \frac{\partial L}{\partial \dot{\vec{x}}} = m\dot{\vec{x}} + \frac{q}{c}\vec{A}(\vec{x}, t). = \text{canonical mom.}$$

\uparrow
kinetic mom.

The canonical momentum is gauge-dependent:

of

$$\vec{p}' = m\dot{\vec{x}} + \frac{q}{c}\vec{A}', \quad \text{then}$$

$$\vec{p}' = \vec{p} + \frac{q}{c} \nabla f.$$

Classical Hamiltonian:

$$H = \frac{1}{2m} \left[\vec{p} - \frac{q}{c}\vec{A}(\vec{x}, t) \right]^2 + q\phi(\vec{x}, t).$$

The first term is a complicated way of writing the kinetic energy; notice that

$$\vec{p} - \frac{q}{c}\vec{A} = m\vec{v} = \text{kinetic momentum},$$

so $\frac{1}{2m} \left[\vec{p} - \frac{q}{c}\vec{A} \right]^2 = \frac{1}{2}mv^2.$

Charged Particle in EM field; Quantum Mechanics.

We guess that the classical formula also works in QM, with a reinterpretation of symbols. Since \vec{p} and \vec{A} do not commute in QM, we must be careful about the order. We interpret:

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$$\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 = p^2 - \frac{q}{c}\vec{p}\cdot\vec{A} - \frac{q}{c}\vec{A}\cdot\vec{p} + \frac{q^2}{c^2}A^2,$$

because this is Hermitian. It's a guess that all this will work, and in any case we are neglecting spin.

The Schrödinger equation for the wave function $\psi(\vec{x},t)$ is

$$\frac{1}{2m} \left[-it\nabla - \frac{q}{c}\vec{A}(\vec{x},t) \right]^2 \psi + q\phi(\vec{x},t)\psi = it\frac{\partial\psi}{\partial t}.$$

It's curious that the Sch. eqn. (and the classical Ham.) require the use of potentials \vec{A}, ϕ , when the classical particle only feels the \vec{E}, \vec{B} fields. So we should understand how the quantum description changes under a gauge transformation, which should have no effect on the physics. (At least, it has no effect at the classical level, we should see what happens in QM.)

Define a new wave fn. $\psi'(\vec{x},t)$ by

$$\psi'(\vec{x},t) = e^{i\frac{q}{hc}f(\vec{x},t)} \psi(\vec{x},t).$$

The new and old wave fns differ by a t-dep and spatially dependent phase factor. Here $f(\vec{x},t)$ is a function that will turn out to be the gauge scalar.

Consider letting the kinetic momentum operator $\rightarrow \vec{p} - \frac{q}{c}\vec{A}$ act on ψ , and pull the phase factor to the left:

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$$\left(-i\hbar\nabla - \frac{q}{c}\vec{A}\right) e^{-\frac{iqf}{\hbar c}} \psi'$$

$$= e^{-\frac{iqf}{\hbar c}} \left(-i\hbar\nabla - \frac{q}{c}\vec{A} - \frac{q}{c}\nabla f\right) \psi'$$

$$= e^{-\frac{iqf}{\hbar c}} \left(-i\hbar\nabla - \frac{q}{c}\vec{A}'\right) \psi'. \quad \vec{A}' = \vec{A} + \nabla f.$$

Now multiply by $\left(-i\hbar\nabla - \frac{q}{c}\vec{A}\right)$ again and pull phase factor through this, too:

$$\left(-i\hbar\nabla - \frac{q}{c}\vec{A}\right)^2 e^{-\frac{iqf}{\hbar c}} \psi'$$

$$= e^{-\frac{iqf}{\hbar c}} \left(-i\hbar\nabla - \frac{q}{c}\vec{A}'\right)^2 \psi'.$$

So the Sch. eqn. can be written in terms of ψ' ,

$$e^{-\frac{iqf}{\hbar c}} \left\{ \frac{1}{2m} \left(-i\hbar\nabla - \frac{q}{c}\vec{A}'\right)^2 \psi' + q\phi\psi' \right\}$$

$$= i\hbar \frac{\partial}{\partial t} \left(e^{-\frac{iqf}{\hbar c}} \psi' \right)$$

$$= e^{-\frac{iqf}{\hbar c}} \left(\frac{q}{c} \frac{\partial f}{\partial t} \psi' + i\hbar \frac{\partial \psi'}{\partial t} \right).$$

Phase factors cancel, bring $\frac{\partial f}{\partial t}$ term to LHS, use

$$\phi' = \phi - \frac{1}{c} \frac{\partial f}{\partial t},$$

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you get,

$$\frac{1}{2m} \left[-i\hbar\nabla - \frac{q}{c}\vec{A}' \right]^2 \psi' + q\phi'\psi' = i\hbar \frac{\partial \psi'}{\partial t},$$

a new Sch. eqn in the primed gauge.

So if you do a gauge transformation on the EM fields, you must also change the phase of ψ to restore the form of the Schrödinger eqn.

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Probability density, current. (Single particle moving in 3D).

Wave fn ψ is a scalar field, but not like a classical field, e.g. cannot be measured in same way. Nevertheless, $|\psi|^2$ often makes sense as a particle density, $q|\psi|^2$ as a charge density, which has an associated current. Define

$$\vec{v} = \frac{1}{m} (\vec{p} - \frac{q}{c} \vec{A}) = \frac{1}{m} (-i\hbar \nabla - \frac{q}{c} \vec{A}).$$

Then

$$\vec{J} = \frac{1}{2} [\psi^* (\vec{v} \psi) + (\vec{v} \psi^*)^* \psi] = \text{Re } \psi^* (\vec{v} \psi) = \vec{J}(\vec{x}, t).$$

$$\rho = |\psi|^2$$

$$\nabla \cdot \vec{J} + \frac{\partial \rho}{\partial t} = 0. \quad \text{Exercise to prove.}$$

Ehrenfest relations. Let $H = \frac{\vec{p}^2}{2m} + V(\vec{x})$ (in 3D).

In Heisenberg picture,

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} - \frac{i}{\hbar} [A, H] \quad (\text{omit } H \text{ subscripts, Heis. picture understood}).$$

Use commutators,

$$[x_i, f(\vec{p})] = i\hbar \frac{\partial f}{\partial p_i}$$

$$[p_i, g(\vec{x})] = -i\hbar \frac{\partial g}{\partial x_i}$$

Then :

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$$\dot{\vec{x}} = \frac{i}{\hbar} \left[\frac{p^2}{2m}, \vec{x} \right] = \frac{\vec{p}}{m}$$

$$\dot{\vec{p}} = \frac{i}{\hbar} \left[V(\vec{x}), \vec{p} \right] = -\nabla V(\vec{x}).$$

or,

$$m \ddot{\vec{x}} = -\nabla V(\vec{x})$$

An operator version of Newton's laws. Now take expectation values w.r.t.

$$|\psi\rangle = |\psi_H\rangle = |\psi_S(0)\rangle:$$

$$\langle \psi_H | m \frac{d^2}{dt^2} \vec{x} | \psi_H \rangle = m \frac{d^2}{dt^2} \langle \psi | \vec{x} | \psi \rangle = m \frac{d^2}{dt^2} \langle \vec{x} \rangle.$$

$$= - \langle \nabla V(\vec{x}) \rangle, \quad \text{or}$$

$$m \frac{d^2}{dt^2} \langle \vec{x} \rangle = - \langle \nabla V(\vec{x}) \rangle$$

Ehrenfest relation on
expectation values.

Notice that the expectation values can be computed in the Schrödinger picture, since they are independent of which picture we use. Do not say that expectation values follow the classical motion (Sakurai is mistaken), because

$$\langle \nabla V(\vec{x}) \rangle \neq \nabla V(\langle \vec{x} \rangle)$$

in general. However, in special case that $V(\vec{x})$ is at most a quadratic polynomial in \vec{x} :

$$\nabla(\vec{x}) = \frac{1}{2} \sum_{ij} a_{ij} x_i x_j + \sum_i b_i x_i + c,$$

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$$\frac{\partial V}{\partial x_i} = \sum_j a_{ij} x_j + b_i,$$

then it is true that $\langle \nabla V(\vec{x}) \rangle = \nabla V(\langle \vec{x} \rangle)$, and $\langle \vec{x} \rangle(t)$ does follow the classical motion. These cases include:

1. Free particle
2. Particle in uniform electric or gravitational field
3. Harmonic oscillators and various generalizations.

Another case is particle in uniform magnetic field (not proven here).

Some small topics first.

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1. The single-valuedness of the wavefunction. Work in 3D.

Let $|4\rangle$ be the state vector for the system. Expand it as a lin. comb. of position eigenstates $|\vec{x}\rangle$:

$$|4\rangle = \int d^3\vec{x} |\vec{x}\rangle \Psi(\vec{x}).$$

The wave function $\Psi(\vec{x})$ is the expansion coefficients. This is the definition of the wave fn. It is single-valued because the position eigenvects are single-valued.

In the remaining topics today, we work with the 1D Schrödinger eqn.

2. Degeneracies in 1D. Let ψ, ϕ be two solns of the Sch. eqn. with energy E ,

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

$$-\frac{\hbar^2}{2m} \phi'' + V(x)\phi = E\phi$$

Mult 1st eqn. by ϕ , 2nd by ψ , subt., get

$$\phi\psi'' - \psi\phi'' = \frac{dW}{dx} = 0$$

where

$$W \equiv \text{Wronskian} = \phi\psi' - \psi\phi'.$$

So, $W = \text{const}$ (indep. of x). Now suppose (usually due to bdry cond's) that ϕ, ψ both vanish at same pt x , including possibilities $x \rightarrow \infty$, $x \rightarrow -\infty$, or both. Then $W=0$ (everywhere), or,

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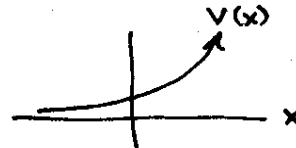
$$\frac{\psi'}{\psi} = \frac{\phi'}{\phi} \Rightarrow \psi = c\phi \quad (c=\text{const})$$

$\Rightarrow \psi, \phi$ are lin. dep.

Conclusion: If today cond's force ψ to vanish at some x , including $x \rightarrow \pm\infty$, then energy eigenfs are nondegenerate.

Examples: 1. Bound states of oscillators are non-degen, since $\psi(\pm\infty) = 0$.

2. Scattering problem like



have nondegen. eigenstates, since $\psi(x \rightarrow +\infty) = 0$.

3. Free particle does not require ψ to vanish anywhere, including $\pm\infty$, so degen. is allowed. In fact, there is a degen.,

$$e^{\pm ipx/\hbar} \quad (2 \text{ solns w. same energy } E = p^2/2m).$$

3. Reality of wave fn. Sch. eqn is real, so if ψ is a soln, then so is ψ^* .

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

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

Suppose E is nondegenerate. Then ψ, ψ^* must be lin. dep., i.e.,

$$\psi = c\psi^* \quad \text{some } c.$$

$$\Rightarrow |\psi|^2 = |c|^2 |\psi^*|^2 \Rightarrow |c|^2 = 1 \Rightarrow c = e^{i\alpha}.$$

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If $\psi = e^{i\alpha} \psi^*$ then

$$e^{-i\alpha/2} \psi = e^{i\alpha/2} \psi^* \equiv \phi(x) = \text{real.}$$

Conclusion: If ψ is a nondegenerate energy eigenfn. in 1D, then by a phase convention can make ψ real.

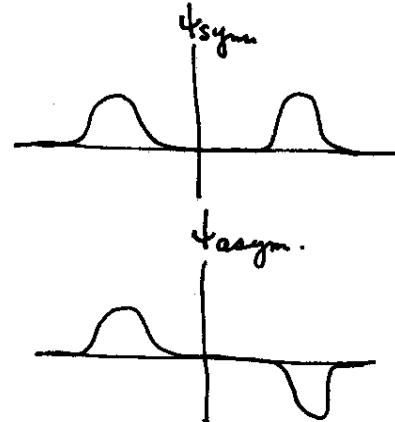
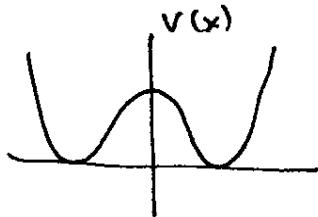
4. Interleaving of Nodes

The nodes of a wave fn. are the places where $\psi=0$.

For bound state eigenfns of 1D Sch. equ., ψ_0, ψ_1, \dots with $E_0 < E_1 < E_2 < \dots$, the n -th eigenfn. has n nodes (none for ground state), and the nodes of ψ_{n+1} interleave the nodes of ψ_n , like this:

$$\begin{array}{cccccc} \cdot & \cdot & \cdot & \cdot & \cdot & \text{nodes of } \psi_4 \\ \times & \times & \times & \times & \times & \text{nodes of } \psi_5 \end{array}$$

This is independent of the potential. Proof can be found in Morse and Feshbach. Application: In double well potential, symm. and antisymm lin. comb. of ground state wave fn. in each well are nearly degenerate, but split by small tunneling.



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Q: which has lower energy? (which is the true ground state?)

A: The symmetric one, with 0 nodes. The antisymmetric one, with one node, is the first excited state.