P423 – Lecture 3 Propagators; charged particle in a magnetic field.

Propagators and quantum dynamics

Previous class: $|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle$

where $\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}(t-t_0)\hat{H}}$ when $\hat{H}$ does not depend explicitly on time.

Now assume that at $t=t_0$ $|\psi\rangle = |\vec{r}_0\rangle$.

what is the probability of measuring $|\psi\rangle = |\vec{r}\rangle$ at $t > t_0$? It is given by the modulus squared of the Propagator:

$$\langle \vec{r} | \hat{U}(t,t_0) | \vec{r}_0\rangle \equiv G(\vec{r},t;\vec{r}_0,t_0)$$

We can show that this is the Green's fnc associated to the Schrödinger's eqn., in that

$$\left[-\frac{\hbar^2}{2m}\nabla_r^2 + V(\vec{r}) - i\hbar\frac{\partial}{\partial t}\right] G(\vec{r},t;\vec{r}_0,t_0) = -i\hbar\,\delta(\vec{r}-\vec{r}_0)\,\delta(t-t_0),$$

with the boundary condition $G(\vec{r},t;\vec{r}_0,t_0) = 0$ for $t < t_0$.

Note:

$$\langle \vec{r}|\psi(t)\rangle = \langle \vec{r}|\hat{U}(t,t_0)|\psi(t_0)\rangle = \int d^3r' \underbrace{\langle \vec{r}|\hat{U}|\vec{r}'\rangle}_{G(\vec{r}t;\vec{r}'t_0)} \langle \vec{r}'|\psi(t_0)\rangle$$

$$= \int d^3r'\, G(\vec{r},t;\vec{r}',t_0)\,\psi(\vec{r}',t_0)$$

Just like your usual Green's function.

For a free particle in $d=1$ we can show that [Problem 1 in A2]:

$$G(x,t;x_0,t_0) = \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}\; e^{i\frac{m(x-x_0)^2}{2\hbar(t-t_0)}} .$$

Note that G is the wave func for a propagating mode that was $|\vec{r}_0\rangle$ at $t=t_0$.

Feynman showed that the propagator can be expressed exactly as

$$\langle \vec{r}\,|U(t,t_0)|\,\vec{r}_0\rangle = \underbrace{\int_{\vec{r}_0}^{\vec{r}} \mathcal{D}[\vec{r}(t)]}_{=\sum_{\text{all paths}}}\; e^{\frac{i}{\hbar}\overbrace{\int_{t_0}^{t} dt\, L[\vec{r},\dot{\vec{r}}]}^{}}$$

action with non-classical trajectories allowed!

where the integral is a sum over all possible paths $\vec{r}(t)$, including non-classical ones.

This is called a Feynman path integral. The nice thing about it is that in the limit $\hbar\to 0$, the exponent blows up; so for the case that $\int_{t_0}^{t} dt\, L$ is minimal for a classical trajectory we will get

$$\langle \vec{r}\,|U(t,t_0)|\vec{r}_0\rangle \approx a\, e^{\frac{i}{\hbar}S(\vec{r},t)} \qquad (\text{Semiclassical limit, } \hbar\to 0).$$

Because the "classical path" minimizes the oscillatory exponent.

Thus as we can see, the Feynman formulation of quantum mechanics makes the semiclassical limit more explicit.

▶ If you want to know more about Feynman path integrals (and see the proof that they satisfy Schrödinger's eqn), I recommend Sakurai's 2.5.

For the purposes of our course we will use the result

$$\langle \vec{r}\,|U(t,t_0)|\vec{r}_0\rangle \propto \sum_{\text{all } \vec{r}(t)} e^{\frac{i}{\hbar}\int_{t_0}^{t} dt\, L[\vec{r},\dot{\vec{r}}]} .$$

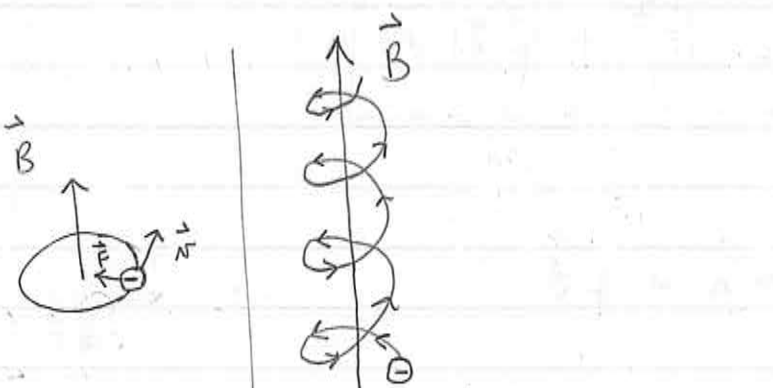
<u>Charged particle in a magnetic field</u>

Why study quantum mechanics of a particle in a B field? Ans: Because it provides the best way to measure $\hbar$ and it gives us the standard of resistance, a fundamental unit of measure (the von Klitzing).

The Lorentz force acting on a charged particle is

$$\vec{F}_{Lorentz} = q\, \vec{v} \times \vec{B} \qquad (q = e = -e_0 \text{ for an electron}).$$

In a constant $\vec{B}$ field, the classical trajectories are circular or screw like:



Case $\vec{v}\cdot\vec{B} = 0$ $(\vec{v} \perp \vec{B})$ | $\vec{v}\cdot\vec{B} \neq 0$ ($\vec{v}$ has a component along $\vec{B}$)

We can <u>not</u> write $\vec{F}_{Lorentz} = -\vec{\nabla}_r V(\vec{r})$. How do we find the quantum eigenstates?

while $\vec{F}$ depends on $\vec{v}$, it is conservative in the sense that $W = \int_{r_i}^{r_f} \vec{F}\cdot d\vec{r} = \int_i^f \vec{F}_{Lorentz} \cdot \frac{d\vec{r}}{dt}\, dt$

$= \int (\vec{v} \times \vec{B}) \cdot \vec{v}\, dt = 0$ for all paths!

$\Rightarrow \vec{F}_{Lorentz}$ never does work on the particle!

For this case, we can incorporate a velocity dependent force in the Lagrangian.

So we will find this Lagrangian, and from it we will get the Hamiltonian to be used in Schrödinger's eqn.

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We want to find $\mathcal{L}$ such that $\frac{\partial \mathcal{L}}{\partial \vec{r}} = \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\vec{r}}}\right) \Rightarrow q\,\vec{v}\times\vec{B} = m\ddot{\vec{r}}$.

For this, recall that $\vec{B} = \vec{\nabla}\times\vec{A}$ where $\vec{A}$ is vector potential ($\vec{\nabla}\cdot\vec{B} = 0$ so we can always do that).

It's easy to see that the Lagrangian is

$$\boxed{\mathcal{L} = \frac{1}{2}m\left(\dot{\vec{r}}\right)^2 + q\,\vec{A}\cdot\dot{\vec{r}}}$$

where $\vec{A} = \vec{A}(\vec{r})$.

$$\vec{p} = \frac{\partial \mathcal{L}}{\partial \dot{\vec{r}}} = m\dot{\vec{r}} + q\vec{A};$$

and the eqn of motion is

$$\frac{d}{dt}(\vec{p}) = \frac{\partial \mathcal{L}}{\partial \vec{r}} \Rightarrow m\ddot{\vec{r}} + q\frac{d\vec{A}}{dt} = q\frac{\partial}{\partial \vec{r}}(\vec{A}\cdot\dot{\vec{r}})$$

Let's compute the x component:

$$m\ddot{x} + q\frac{dA_x}{dt} = q\frac{\partial}{\partial x}\left(\vec{A}\cdot\overset{\text{free of } \vec{r}!}{\vec{v}}\right)$$

$$m\ddot{x} + q\left(\cancel{\frac{\partial A_x}{\partial x}\dot{x}} + \frac{\partial A_x}{\partial y}\dot{y} + \frac{\partial A_x}{\partial z}\dot{z}\right) = q\left(\cancel{\frac{\partial A_x}{\partial x}v_x} + \frac{\partial A_y}{\partial x}v_y + \frac{\partial A_z}{\partial x}v_z\right)$$

$$m\ddot{x} = q\left[v_y\underbrace{\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)}_{(\vec{\nabla}\times\vec{A})_z = B_z} - v_z\underbrace{\left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right)}_{(\vec{\nabla}\times\vec{A})_y = B_y}\right] = q\left(\vec{v}\times\vec{B}\right)_x$$

Do cyclic permutations and conclude that

$$m\ddot{\vec{r}} = q\,\vec{v}\times\vec{B}$$ //

Hence the Hamiltonian is

$$\mathcal{H} = \vec{p}\cdot\dot{\vec{r}} - \mathcal{L} = \vec{p}\cdot\dot{\vec{r}} - \frac{1}{2}m(\dot{\vec{r}})^2 - q\vec{A}\cdot\dot{\vec{r}} = (\vec{p}-q\vec{A})\cdot\dot{\vec{r}} - \frac{1}{2}m(\dot{\vec{r}})^2$$

Plug $\dot{\vec{r}} = \frac{1}{m}(\vec{p}-q\vec{A})$:

$$\mathcal{H} = (\vec{p}-q\vec{A})^2\frac{1}{m} - \frac{1}{2}\cancel{m}\frac{(\vec{p}-q\vec{A})^2}{m^{\cancel{2}}} = \frac{1}{2m}(\vec{p}-q\vec{A})^2$$

$$\boxed{\mathcal{H} = \frac{1}{2m}(\vec{p}-q\vec{A})^2}$$

Note: the canonical momentum $\vec{p} = \frac{\partial\mathcal{L}}{\partial\dot{\vec{r}}} = m\dot{\vec{r}} + q\vec{A}$ is different from the kinetic momentum $m\dot{\vec{r}}$. And also note that $\mathcal{H} = \frac{1}{2}m(\dot{\vec{r}})^2$ (Because $\vec{B}$ field does no work, so energy can not depend on $\vec{B}$!)

Energy levels in a constant $\vec{B}$ field.

Assume $\vec{B} = B\hat{z}$. Since $\vec{B} = \vec{\nabla}\times\vec{A} = \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\hat{z}$ we can choose $A_z = 0$.

Thus

$$\mathcal{H} = \underbrace{\frac{1}{2m}(\hat{\vec{P}}_\perp - q\vec{A})^2}_{\mathcal{H}_\perp} + \frac{1}{2m}\hat{P}_z^2\ ,$$

so the energy eigenstates can be written

$$\varphi_E(\vec{r}) = \psi_\perp(\vec{r}_\perp)\, e^{-\frac{i}{\hbar}p_z z}$$ and the energy is $E = E_\perp + \frac{\hbar^2 p_z^2}{2m}$.

So we can focus on the motion in the $\vec{r}_\perp = (x, y)$ plane. We need to find

$$\mathcal{H}_\perp \psi_\perp = \epsilon\,\psi_\perp \quad \text{where } \psi_\perp = \psi_\perp(\vec{r}_\perp).$$

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$$\mathcal{H}_\perp = \frac{m}{2}\left(\hat{\dot{x}}^2 + \hat{\dot{y}}^2\right), \text{ where}$$

$$\begin{cases} m\hat{\dot{x}} = \hat{p}_x - q\hat{A}_x \\ m\hat{\dot{y}} = \hat{p}_y - q\hat{A}_y \end{cases}$$

But

$$[m\hat{\dot{x}}, m\hat{\dot{y}}] = [\hat{p}_x - q\hat{A}_x, \hat{p}_y - q\hat{A}_y] = [\hat{p}_x, \hat{p}_y - q\hat{A}_y] - q[\hat{A}_x, \hat{p}_y - q\hat{A}_y]$$

$$= \underbrace{[\hat{p}_x, \hat{p}_y]}_{=0} - q[\hat{p}_x, \hat{A}_y] - q\underbrace{[\hat{A}_x, -q\hat{A}_y]}_{=0} - q[\hat{A}_x, \hat{p}_y]$$

But remember that $[\hat{p}_x, f(x)]\psi = \frac{\hbar}{i}\frac{d}{dx}[f(x)\psi(x)] - f(x)\frac{\hbar}{i}\frac{d}{dx}\psi(x)$

$$= \frac{\hbar}{i}\left(\frac{df}{dx}\right)\psi + \cancel{\frac{\hbar}{i}f(x)\frac{d\psi}{dx}} - \cancel{f(x)\frac{\hbar}{i}\frac{d\psi}{dx}} = \left(\frac{\hbar}{i}\frac{df}{dx}\right)\psi$$

So

$$[m\hat{\dot{x}}, m\hat{\dot{y}}] = -q\frac{\hbar}{i}\frac{\partial A_y}{\partial x} + q\frac{\hbar}{i}\frac{\partial A_x}{\partial y} = i\hbar q\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) = i\hbar q\left(\vec{\nabla}\times\vec{A}\right)_z$$

$$\boxed{[m\hat{\dot{x}}, m\hat{\dot{y}}] = i\hbar q B}$$

Now if we define the operators: $\hat{\Pi} = \text{sgn}(q)\frac{m\dot{x}}{\sqrt{|q|B}}$ and $\hat{P}_\Pi = \frac{m\dot{y}}{\sqrt{|q|B}}$ they

$\text{sgn}(q) = \begin{cases} +1 \text{ if } q>0 \\ -1 \text{ if } q<0 \end{cases}$

satisfy:

$$[\hat{\Pi}, \hat{P}_\Pi] = i\hbar$$

$\Rightarrow$ we say that $\hat{P}_\Pi$ is canonically conjugate to $\hat{\Pi}$, and that $\hat{\Pi}$ and $\hat{P}_\Pi$ are canonical variables.

Like momentum

Like position

The Hamiltonian is $\mathcal{H}_\perp = \frac{m}{2}\left(\hat{\dot{x}}^2 + \hat{\dot{y}}^2\right) = \frac{1}{2}\underbrace{\left(\frac{|q|B}{m}\right)}_{\text{dimension of frequency}}\left(\hat{P}^2 + \hat{\Pi}^2\right)$

For $q = -e_0$, the cyclotron frequency is

$$w_c = \frac{e_0 B}{m}$$

(In classical mechanics, w_c its the frequency of rotation of a particle in a B field)

Now we see that $\mathcal{H}_\perp$ is just like an Harmonic oscillator. Define

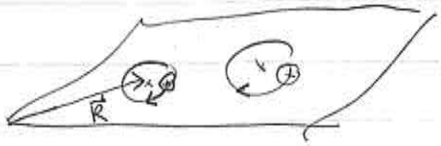
$$\hat{a} = \frac{\hat{\Pi} + i\hat{P}_\Pi}{\sqrt{2\hbar}} \Rightarrow [\hat{a}, \hat{a}^+] = 1, \text{ and}$$

$$\mathcal{H}_\perp = \hbar w_c\left(\hat{a}^+\hat{a} + \frac{1}{2}\right).$$

$$\Rightarrow \boxed{E_\perp = \hbar w_c\left(n + \frac{1}{2}\right) \qquad \text{"Landau levels"}}$$

Is the problem solved? No! Because these levels are highly degenerate. Based on a free particle ($B=0$) we expect two continuum quantum numbers (P_x, P_y). We just showed that one of them got quantized, so we should have another continuum parameter to label the degeneracy – How to find?

Inspired by classical mechanics, let's look at the center of the classical trajectory of the particle in the xy plane:



Classical solution with $q = -e_0$:

$$\left[\vec{r}_\perp(t) - \vec{R}\right]^2 = \left[\frac{\dot{\vec{r}}(t=0)}{\omega_c}\right]^2 \quad \text{where} \quad \vec{R} = \frac{1}{2}\begin{pmatrix} x(0) \\ y(0) \end{pmatrix} - \frac{1}{m\omega_c}\begin{pmatrix} p_y(0) \\ -p_x(0) \end{pmatrix}$$

Note: $\vec{R}(t)$ is a constant of the motion! So $\vec{R}(t) = \vec{R}(t=0)$, i.e. $\frac{d\vec{R}}{dt} = 0$.

We make $\vec{R}$ into an operator, and we get that (for all gauges):

$$\left[\hat{\vec{R}}, H\right] = 0 \qquad \text{(Because classical } \vec{R} \text{ is a constant of the motion!)}$$

$\hat{\vec{R}}$ is denoted the "guiding centre operator".

We can diagonalize $\hat{R}_x$ and H simultaneously (or $\hat{R}_y$ and H). However,

$$[\hat{R}_x, \hat{R}_y] = \left[\frac{x}{2} - \frac{1}{m\omega_c}p_y, \frac{y}{2} + \frac{1}{m\omega_c}p_x\right] = \frac{1}{2m\omega_c}[x, p_x] - \frac{1}{2m\omega_c}[p_y, y] = \frac{1}{2m\omega_c} 2i\hbar = \frac{i\hbar}{m\omega_c}$$

$\Rightarrow$ You can't measure $\hat{R}_x$ and $\hat{R}_y$ simultaneously with high accuracy! We have to pick one of them as our "good" quantum number.

$\Rightarrow$ We can label our wave functions by n and the $\hat{R}_x$ eigenvalue (or alternatively, the $\hat{R}_y$ eigenvalue, but not both!). The R_x will label the degeneracce.

n and R_x "are good quantum numbers" because they span the whole Hilbert space.