Gauge Invariance & Path Integrals

Gauge Invariance

ex: Hydrogen atom in a magnetic field

$$H = \frac{1}{2m_e}\left[\vec{P} - q\vec{A}(\vec{R})\right]^2 + V(\vec{R}) \Leftarrow \frac{P^2}{2m_e} + V(\vec{R})$$

$\vec{A}$ is magnetic vector potential.

Recall from classical E&M:

$$\vec{E}(\vec{r},t) = -\vec{\nabla}\mathcal{U}(\vec{r},t) - \frac{\partial}{\partial t}\vec{A}(\vec{r},t)$$
$$\vec{B}(\vec{r},t) = \vec{\nabla}\times\vec{A}(\vec{r},t)$$

to obtain same $\vec{E}, \vec{B}$ we can specify a scalar function $\chi(r,t)$ such that

$$\mathcal{U}'(\vec{r},t) = \mathcal{U}(\vec{r},t) - \frac{\partial}{\partial t}\chi(\vec{r},t)$$
$$\vec{A}'(\vec{r},t) = \vec{A}(\vec{r},t) + \vec{\nabla}\chi(\vec{r},t)$$

this is called a <u>gauge transformation</u>.

Schrödinger equation depends on $\mathcal{U}, \vec{A}$:
do physical results of theory depend on gauge?

Consider the <u>mechanical</u> momentum

$$\vec{\pi} = \vec{p} - q\vec{A}(r,t)$$

$\vec{p}$ is not gauge invariant, but $\vec{\pi}$ is :

Let's see this !

Classically we have the Lorentz force equation :

$$\vec{F} = q\left[\vec{E}(\vec{r},t) + \vec{v}\times\vec{B}(r,t)\right]$$

$$m\frac{d^2}{dt^2}\vec{r}(t) = \vec{F}$$, depends on $\vec{E}, \vec{B}$

so $(\vec{r},\vec{v})$ are not gauge dependent.

$$r'(t) = r(t)$$

$$p'(t) = p(t) + q\nabla\chi(r(t),t)$$

since

$$\pi(t) = p(t) - qA(\vec{r},t)$$

$$\pi'(t) = p'(t) - q(A'(r',t))$$

and we know $\pi(t) = \pi'(t)$ since

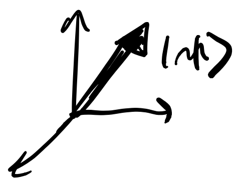
If $\mathcal{L} = \frac{1}{2}mv^2 - q(\mathcal{U}(r,t) - v\cdot A(r,t))$

$$p = \nabla_v\mathcal{L} = m\vec{v} + q\vec{A}(r,t)$$

$$\boxed{m\vec{v} = \vec{\pi}}$$

Gauge invariance in quantum mechanics

Physical system is characterized by a state vector $|\psi\rangle$, which depends on gauge.



There is a unitary transformation from gauge g to gauge g' of the state vector.

Observables are also modified by gauge transformations.

The physical content of quantum mechanics does not depend on gauge chosen.

In the $\{|r\rangle\}$ representation, $\vec{R}$ acts as multiplication by r.

p acts like derivative $\frac{\hbar}{i}\vec{\nabla}$

$$R_{g'} = R_g$$

$$P_{g'} = P_g$$

Mechanical momentum: $\Pi_g = P - qA(R,t)$

$$\Pi_{g'} = \Pi_g - q\nabla\chi(R,t)$$

$$H_g = \frac{1}{2m}\left[P - qA(R,t)\right]^2 + qU(R,t)$$

Transformation of state vector:

$$|\psi'(t)\rangle = T_\chi |\psi(t)\rangle$$

$$T_\chi^\dagger T_\chi = \mathbb{1}$$

$$T_\chi = e^{\frac{iq}{\hbar}\chi(R,t)}$$

$$\psi'(r,t) = e^{\frac{iq\chi(R,t)}{\hbar}} \psi(r,t)$$

Transformation of observables:

Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H_g(t)|\psi(t)\rangle$$

we have a new equation in other gauge g':

$$i\hbar \frac{\partial}{\partial t} |\psi'(t)\rangle = H_{g'}(t)|\psi'(t)\rangle$$

Consider L.H.S.

$$i\hbar \frac{\partial}{\partial t} |\psi'(t)\rangle = i\hbar \frac{\partial}{\partial t} \left\{ T_\chi |\psi(t)\rangle \right\}$$

$$= i\hbar\left(\frac{\partial}{\partial t} T_\chi\right)|\psi\rangle + i\hbar T_\chi \frac{\partial}{\partial t}|\psi(t)\rangle$$

$$= -q\frac{\partial}{\partial t}\chi(R,t)\,T_\chi|\psi\rangle + T_\chi H_g|\psi\rangle$$

Define $\tilde{H}_g = T_\chi H_g T_\chi^\dagger$

$$= \left\{-q\frac{\partial}{\partial t}\chi(R,t) + \tilde{H}_g(t)\right\}|\psi'(t)\rangle$$

Consider

$$\tilde{H} = \frac{1}{2m}\left[\tilde{p} - qA(\tilde{R},t)\right] + qU(\tilde{R},t)$$

$$\tilde{R} = T_\chi R T_\chi^\dagger = R$$

$$\tilde{p} = T_\chi p T_\chi^\dagger = p - q\nabla\chi(R,t)$$

$$\Rightarrow \tilde{H}_g = \frac{1}{2m}\left[p - q(A - \nabla\chi)\right] + qU$$

$$H_g' = \tilde{H}_g - q\frac{\partial}{\partial t}\chi(R,t)$$

observables : $\underline{\tilde{K} = T_\chi K T_\chi^\dagger}$

$\tilde{R}_g = R_g'$ but $\tilde{P}_g \neq P_g'$

not a true physical quantity.

$\tilde{\Pi}_g = \Pi_g'$

true physical quantities

When we measure a true physical quantity G.
Let g be the gauge. State is $|\psi\rangle$,
observable G_g. Suppose $|\varphi_n\rangle$ is an eigenvector
of G_g with eigenvalue g_n. Assume non-degenerate.

$$G_g |\varphi_n\rangle = g_n |\varphi_n\rangle.$$

Probability to obtain g_n : $P_n = |\langle\varphi_n|\psi\rangle|^2$

But what happens in a gauge transformation?

If gauge changes to g',

$$|\varphi_n'\rangle = T_\chi |\varphi_n\rangle$$

$$G_{g'} |\varphi_n'\rangle = T_\chi G_g T_\chi^\dagger \left(T_\chi |\varphi_n\rangle\right)$$

$$= T_\chi g_n |\varphi_n\rangle = g_n |\varphi_n'\rangle$$

$$\langle\varphi_n'|\psi'\rangle = \langle\varphi_n | T_\chi^\dagger T_\chi | \psi\rangle$$

$$= \langle\varphi_n|\psi\rangle$$

So measurement result g_n and probability
$|\langle\varphi_n|\psi\rangle|^2$ are <u>gauge invariant</u>.

Example 1 : Hydrogen atom in a magnetic field.

$$H = \frac{1}{2m_e}\left[\vec{P} - q\vec{A}(\vec{R})\right]^2 + V(R)$$

Assume a uniform magnetic field $\vec{B} = \vec{\nabla}\times\vec{A}(r)$

$$\vec{A}(r) = -\frac{1}{2}\,\vec{r}\times\vec{B}$$

($\vec{B}$ isn't an operator here)

$$\left[\vec{P} - q\vec{A}(\vec{R})\right]^2 = P^2 + \frac{q}{2}\left[\vec{B}\cdot(\vec{P}\times\vec{R}) - (\vec{R}\times\vec{P})\cdot\vec{B}\right]$$
$$+ \frac{q^2}{4}\left[R^2B^2 - (\vec{R}\cdot\vec{B})^2\right]$$

$$H = H_0 + H_1 + H_2$$

$$H_0 = \frac{P^2}{2m_e} + V(\vec{R})$$

$$H_1 = -\frac{\mu_B}{\hbar}\vec{L}\cdot\vec{B} \qquad \mu_B \equiv \frac{q\hbar}{2m_e} \text{ (Bohr magneton)}$$

$$H_2 = \frac{q^2B^2R_\perp^2}{8m_e} \qquad R_\perp^2 = R^2 - \frac{(\vec{R}\cdot\vec{B})^2}{B^2}$$

projection $\vec{R}$ on plane $\perp$ to $\vec{B}$.

Note : $\vec{\Pi} = m_e\vec{V}$ is "mechanical momentum"

$$\frac{\Pi^2}{2m_e} = \frac{1}{2m_e}\left(\vec{P} - q\vec{A}(\vec{R})\right)^2$$

Consider relative sizes of these terms

Hydrogen H_0 $\frac{\Delta E}{h} \simeq 10^{14} - 10^{15}$ Hz

$$\simeq \frac{\hbar^2}{m_e a_0^2} \frac{1}{h}$$

$$\frac{\Delta E_1}{h} = \frac{1}{h}\left(\frac{\mu_B}{\hbar} \hbar B\right) = \frac{\omega_L}{2\pi}$$

$$\frac{\omega_L}{2\pi B} = 1.4 \text{ MHz/ Gauss}$$

so $\Delta E_1 << \Delta E_0$

Also $\Delta E_2 << \Delta E_1$

since $\Delta E_2 = \frac{q^2 B_0^2 a_0^2}{m_e}$,

$$\frac{\Delta E_2}{\Delta E_1} \sim 2\hbar \frac{qB}{m_e} \frac{m_e a_0^2}{\hbar^2} \simeq \frac{\Delta E_1}{\Delta E_0}$$

typically we can neglect H_2 when H_1 has a nonzero contribution.

Consider H_1 : $-\frac{\mu_B}{\hbar} \vec{L} \cdot \vec{B} = -\vec{M}_1 \cdot \vec{B}$

for a magnetic moment $\vec{M}_1$.

Related to classical revolution of an electron in orbit.

Classical argument :

the current $i = q\dfrac{v}{2\pi r}$

$$|M| = i \times A = q\frac{v}{2\pi r}\pi r^2 = \frac{q}{2} r v$$

Classical angular momentum

$|\mathcal{L}| = m_e r v$

Moment $\mathcal{M} = \dfrac{q\mathcal{L}}{2m_e}$ $\left(\vec{M}_1 = \dfrac{q}{2m_e}\vec{L} \right)$

Still classical

But we must not confuse angular momentum $\vec{r}\times\vec{p} = \vec{\mathcal{L}}$ with mechanical momentum $\vec{r}\times m_e\vec{v}$

$$\vec{r}\times m_e\vec{v} = \vec{\mathcal{L}} - q\vec{r}\times A(\vec{r})$$

But this is a small error !

$\mathcal{M}$ is propotional to $\vec{r}\times m_e\vec{v}$ not $\vec{r}\times\vec{p}$

$$\vec{\mathcal{M}} = \frac{q}{2m_e}(\vec{r}\times m_e\vec{v}) = \frac{q}{2m_e}\left[\vec{\mathcal{L}} - q\vec{r}\times\vec{A}(r)\right]$$

in our gauge, this is $= \dfrac{q}{2m_e}\left[\vec{r}\times\vec{p} - q\vec{r}\times\vec{A}(\vec{r})\right]$

$\vec{A} = -\frac{1}{2}\vec{r}\times\vec{B}$

$$= \frac{q}{2m_e}\left[\vec{r}\times\vec{p}\right] + \frac{q^2}{4m_e}\vec{r}\times(\vec{r}\times\vec{B})$$

$$= \underbrace{\frac{q}{2m_e}\left(\vec{r}\times\vec{p}\right]}_{m_1} + \underbrace{\frac{q^2}{4m_e}\left[(\vec{r}\cdot\vec{B})\vec{r} - r^2\vec{B}\right]}_{m_2}$$

proportional to B.

m_2 induced moment,

energy $-\frac{1}{2}m_2\cdot B$

$$= \frac{q^2}{8m_e}\left[r^2B^2 - (\vec{r}\cdot\vec{B})^2\right] = \frac{q}{8m_e}R_\perp^2 B^2$$

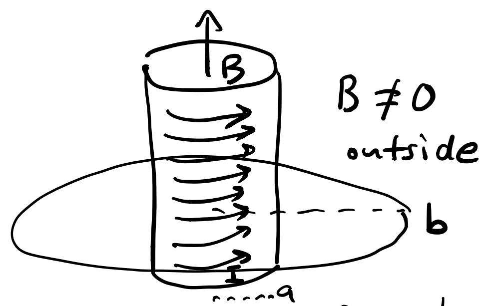
Induced moment, according to Lenz's law opposes the applied field. H_2 is called the diamagnetic term.

Example 2

Aharonov Bohm effect & Geometric Phase

The vector potential $\vec{A}$ can affect the quantum behavior of a particle that never sees a magnetic field!

Consider a particle confined to move on a circular track outside of a solenoid



Let b be the radius of the circular track.
charge on particle is q.

The vector potential can be chosen e.g. as

$$\vec{A} = \frac{\Phi}{2\pi r}\hat{\phi}.$$

Φ is the magnetic flux through the solenoid.

$$\Phi = \pi a^2 B$$

Assume no scalar potential. $\mathcal{U} = 0$

$$\vec{\nabla}\times\vec{A} = \hat{z}\,\frac{1}{r}\frac{\partial}{\partial r}\left(r\,\frac{\Phi}{2\pi r}\right)$$

$= 0$ outside solenoid, since Φ is independent of r.

$$= \hat{z}\,\frac{1}{r}\frac{\partial}{\partial r}\left(r\,\frac{\pi r^2 B}{2\pi r}\right) = B\hat{z}$$ inside solenoid.

The Hamiltonian is

$$H = \frac{1}{2m}(p - qA)^2 + q\mathcal{U}, \qquad \mathcal{U} = 0$$

$$= \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} - q\vec{A}\right)^2$$

$$= \frac{1}{2m}\left(-\hbar^2\nabla^2 + q^2A^2 + i\hbar q\,\vec{A}\cdot\vec{\nabla} + i\hbar q\,\vec{\nabla}\cdot\vec{A}\right)$$

Consider e.g. $\vec{\nabla}\cdot(f\vec{A}) = \vec{\nabla}f\cdot\vec{A} + f(\vec{\nabla}\cdot\vec{A})$

f, A will be functions of (r,ϕ), $\vec{\nabla}\cdot\vec{A}=0$ in this gauge, we can write

$$H = \frac{1}{2m}\left(-\hbar^2\nabla^2 + q^2A^2 + 2i\hbar q\,\vec{A}\cdot\vec{\nabla}\right)$$

Schrödinger equation:

$$\frac{1}{2m}\left[-\frac{\hbar^2}{b^2}\frac{d^2}{d\phi^2} + \left(\frac{q\Phi}{2\pi b}\right)^2 + \frac{i\hbar q\,\Phi}{\pi b^2}\frac{d}{d\phi}\right]\psi(\phi) = E\psi(\phi)$$

This can be simplified!

$$\frac{d^2\psi}{d\phi^2} + 2i\beta\frac{d\psi}{d\phi} + \epsilon\psi = 0$$

$$\beta \equiv \frac{q\Phi}{2\pi\hbar} \qquad \epsilon = \frac{2mb^2E}{\hbar^2} - \beta^2$$

The solution of this is

$$\psi = A e^{i\lambda\phi} \qquad \lambda = \beta \pm \sqrt{\beta^2+\epsilon}$$

$$\lambda = \beta \pm \frac{b}{\hbar}\sqrt{2mE}$$

we require $\psi(\phi) = \psi(\phi+2\pi)$

$$\beta \pm \frac{b}{\hbar}\sqrt{2mE} = n \qquad \text{for } n = 0, \pm1, \pm2, \ldots$$

The energy is

$$E_n = \frac{\hbar^2}{2mb^2}\left(n - \frac{q\Phi}{2\pi\hbar}\right)^2$$

there is a degeneracy lifted by the presence of the solenoid. Particle going same direction as current $(n > 0)$ has lower energy than particle going against the current $(n < 0)$.

The allowed energies depend on the solenoid flux even though the field is zero at the location of the particle!

For the Aharonov-Bohm effect we can consider the phase accumlated by an electron matter wave as it traverses a region around a magnetic flux.

There is also a scalar Aharonov-Bohm effect

(more on this later, path integrals)