§ 海森堡方程.

H picture下, H方程.

$$\frac{d\cancel{A}Q}{dt} = \frac{1}{i\hbar}[\overset{Q}{\cancel{A}}, H]$$

Erenfest 定理, 以上对应经典方程. $\frac{dQ}{dt} = \{Q, H\}$

我们来验证一下. 带电粒子在电磁场中的运动方程 (H picture)

$$[\hat{x}_i, \hat{p}_i] = i\hbar \quad \leftarrow [x_i, p_j] = i\hbar\delta_{ij}$$

$$\frac{dx_i}{dt} = \frac{1}{i\hbar}[x_i, H], \quad H = \frac{(P - \frac{qA}{c})^2}{2\mu} + q\phi$$

$$[x_i, \phi] = 0. \quad [x_i, \vec{A}] = 0, \quad \vec{v}^2 = \vec{v}\cdot\vec{v} = \sum_i v_i^2$$

$$\left[x_i, (P - \frac{qA}{c})^2\right] = (P_i - \frac{qA_i}{c})[x_i, P_i - \frac{qA_i}{c}]$$

$$+ [x_i, P_i - \frac{qA_i}{c}](P_i - \frac{qA_i}{c})$$

$$= 2i\hbar(P_i - \frac{qA_i}{c})$$

$$\therefore \frac{dx_i}{dt} = \frac{1}{\mu}(P_i - \frac{qA_i}{c}) = \frac{\pi_i}{\mu}$$

用到 $[x, p] = i\hbar$

用量子力学得到 $\hat{P}$ 与 $\hat{\pi}$ 的关系, 说明 $\hat{P} = -i\hbar\nabla$ 正确

(从H导出 $\hat{P}$ 与 $\hat{\pi}$ 算符的关系). H也是正确的

再来验证 $\mu\ddot{\vec{r}} = q\vec{E} + q\vec{v}\times\vec{B}$ 与海森堡方程形式相同.

$\Rightarrow \frac{d\vec{\pi}}{dt}$

• 首先计算 $[\pi_i, \pi_j] = \frac{i\hbar q}{c}\varepsilon_{ijk} B_k$ (1)

$$\varepsilon_{123} = 1,\quad \varepsilon_{213} = -1,\quad \varepsilon_{231} = 1 \quad \cdots$$
$$\varepsilon_{ijk} = -\varepsilon_{jik}$$

证明:

$$[\pi_1, \pi_2] = \left[p_1 - \frac{qA_1}{c},\ p_2 - \frac{qA_2}{c}\right]$$

$$= [p_1, p_2] - \left[p_1, \frac{qA_2}{c}\right] - \left[\frac{qA_1}{c}, p_2\right] + \left[\frac{qA_1}{c}, \frac{qA_2}{c}\right]$$

利用: $[p_1, A_2]\psi = -i\hbar\partial_x(A_2\psi) + A_2 i\hbar\partial_x\psi = (-i\hbar\partial_x A_2)\psi$

(坐标表象看) (或者: $[p_x, f(x)] = -i\hbar\partial_x f(x)$ ← 由 $[x, p_x] = i\hbar$ 导出)

$$-\left[\frac{qA_1}{c}, p_2\right]\psi = \left[p_2, \frac{qA_1}{c}\right]\psi = \frac{q}{c}(-i\hbar\partial_y A_1)\psi$$

$$\left.\begin{aligned}[\pi_1, \pi_2] &= \frac{qi\hbar}{c}(\partial_x A_2 - \partial_y A_1)\\ \vec{B} &= \nabla\times\vec{A}\end{aligned}\right\} = \frac{qi\hbar}{c} B_3$$

证毕

• $[\pi_i, \phi] = \left[p_i - \frac{qA}{c}, \phi\right] = -i\hbar\partial_i\phi$

$$\Rightarrow \frac{d\pi_i}{dt} = \frac{1}{i\hbar}\left[\pi_i, \frac{\pi^2}{2\mu} + q\phi\right], \quad \pi^2 = \pi_1^2 + \pi_2^2 + \pi_3^2$$

以 $\frac{d\pi_1}{dt} = \frac{1}{i\hbar}\left(\left[\pi_1, \frac{\pi_2^2}{2\mu}\right] + \left[\pi_1, \frac{\pi_3^2}{2\mu}\right] + [\pi_1, q\phi]\right)$

然而: $\vec{\pi} = \vec{p} - \frac{q\vec{A}}{c}$, 当 $\frac{\partial\vec{A}(x,t)}{\partial t} \neq 0$, $\frac{d\pi_i}{dt} = \frac{1}{i\hbar}[\pi_i, H] - \frac{q\partial A_i}{c\partial t}$

$$[\pi_1, \pi_2^2] = \pi_2[\pi_1, \pi_2] + [\pi_1, \pi_2]\pi_2$$

$$= (\pi_2 B_3 + B_3 \pi_2)\frac{i\hbar q}{c}$$

$$[\pi_1, \pi_3^2] = -(\pi_3 B_2 + B_2 \pi_3)\frac{i\hbar q}{c}$$

$$\frac{d\pi_1}{dt} = \frac{1}{i\hbar}\left(-i\hbar \underbrace{\partial_x q\phi}_{-(\nabla\phi)_1} + \frac{i\hbar q}{2\mu c}\left[\underbrace{(\pi_2 B_3 - \pi_3 B_2)}_{(\vec\pi\times\vec B)_1} - \underbrace{(B_2\pi_3 - B_3\pi_2)}_{(\vec B\times\vec\pi)_1}\right]\right) - \frac{q}{c}\frac{\partial A_1}{\partial t}$$

$$\boxed{\frac{d\vec\pi}{dt} = q\vec E + \frac{q}{c\cdot 2\mu}(\vec\pi\times\vec B - \vec B\times\vec\pi)}$$ ← 牛顿方程，含Lorentz力

$\because \vec E = -\nabla\phi - \frac{\partial\vec A}{c\,\partial t}$，$\frac{\vec\pi}{\mu} = \frac{d\vec x}{dt}$，

$$\vec\pi\times\vec B = \begin{vmatrix} i & j & k \\ \pi_1 & \pi_2 & \pi_3 \\ B_1 & B_2 & B_3 \end{vmatrix}, \quad \vec B\times\vec\pi = \begin{vmatrix} i & j & k \\ B_1 & B_2 & B_3 \\ \pi_1 & \pi_2 & \pi_3 \end{vmatrix}$$

- $\vec B\times\vec\pi \overset{?}{=} -\vec\pi\times\vec B$
- 验证了 Erenfest 定理.
- $\hat p = -i\hbar\nabla$ 正确. ← 对易式.

§ 规范变换，规范不变.

用 ϕ 与 $\vec{A}$ 描述电磁场：$\vec{E}=-\nabla\phi-\frac{1}{c}\frac{\partial\vec{A}}{\partial t}$，$\vec{B}=\nabla\times\vec{A}$

带电粒子的运动可由哈密顿量 $H=\frac{1}{2\mu}\left(\vec{p}-\frac{q\vec{A}}{c}\right)^2+q\phi$

描述：$\dot{\vec{r}}=\frac{\partial H}{\partial\vec{p}}$，$\dot{\vec{p}}=-\frac{\partial H}{\partial\vec{r}}$. $\vec{\pi}=\vec{p}-\frac{q\vec{A}}{c}$ 为机械动量

等价于牛顿方程（含 Lorentz 力）.

进而我们得到 schrödinger 方程.

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

在坐标表象下，$\vec{p}\to-i\hbar\nabla$，$\vec{p}-\frac{q\vec{A}}{c}\to-i\hbar\nabla-\frac{q\vec{A}}{c}=\vec{\pi}$

$|\psi(x)|^2=\rho$ 仍有几率解释. 满足：

$$\frac{\partial\rho}{\partial t}+\nabla\cdot\vec{j}=0$$

其中 $\vec{j}=\frac{1}{2\mu}\left(\psi^*\vec{\pi}\psi+\psi\vec{\pi}^*\psi^*\right)$

将 ψ 写成 $\psi=\sqrt{\rho}\,e^{iS/\hbar}$，则

$$\vec{j}=\frac{\rho}{\mu}\left(\nabla S-\frac{q\vec{A}}{c}\right)\quad\left(\text{在 }\vec{A}=0\text{ 时退化为 }\vec{j}=\frac{\rho}{\mu}\nabla S\right)$$

我们知道电磁场 $(\vec{E},\vec{B})$ $(\phi,\vec{A})$ 在规范变换 (gauge transformation)

$$\phi\to\phi'=\phi-\frac{\partial\Lambda}{c\,\partial t},\quad\vec{A}\to\vec{A}'=\vec{A}+\nabla\Lambda$$

原则上 $\Lambda(\vec{x},t)$.

下不变，因为 $\vec{E}=-\nabla\phi-\frac{1}{c}\frac{\partial\vec{A}}{\partial t}$，$\vec{B}=\nabla\times\vec{A}$

两个例子：① $\frac{\partial\Lambda}{\partial t}=$ 常数入，$\nabla\Lambda=0$，势能零点移动，$\vec{A}$ 不变. ② Λ 只是 $\vec{x}$ 函数. $\frac{\partial\Lambda}{\partial t}=0$. ϕ 不变.

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

设 $|\alpha\rangle$ 是由 $\vec{A}$ 描述的电磁场中的态矢. 若用 $\vec{A}' = \vec{A} + \nabla\Lambda$ 描述, 则态矢变成 $|\alpha'\rangle$, 它们可以有 $|\alpha'\rangle = g|\alpha\rangle$

态矢的规范变换

首先我们可以要求(态矢归一)

$$\langle\alpha|\alpha\rangle = \langle\alpha'|\alpha'\rangle.$$

(否则无法保证测量不变).

那么 $\langle\alpha'|\alpha'\rangle = \langle\alpha|g^{+}\cdot g|\alpha\rangle \Rightarrow g^{+}g = \mathbb{1}$

即 变换 g 是幺正的 (Unitary)

☆ 物理量在不同规范下期望值不应变化, 即

(还有概率)

$$\langle\alpha|\vec{x}|\alpha\rangle = \langle\alpha'|\vec{x}|\alpha'\rangle$$

$$\langle\alpha|\underbrace{(\vec{p} - \frac{q\vec{A}}{c})}_{\vec{\pi}}|\alpha\rangle = \langle\alpha'|\underbrace{(\vec{p} - \frac{q\vec{A}'}{c})}_{\vec{\pi}'}|\alpha'\rangle$$

称为 gauge invariant (规范不变). (同时假设 $\vec{x}, \vec{p}$ 不变, $[x_i, p_j] = i\hbar\delta_{ij}$)

也就是要求: $g^{+}\vec{x}g = \vec{x}$

$$g^{+}(\vec{p} - \frac{q\vec{A}}{c} - \frac{q\nabla\Lambda}{c})g = \vec{p} - \frac{q\vec{A}}{c}$$

假设 $g = e^{\frac{iq\Lambda(\vec{x})}{\hbar c}}$, 则上两式可满足.

- $g^{+}g = \mathbb{1}$ 且是幺正的

- $[\vec{x}, g] = 0 \Rightarrow g^{+}\vec{x}g = \vec{x}$

注: $\Lambda(\vec{x})$ 中 $\vec{x}$ 是算符

• $e^{-\frac{iq\Lambda}{\hbar c}}\,\vec{p}\,e^{\frac{iq\Lambda}{\hbar c}} = e^{-\frac{iq\Lambda}{\hbar c}}\left[\vec{p}, e^{\frac{iq\Lambda}{\hbar c}}\right] + \vec{p}$

$$= -e^{-\frac{iq\Lambda}{\hbar c}}\, i\hbar\nabla\, e^{\frac{iq\Lambda}{\hbar c}} + \vec{p}$$

$$= \vec{p} + \frac{q\nabla\Lambda}{c}$$

注：用到 $[x, p_x] = i\hbar$

$\Rightarrow \vec{p}\cdot f(x) - f(x)\vec{p} = -i\hbar\nabla f(x)$

因此 $\langle \pi \rangle$ 规范不变 .

☆ 态可以变，但测量不变

(补充)

证明 $[P_x, f(x)] = -i\hbar \dfrac{\partial f(x)}{\partial x}$

$$f(x) = \sum_n \frac{1}{n!} f^{(n)}(0)\, x^n$$

$$[P_x, f(x)] = \sum_n \frac{1}{n!} f^{(n)}(0)\, [P_x, x^n]$$

由于 $[P_x, x] = -i\hbar$, $[P_x, x^2] = x[P_x, x] - [P_x, x]x = -2i\hbar x$

设 $[P_x, x^n] = -i\hbar n x^{n-1}$

则 $[P_x, x^{n+1}] = [P_x, x^n \cdot x] = P_x x^n x - x^n x P_x + x^n P_x x - x^n P_x x$

$= -i\hbar n x^{n-1} \cdot x - i\hbar x^n$

$= -i\hbar (n+1) \cdot x^n$

$$\Rightarrow [P_x, f(x)] = \sum_n \frac{1}{n!} f^{(n)}(0)\, (-i\hbar n)\, x^{n-1}$$

$$= -i\hbar \partial_x f(x)$$