Chapter 1: Phase in Quantum Mechanics

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$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H(t)|\psi\rangle \tag{1}$$

$$|\psi(t)\rangle = |\psi(t)|e^{i\phi(t)} \tag{2}$$

1 Berry's Phase

H 不含时

$$H|n\rangle = E_n|n\rangle \tag{3}$$

E_n 是本征值，$|n\rangle$ 是本征态。本征态构成正交完备基，可以用来展开

$$|\psi(t)\rangle = \sum_n c_n(t)|n\rangle \tag{4}$$

$$c_n(t) = \langle n|\psi(t)\rangle \tag{5}$$

$$|\psi(t)\rangle = \sum_n \langle n|\psi(t)\rangle|n\rangle = \sum_n |n\rangle\langle n|\psi(t)\rangle \tag{6}$$

得到单位算符 $\sum_n |n\rangle\langle n| = 1$。将 $|\psi\rangle(t)$ 代入薛定谔方程

$$i\hbar\frac{\partial}{\partial t}\sum_n c_n(t)|n\rangle = H\sum_n c_n(t)|n\rangle = \sum_n c_n(t)H|n\rangle = \sum_n c_n(t)E_n|n\rangle \tag{7}$$

将 $\langle m|$ 作用在方程两边

$$i\hbar\frac{\partial}{\partial t}\sum_n c_n(t)\langle m|n\rangle = \sum_n c_n(t)E_n\langle m|n\rangle \tag{8}$$

$$i\hbar\frac{\partial}{\partial t}c_m(t) = E_m c_m(t) \tag{9}$$

$$i\hbar\frac{1}{c_m(t)}\frac{\partial}{\partial t}c_m(t) = E_m \tag{10}$$

$$\int_0^t i\hbar\frac{1}{c_m(t')}\frac{\partial}{\partial t'}c_m(t')\mathrm{d}t' = \int_0^t E_m\mathrm{d}t' \tag{11}$$

$$i\hbar|\ln c_m(t) - \ln c_m(0)| = E_m(t)t \tag{12}$$

$$c_m(t) = c_m(0)e^{-i\frac{E_m(t)}{\hbar}t} \tag{13}$$

$$|\psi(t)\rangle = \sum_n c_n(t) |n\rangle = \sum_n c_n(0) e^{-i\frac{E_n(t)}{\hbar}t} |n\rangle \tag{14}$$

设 $|\psi(t)\rangle$ 在一个态上演化

$$c_n(t=0) = \delta_{n,m} \tag{15}$$

$$|\psi(t)\rangle = \sum_n \delta_{n,m} e^{-i\frac{E_n(t)}{\hbar}t} |n\rangle = e^{-i\frac{E_m(t)}{\hbar}t} |m\rangle \tag{16}$$

Slow varying Hamiltonian

$$H(t=0) |n(t=0)\rangle = E_n(t=0) |n(t=0)\rangle \tag{17}$$

当 $H(t) = H$ 时，

$$|\psi(t)\rangle = e^{-i\frac{E_n}{\hbar}t} |n\rangle \tag{18}$$

当 $H(t)$ 含时时，近似

$$|\psi(t)\rangle \doteq \exp\left[-\frac{i}{\hbar}\int_o^t E_n(t')\mathrm{d}t' + i\gamma_n(t)\right] |n(t)\rangle = c_n(t) |n(t)\rangle \tag{19}$$

$$H(t) |\psi(t)\rangle = i\hbar\frac{\partial}{\partial t} |\psi(t)\rangle \tag{20}$$

$$H(t)c_n(t) |n(t)\rangle = i\hbar\frac{\partial}{\partial t} c_n(t) |n(t)\rangle = i\hbar\dot{c}_n(t) |n(t)\rangle + i\hbar c_n(t) |\dot{n}(t)\rangle = E_n(t)c_n(t) |n(t)\rangle \tag{21}$$

$$\dot{c}_n(t) = c_n(t)\left[-\frac{i}{\hbar}E_n(t) + i\dot{\gamma}_n(t)\right] \tag{22}$$

代入 Eq.(21)

$$E_n(t)c_n(t) |n(t)\rangle = E_n(t)c_n(t) |n(t)\rangle - \hbar\dot{\gamma}_n(t)c_n(t) |n(t)\rangle + i\hbar c_n(t) |\dot{n}(t)\rangle \tag{23}$$

即

$$\dot{\gamma}_n(t) |n(t)\rangle = i |\dot{n}(t)\rangle \tag{24}$$

哈密顿量依赖时间往往是通过形式 $H(t) = H(\vec{R}(t))$

$$H(\vec{R}(t)) \left|n(\vec{R}(t))\right\rangle = E_n(\vec{R}(t)) \left|n(\vec{R}(t))\right\rangle \tag{25}$$

$$\left|\dot{n}(\vec{R}(t))\right\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\vec{R}(t)\cdot\nabla_{\vec{R}} \left|n(\vec{R}(t))\right\rangle \tag{26}$$

$$\dot{\gamma}_n(t) \left|n(\vec{R}(t))\right\rangle = i\frac{\mathrm{d}}{\mathrm{d}t}\vec{R}(t)\cdot\nabla_{\vec{R}} \left|n(\vec{R}(t))\right\rangle = i\frac{\mathrm{d}}{\mathrm{d}t}\vec{R}(t)\cdot\left|\nabla_{\vec{R}} n(\vec{R}(t))\right\rangle \tag{27}$$

将 $\left\langle n(\vec{R}(t))\right|$ 作用在方程两边

$$\dot{\gamma}_n(t) = i\left\langle n(\vec{R}(t))\middle|\nabla_{\vec{R}} n(\vec{R}(t))\right\rangle\cdot\dot{\vec{R}}(t) \tag{28}$$

$$\begin{aligned}\gamma_n(t) &= i\int_0^t \left\langle n(\vec{R}(t'))\middle|\nabla_{\vec{R}} n(\vec{R}(t'))\right\rangle\cdot\dot{\vec{R}}(t')\mathrm{d}t' \\ &= i\int_{\vec{R}(0)}^{\vec{R}(t)} \left\langle n(\vec{R}(t'))\middle|\nabla_{\vec{R}} n(\vec{R}(t'))\right\rangle \mathrm{d}\vec{R}(t') \\ &= i\int_0^t \langle n(t')|\dot{n}(t')\rangle \,\mathrm{d}t'\end{aligned} \tag{29}$$

代入近似解

$$|\psi(t)\rangle \doteq \exp\left[-\frac{i}{\hbar}\int_o^t E_n(t')\mathrm{d}t'\right]\exp\left[-\int_0^t \langle n(t')|\dot{n}(t')\rangle\,\mathrm{d}t'\right]|n(t)\rangle \tag{30}$$

$$\alpha_n(t) = -\frac{1}{\hbar}\int_o^t E_n(t')\mathrm{d}t' \tag{31}$$

$$\gamma_n(t) = i\int_0^t \langle n(t')|\dot{n}(t')\rangle\,\mathrm{d}t' \neq 0 \tag{32}$$

$\alpha_n(t)$ 被称为动力学因子 (Dynamic phase factor)，$\gamma_n(t)$ 被称为几何因子 (Geometry phase factor)，也叫 Berry's Phase。

给定一特殊情况，$\vec{R}(0)=\vec{R}(T), H(0)=H(T)$，$T$ 时刻

$$\gamma_n(T) = i\int_0^T \left\langle n(\vec{R}(t'))\middle|\nabla_{\vec{R}} n(\vec{R}(t'))\right\rangle\cdot\mathrm{d}\vec{R}(t') \tag{33}$$

环路积分

$$\gamma_n(C) = i\oint_C \left\langle n(\vec{R})\middle|\nabla_{\vec{R}} n(\vec{R})\right\rangle\cdot\mathrm{d}\vec{R} \tag{34}$$

2 Adiabatic Condition 绝热条件

我们已经得到

$$|\psi(t)\rangle \doteq \exp\left[-\frac{i}{\hbar}\int_o^t E_n(t')\mathrm{d}t'\right]\exp\left[-\int_0^t \langle n(t')|\dot{n}(t')\rangle\,\mathrm{d}t'\right]|n(t)\rangle \tag{35}$$

那么上述近似在什么情况下是一个好的近似? $H(t)$ 变化缓慢（极端情况 $H(t)=H$）。

假定

$$|\psi(0)\rangle = |m\rangle \tag{36}$$

即 $|\psi\rangle$ 在态 $|m\rangle$ 上演化。当 $t\leq 0$ 时，$H(t)=H(0)$；当 $t>0$ 时，$H(t)$ 含时。

$$H(0)\,|m\rangle = E_m(0)\,|m\rangle \tag{37}$$

将 $|\psi\rangle$ 用一组正交完备积 $|l\rangle$ 展开

$$|\psi(t)\rangle = \sum_l c_l(t)\,|l(t)\rangle \tag{38}$$

其中

$$c_l(t) = a_l(t)\exp\left[-\frac{i}{\hbar}\int_0^t E_l(t')\mathrm{d}t'\right] \tag{39}$$

将 $|\psi(t)\rangle$ 代入薛定谔方程 $i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle$

$$\begin{aligned} &i\hbar\sum_l\left\{\dot{a}_l\exp\left[-\frac{i}{\hbar}\int_0^t E_l(t')\mathrm{d}t'\right]|l\rangle - \frac{i}{\hbar}a_l E_l\exp\left[-\frac{i}{\hbar}\int_0^t E_l(t')\mathrm{d}t'\right]|l\rangle + a_l\exp\left[-\frac{i}{\hbar}\int_0^t E_l(t')\mathrm{d}t'\right]\left|\dot{l}\right\rangle\right\} \\ &=\sum_l a_l\exp\left[-\frac{i}{\hbar}\int_0^t E_l(t')\mathrm{d}t'\right]H(t)\,|l\rangle = \sum_l a_l\exp\left[-\frac{i}{\hbar}\int_0^t E_l(t')\mathrm{d}t'\right]E_l\,|l\rangle \end{aligned} \tag{40}$$

即

$$i\hbar\sum_l\left\{\dot{a}_l\exp\left[-\frac{i}{\hbar}\int_0^t E_l(t')\mathrm{d}t'\right]|l\rangle + a_l\exp\left[-\frac{i}{\hbar}\int_0^t E_l(t')\mathrm{d}t'\right]\left|\dot{l}\right\rangle\right\} = 0 \tag{41}$$

将 $\langle n|$ 作用在方程左右两边

$$\sum_l \dot{a}_l(t)\exp\left[-\frac{i}{\hbar}\int_0^t E_l(t')\mathrm{d}t'\right]\delta_{n,l}+\sum_l a_l(t)\exp\left[-\frac{i}{\hbar}\int_0^t E_l(t')\mathrm{d}t'\right]\left\langle n(t)\middle|\dot{l}(t)\right\rangle=0 \tag{42}$$

即

$$\dot{a}_n(t)\exp\left[-\frac{i}{\hbar}\int_0^t E_n(t')\mathrm{d}t'\right]+\sum_l a_l(t)\exp\left[-\frac{i}{\hbar}\int_0^t E_l(t')\mathrm{d}t'\right]\left\langle n(t)\middle|\dot{l}(t)\right\rangle=0 \tag{43}$$

$$\dot{a}_n(t)=-a_n(t)\langle n(t)|\dot{n}(t)\rangle-\sum_{l(\neq n)} a_l(t)\exp\left\{\frac{i}{\hbar}\int_0^t [E_n(t')-E_l(t')]\mathrm{d}t'\right\}\left\langle n(t)\middle|\dot{l}(t)\right\rangle \tag{44}$$

由于我们讨论的是 $|\psi(0)\rangle=|m\rangle$，当 $|n\rangle=|m\rangle$ 时

$$\dot{a}_m(t)=-a_m(t)\langle m(t)|\dot{m}(t)\rangle-\sum_{l(\neq m)} a_l(t)\exp\left\{\frac{i}{\hbar}\int_0^t [E_m(t')-E_l(t')]\mathrm{d}t'\right\}\left\langle m(t)\middle|\dot{l}(t)\right\rangle \tag{45}$$

好的近似要求对于任意 $n\neq m$，$a_n(t)$ 都很小，同样 $\dot{a}_n(t)$ 也很小

$$\begin{aligned}\dot{a}_n(t)=-a_n(t)\langle n(t)|\dot{n}(t)\rangle\quad&-\sum_{l(\neq n)} a_l(t)\exp\left\{\frac{i}{\hbar}\int_0^t [E_n(t')-E_l(t')]\mathrm{d}t'\right\}\left\langle n(t)\middle|\dot{l}(t)\right\rangle\\=-a_n(t)\langle n(t)|\dot{n}(t)\rangle\quad&-\sum_{l(\neq n,m)} a_l(t)\exp\left\{\frac{i}{\hbar}\int_0^t [E_n(t')-E_l(t')]\mathrm{d}t'\right\}\left\langle n(t)\middle|\dot{l}(t)\right\rangle\\&-a_m(t)\exp\left\{\frac{i}{\hbar}\int_0^t [E_n(t')-E_m(t')]\mathrm{d}t'\right\}\langle n(t)|\dot{m}(t)\rangle\end{aligned} \tag{46}$$

当 $n,l\neq m$ 时，$a_n(t)$ 和 $a_l(t)$ 是小量，因此第一项和第二项是小量，而 $a_m(t)$ 是大量，因此要求 $\langle n|\dot{m}\rangle$ 是小量。

由于 $\langle n|\dot{m}\rangle$ 的量纲是 $\left[\frac{1}{T}\right]$，不能形容大小，因此我们需要寻找参数组成一个无量纲量，如

$$\left|\frac{\langle n|\dot{m}\rangle\hbar}{E_n-E_m}\right|\ll 1 \tag{47}$$

可以将它等价写成

$$\left|\frac{\hbar\langle n|\dot{H}|\dot{m}\rangle}{(E_n-E_n)^2}\right|\ll 1 \tag{48}$$

即“**绝热条件**”。

接下来证明二者等价：

$$H(t)|n(t)\rangle=E_n(t)|n(t)\rangle \tag{49}$$

对时间求导

$$\dot{H}(t)|n(t)\rangle+H(t)|\dot{n}(t)\rangle=\dot{E}_n(t)|n(t)\rangle+E_n(t)|\dot{n}(t)\rangle \tag{50}$$

将 $\langle m|$ 作用在方程两边

$$\langle m(t)|\dot{H}(t)|n(t)\rangle+H(t)\langle m(t)|\dot{n}(t)\rangle=\dot{E}_n(t)\langle m(t)|n(t)\rangle+E_n(t)\langle m(t)|\dot{n}(t)\rangle \tag{51}$$

即

$$\langle m(t)|\dot{H}(t)|n(t)\rangle+E_m\langle m(t)|\dot{n}(t)\rangle=E_n(t)\langle m(t)|\dot{n}(t)\rangle \tag{52}$$

$$\langle m(t)|\dot{H}(t)|n(t)\rangle=[E_n(t)-E_m(t)]\langle m(t)|\dot{n}(t)\rangle \tag{53}$$

$$\langle m(t)|\dot{n}(t)\rangle = \frac{\langle m|\dot{H}|n\rangle}{E_n - E_m} \tag{54}$$

证毕。

$$\begin{aligned}\dot{a}_m(t) &= -a_m(t)\langle m|m\rangle(t)\dot{m}(t) - \sum_{l(\neq m)} a_l(t)\exp\left\{\frac{i}{\hbar}\int_0^t [E_m(t') - E_l(t')]\mathrm{d}t'\right\}\left\langle m(t)\middle|\dot{l}(t)\right\rangle \\ &= -a_m(t)\langle m(t)|\dot{m}(t)\rangle \qquad \text{（第二项是小量）}\end{aligned} \tag{55}$$

$$\ln a_m(t')\Big|_0^t = -\int_0^t \langle m(t')|\dot{m}(t')\rangle\,\mathrm{d}t' \tag{56}$$

$$a_m(t) = \exp\left[-\int_0^t \langle m(t')|\dot{m}(t')\rangle\,\mathrm{d}t'\right]a_m(0) \tag{57}$$

$$\begin{aligned}|\psi(t)\rangle &= \sum_n a_n(t)\exp\left[-\frac{i}{\hbar}\int_0^t E_n(t)\mathrm{d}t'\right]|n(t)\rangle \\ &= a_m(t)\exp\left[-\frac{i}{\hbar}\int_0^t E_m(t)\mathrm{d}t'\right]|m(t)\rangle \qquad (n \neq m \text{ 都是小量}) \\ &= a_m(t)e^{i\alpha_m(t)}|m(t)\rangle\end{aligned} \tag{58}$$

$$|\psi(t)\rangle = e^{i[\alpha_m(t)+\gamma_m(t)]}|m(t)\rangle \tag{59}$$

Example

已知

$$H(\vec{B}(t)) = -\mu_B\vec{\sigma}\cdot\vec{B}(t) \tag{60}$$

$$\vec{B}(t) = (B_1\cos 2\omega_0 t, B_1\sin 2\omega_0 t, B_0) \tag{61}$$

绝热条件成立，求几何因子。

$$\begin{aligned}H((t)) &= -\mu_B[B_x\sigma_x + B_y\sigma_y + B_z\sigma_z](t) \\ &= -\mu_B\left(B_x\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} + B_y\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix} + B_z\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\right)(t) \\ &= -\mu_B\begin{bmatrix}B_0 & B_1e^{-i2\omega_0 t}\\ B_1e^{i2\omega_0 t} & -B_0\end{bmatrix}\end{aligned} \tag{62}$$

求解方程

$$H(t)|\psi_\pm(t)\rangle = E_\pm|\psi_\pm(t)\rangle \tag{63}$$

得到本征矢和本征值

$$|\psi_-(t)\rangle = \begin{bmatrix}\cos\theta\\ \sin\frac{\theta}{2}e^{-i2\omega_0 t}\end{bmatrix} \qquad E_-(t) = -\mu_B\sqrt{B_0^2 + B_1^2} \tag{64}$$

$$|\psi_+(t)\rangle = \begin{bmatrix}-\sin\theta\\ \cos\frac{\theta}{2}e^{i2\omega_0 t}\end{bmatrix} \qquad E_+(t) = \mu_B\sqrt{B_0^2 + B_1^2} \tag{65}$$

$$\theta = \tan^{-1}\frac{B_1}{B_0} \tag{66}$$

假定 $|\psi(t)\rangle$ 在 $|\psi_-(t)\rangle$ 上演化

$$|\psi(t=0)\rangle = |\psi_-(t=0)\rangle \tag{67}$$

$$\begin{aligned}\gamma_-(t) &= i\int_0^t \left\langle \psi_-(t') \middle| \dot{\psi}_-(t') \right\rangle \mathrm{d}t' \\ &= i\int_0^t \begin{bmatrix}\cos\theta & \sin\frac{\theta}{2}e^{i2\omega_0 t'}\end{bmatrix} \begin{bmatrix}0 \\ -i2\omega\sin\frac{\theta}{2}e^{-i2\omega_0 t'}\end{bmatrix} \mathrm{d}t' \\ &= i\int_0^t (-2i)\omega_0 \sin^2\frac{\theta}{2}\mathrm{d}t' \\ &= 2\omega_0 t\sin^2\frac{\theta}{2}\end{aligned} \tag{68}$$

$$\begin{aligned}|\psi(t)\rangle &= \exp[i\gamma_-(t)]\exp\left[-\frac{i}{\hbar}\int_0^t E_-(t')\mathrm{d}t'\right]|\psi_-(t)\rangle \\ &= \exp\left[i2\omega_0 t\sin^2\frac{\theta}{2}\right]\exp\left[\frac{i}{\hbar}\mu_B\sqrt{B_0^2+B_1^2}t\right]|\psi_-(t)\rangle\end{aligned} \tag{69}$$

$$|\psi(T)\rangle = \exp[i\pi(1-\cos\theta)]\exp\left[\frac{i}{\hbar}\mu_B\sqrt{B_0^2+B_1^2}T\right]|\psi_-(t)\rangle \tag{70}$$

几何因子

$$\gamma(t) = \pi(1-\cos\theta) \tag{71}$$

3 Effective field and Degeneracy point

$$\begin{aligned}\gamma_n(C) &= \oint_C i\left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R})\right\rangle \cdot \mathrm{d}\vec{R} \\ &= -\oint_C \vec{A}_n(\vec{R})\cdot\mathrm{d}\vec{R} \\ &= -\iint_S \left[\nabla_{\vec{R}}\times\vec{A}_n(\vec{R})\right]\cdot\mathrm{d}\vec{S} \\ &= -\iint_S \vec{B}_n(\vec{R})\cdot\mathrm{d}\vec{S}\end{aligned} \tag{72}$$

其中

$$\vec{A}_n(\vec{R}) = i\left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R})\right\rangle \tag{73}$$

$$\vec{B}_n(\vec{R}) = \nabla_{\vec{R}}\times\vec{A}_n(\vec{R}) \tag{74}$$

$\vec{A}_n(\vec{R})$ 为矢势 (vector potential)，$\vec{B}_n(\vec{R})$ 为有效场。由于 $\vec{A}_n(\vec{R})$ 是实数，接下来证明 $\left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R})\right\rangle$ 是纯虚数。即证明

$$\left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R})\right\rangle = -\left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R})\right\rangle^\dagger \tag{75}$$

已知

$$\left\langle n(\vec{R}) \middle| n(\vec{R})\right\rangle = 1 \tag{76}$$

方程两边作用 $\nabla_{\vec{R}}$

$$\begin{aligned}\nabla_{\vec{R}}\left\langle n(\vec{R}) \middle| n(\vec{R})\right\rangle &= \left\langle \nabla_{\vec{R}} n(\vec{R}) \middle| n(\vec{R})\right\rangle + \left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R})\right\rangle \\ &= \left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R})\right\rangle^\dagger + \left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R})\right\rangle = 0\end{aligned} \tag{77}$$

因此

$$\left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R})\right\rangle = -\left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R})\right\rangle^\dagger \tag{78}$$

即

$$\left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R}) \right\rangle = i \operatorname{Im} \left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R}) \right\rangle \tag{79}$$

$$\gamma_n(C) = -\operatorname{Im} \oint_C \left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R}) \right\rangle \cdot \mathrm{d}\vec{R} \tag{80}$$

$$\vec{A}_n(\vec{R}) = \operatorname{Im} \left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R}) \right\rangle \tag{81}$$

$$\begin{aligned} \vec{B}_n(\vec{R}) &= \nabla_{\vec{R}} \times \vec{A}_m(\vec{R}) = \nabla_{\vec{R}} \times \operatorname{Im} \left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R}) \right\rangle \\ &= \operatorname{Im} \nabla_{\vec{R}} \times \left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R}) \right\rangle \end{aligned} \tag{82}$$

接下来证明 $\vec{B}_n(\vec{R})$ 另外一种形式:

$$\vec{B}_n(\vec{R}) = \operatorname{Im} \sum_{m(\neq n)} \frac{\left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} H \middle| m(\vec{R}) \right\rangle \times \left\langle m(\vec{R}) \middle| \nabla_{\vec{R}} H \middle| n(\vec{R}) \right\rangle}{\left[E_n(\vec{R}) - E_m(\vec{R})\right]^2} \tag{83}$$

证明如下

$$\begin{aligned} \vec{B}_n(\vec{R}) &= \operatorname{Im} \nabla_{\vec{R}} \times \left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R}) \right\rangle \\ &= \operatorname{Im} \left[\left\langle \nabla_{\vec{R}} n(\vec{R}) \right| \times \left| \nabla_{\vec{R}} n(\vec{R}) \right\rangle + \left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} \times \nabla_{\vec{R}} n(\vec{R}) \right\rangle \right] \end{aligned} \tag{84}$$

其中

$$\nabla_{\vec{R}} \times \nabla_{\vec{R}} n(\vec{R}) = 0 \tag{85}$$

当 $\vec{v}$ 不是纯虚数或实数时，$\vec{v} \times \vec{v}^{\dagger} \neq 0$

$$\begin{aligned} \vec{B}_n(\vec{R}) &= \operatorname{Im} \left[\left\langle \nabla_{\vec{R}} n(\vec{R}) \right| \times \left| \nabla_{\vec{R}} n(\vec{R}) \right\rangle \right] \\ &= \operatorname{Im} \left[\left\langle \nabla_{\vec{R}} n(\vec{R}) \right| \left(\sum_m \left| m(\vec{R}) \right\rangle \left\langle \vec{R} \right| \right) \times \left| \nabla_{\vec{R}} n(\vec{R}) \right\rangle \right] \\ &= \operatorname{Im} \sum_m \left[\left\langle \nabla_{\vec{R}} n(\vec{R}) \middle| m(\vec{R}) \right\rangle \times \left\langle m(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R}) \right\rangle \right] \\ &= \operatorname{Im} \left[\sum_{m(\neq n)} \left\langle \nabla_{\vec{R}} n(\vec{R}) \middle| m(\vec{R}) \right\rangle \times \left\langle m(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R}) \right\rangle + \left\langle \nabla_{\vec{R}} n(\vec{R}) \middle| n(\vec{R}) \right\rangle \times \left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R}) \right\rangle \right] \\ &= \operatorname{Im} \sum_{m(\neq n)} \left\langle \nabla_{\vec{R}} n(\vec{R}) \middle| m(\vec{R}) \right\rangle \times \left\langle m(\vec{R}) \middle| \nabla_{\vec{R}} n(\vec{R}) \right\rangle \end{aligned} \tag{86}$$

又由于我们需要证明

$$\vec{B}_n(\vec{R}) = \operatorname{Im} \sum_{m(\neq n)} \frac{\left\langle n(\vec{R}) \middle| \nabla_{\vec{R}} H \middle| m(\vec{R}) \right\rangle \times \left\langle m(\vec{R}) \middle| \nabla_{\vec{R}} H \middle| n(\vec{R}) \right\rangle}{\left[E_n(\vec{R}) - E_m(\vec{R})\right]^2} \tag{87}$$

即证

$$\frac{\langle m| (\nabla_{\vec{R}} H) |n\rangle}{E_n - E_m} = \langle m| \nabla_{\vec{R}} |n\rangle \tag{88}$$

由

$$H |n\rangle = E_n(\vec{R}) |n\rangle \tag{89}$$

方程两边作用 $\nabla_{\vec{R}}$

$$(\nabla_{\vec{R}} H) |n\rangle + H \nabla_{\vec{R}} |n\rangle = \nabla_{\vec{R}} E_n(\vec{R}) |n\rangle + E_n(\vec{R}) \nabla_{\vec{R}} |n\rangle \tag{90}$$

方程两边作用 $\langle m|$

$$\langle m| (\nabla_{\vec{R}} H) |n\rangle + \langle m| H \nabla_{\vec{R}} |n\rangle = \langle m| \nabla_{\vec{R}} E_n(\vec{R}) |n\rangle + \langle m| E_n(\vec{R}) \nabla_{\vec{R}} |n\rangle \tag{91}$$

由于 Hamiltion 是厄米的，又由于 $\nabla_{\vec{R}} E_n(\vec{R})$ 与内积空间无关

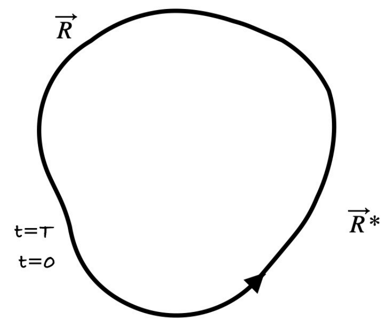
$$\langle m| (\nabla_{\vec{R}} H) |n\rangle + \langle m| E_m(\vec{R}) \nabla_{\vec{R}} |n\rangle = \langle m| E_n(\vec{R}) \nabla_{\vec{R}} |n\rangle \tag{92}$$

即

$$\langle m| (\nabla_{\vec{R}} H) |n\rangle = (E_n - E_m) \langle m| \nabla_{\vec{R}} |n\rangle \tag{93}$$

$$\langle m| (\nabla_{\vec{R}} H) |n\rangle^\dagger = (E_n - E_m) \langle m| \nabla_{\vec{R}} |n\rangle^\dagger \tag{94}$$

证毕。



假定 $\vec{R}(0) = \vec{R}(T)$，$H(0) = H(T)$，在 $\vec{R}$ 空间中有一点 $\vec{R}^*$，$\vec{R}^*$ 不在环上但接近环，假定 $\vec{R}^*$ 有两个态 $|m\rangle$ 和 $|n\rangle$，$|m\rangle$ 和 $|n\rangle$ 简并且 $|m\rangle \neq |n\rangle$。

$$H(\vec{R}^*) \left|m(\vec{R}^*)\right\rangle = E_m(\vec{R}^*) \left|m(\vec{R}^*)\right\rangle \tag{95}$$

$$H(\vec{R}^*) \left|n(\vec{R}^*)\right\rangle = E_n(\vec{R}^*) \left|n(\vec{R}^*)\right\rangle \tag{96}$$

$$E_m(\vec{R}^*) = E_n(\vec{R}^*) = E(\vec{R}^*) \tag{97}$$

只考虑简并态 $|m\rangle$ 和 $|n\rangle$，记为 $|+\rangle$ 和 $|-\rangle$。

$$\vec{B}_+(\vec{R}) = \mathrm{Im} \frac{\langle +| \nabla_{\vec{R}} H |-\rangle \times \langle -| \nabla_{\vec{R}} H |+\rangle}{\left[E_+(\vec{R}) - E_-(\vec{R})\right]^2} \tag{98}$$

$$\vec{B}_-(\vec{R}) = \mathrm{Im} \frac{\langle -| \nabla_{\vec{R}} H |+\rangle \times \langle +| \nabla_{\vec{R}} H |-\rangle}{\left[E_-(\vec{R}) - E_+(\vec{R})\right]^2} \tag{99}$$

$$H(\vec{R}^*) \left|\pm(\vec{R}^*)\right\rangle = E_\pm(\vec{R}^*) \left|\pm(\vec{R}^*)\right\rangle = E(\vec{R}^*) \left|\pm(\vec{R}^*)\right\rangle \tag{100}$$

普遍情况下

$$H(\vec{R}) = \begin{bmatrix} H_{++}(\vec{R}) & H_{+-}(\vec{R}) \\ H_{-+}(\vec{R}) & H_{--}(\vec{R}) \end{bmatrix} \tag{101}$$

假定

$$H(\vec{R}^*) = \begin{bmatrix} H_{++}(\vec{R}^*) & 0 \\ 0 & H_{--}(\vec{R}^*) \end{bmatrix} = \begin{bmatrix} E(\vec{R}^*) & 0 \\ 0 & E(\vec{R}^*) \end{bmatrix} \tag{102}$$

取 $H(\vec{R}^*)=0$，由于 $\vec{R}^*$ 与 $\vec{R}$ 离得很近，$H(\vec{R})$ 可用 $\vec{R}^*$ 展开

$$H(\vec{R})=a\sqrt{\left(\vec{R}-\vec{R}^*\right)^2}+b\vec{\sigma}\cdot\left(\vec{R}-\vec{R}^*\right) \tag{103}$$

移动坐标系令 $\vec{R}^*=0$，则

$$H(\vec{R})=aR+b\vec{\sigma}\cdot\vec{R} \tag{104}$$

令 $a=0,b=1$，简化 $H(\vec{R})$(只要物理本质存在，如何简化并不重要)

$$H(\vec{R})=\vec{\sigma}\cdot\vec{R}=\begin{bmatrix} z & x-iy \\ x+iy & -z \end{bmatrix} \tag{105}$$

求 $H(\vec{R})$ 的本征态和本征值

$$H(\vec{R})=\vec{\sigma}\cdot\vec{R}=\begin{vmatrix} z-E & x-iy \\ x+iy & -z-E \end{vmatrix}=E^2-(x^2+y^2+z^2)=0 \tag{106}$$

$$E_+=-E_-=R \tag{107}$$

$$\nabla_{\vec{R}}H(\vec{R})=\nabla_{\vec{R}}(\vec{\sigma}\cdot\vec{R})=\vec{\sigma} \tag{108}$$

代回 Eq.(98)，得

$$\vec{B}_{+x}(\vec{R})=\mathrm{Im}\,\frac{\langle +|\,\sigma_y\,|-\rangle\,\langle -|\,\sigma_z\,|+\rangle}{2R^2}=0 \tag{109}$$

$$\vec{B}_{+y}(\vec{R})=\mathrm{Im}\,\frac{\langle +|\,\sigma_z\,|-\rangle\,\langle -|\,\sigma_x\,|+\rangle}{2R^2}=0 \tag{110}$$

$$\vec{B}_{+z}(\vec{R})=\mathrm{Im}\,\frac{\langle +|\,\sigma_x\,|-\rangle\,\langle -|\,\sigma_y\,|+\rangle}{2R^2}=\frac{1}{2R^2} \tag{111}$$

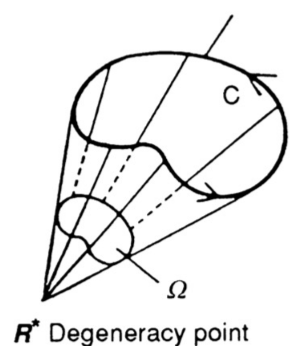
即

$$\vec{B}_+(\vec{R})=\frac{\vec{R}}{2R^3} \tag{112}$$

这种形式的磁场是由磁单极 $\rho_m(\vec{R})=-\frac{1}{2}\delta(\vec{R})$ 引起的，而自然界中并不存在磁单极，因此也不存在形如上式的磁场。

Anyway，我们来计算 Berry's phase

$$\gamma_+(C)=-\gamma_-(C)=-\iint_S\vec{B}_+(\vec{R})\cdot\mathrm{d}\vec{S}=-\iint_S\frac{\vec{R}}{2R^3}\cdot\mathrm{d}\vec{S}=-\frac{1}{2}\Omega(C) \tag{113}$$



4 Aharanov-Ananda Phase

接下来讨论和 Berry's phase 关系很大的一个概念：Aharanov-Ananda Phase。

哈密顿量变化很慢时，

$$|\psi(t)\rangle \doteq \exp[i\gamma_n(t)]\exp[i\alpha_n(t)]\,|n(t)\rangle \tag{114}$$

当 $H(T)=H(0)$ 时

$$\begin{aligned}|\psi(T)\rangle &\doteq \exp[i\gamma_n(C)]\exp[i\alpha_n(t)]\,|n(T)\rangle \\ &= \exp[i\gamma_n(C)]\exp[i\alpha_n(t)]\,|n(0)\rangle \\ &= \exp[i\gamma_n(C)]\exp[i\alpha_n(t)]\,|\psi(0)\rangle\end{aligned} \tag{115}$$

$$\alpha_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')\mathrm{d}t' \tag{116}$$

将 $|\phi(t)\rangle$ 写成

$$|\psi(t)\rangle = e^{i\phi}\,|\psi(0)\rangle \qquad (\phi\neq\alpha) \tag{117}$$

接下来讨论 $|\psi(t)\rangle$ 不在一个态上演化。由于 $|\psi(t)\rangle$ 不在一个态上演化，动力学因子 α 不再写成如上形式，因此我们需要重新定义动力学因子：

$$\alpha(T) = -\frac{1}{\hbar}\int_0^T \mathrm{d}t < \psi(x)|H(t)|\psi(t)> \tag{118}$$

因此几何因子

$$\gamma = \phi - \alpha \tag{119}$$

定义

$$\left|\tilde{\psi}(t)\right\rangle = e^{-if(t)}\,|\psi(t)\rangle \tag{120}$$

要求

$$f(T) - f(0) = \phi \tag{121}$$

将 $|\psi(t)\rangle = e^{if(t)}\left|\tilde{\psi}(t)\right\rangle$ 代入薛定谔方程

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\left[e^{if(t)}\left|\tilde{\psi}(t)\right\rangle\right] = -\hbar\dot{f}(t)\,|\psi(t)\rangle + i\hbar e^{if(t)}\frac{\partial}{\partial t}\left|\tilde{\psi}(t)\right\rangle = H(t)\,|\psi(t)\rangle \tag{122}$$

方程两边作用 $\langle\psi(t)|$

$$-\hbar\dot{f}(t) + i\hbar\,\langle\psi(t)|\,e^{if(t)}\frac{\partial}{\partial t}\left|\tilde{\psi}(t)\right\rangle = -\hbar\dot{f}(t) + i\hbar\left\langle\tilde{\psi}(t)\right|\frac{\partial}{\partial t}\left|\tilde{\psi}(t)\right\rangle = \langle\psi(t)|\,H(t)\,|\psi(t)\rangle \tag{123}$$

方程两边积分 $\int_0^t \mathrm{d}t'$

$$f(T) - f(0) = \int_0^t \mathrm{d}t'\left\langle\tilde{\psi}(t')\right| i\frac{\partial}{\partial t'}\left|\tilde{\psi}(t')\right\rangle - \frac{1}{\hbar}\int_0^t \mathrm{d}t'\,\langle\psi(t')|\,H(t')\,|\psi(t')\rangle \tag{124}$$

即

$$\phi = \int_0^t \mathrm{d}t'\left\langle\tilde{\psi}(t')\right| i\frac{\partial}{\partial t'}\left|\tilde{\psi}(t')\right\rangle + \alpha \tag{125}$$

故

$$\alpha(T) = -\frac{1}{\hbar}\int_0^T \mathrm{d}t < \psi(t)|H(t)|\psi(t)> \tag{126}$$

$$\gamma(T)=\int_0^T \mathrm{d}t\left\langle\tilde{\psi}(t)\right| i\frac{\partial}{\partial t}\left|\tilde{\psi}(t)\right\rangle \tag{127}$$

当哈密顿量 $H(t)=H$ 时，γ 也不为 0。

假定存在特殊情况 $H(t)=H$，且 $|\psi(t)\rangle$ 在两个态上演化

$$H\left|\psi_{\pm}\right\rangle=E_{\pm}\left|\psi_{\pm}\right\rangle \tag{128}$$

设

$$|\psi(0)\rangle=\cos\frac{\theta}{2}\left|\psi_{-}\right\rangle+\sin\frac{\theta}{2}\left|\psi_{+}\right\rangle \tag{129}$$

$$\begin{aligned}|\psi(t)\rangle&=e^{-\frac{iE_-t}{\hbar}}\cos\frac{\theta}{2}\left|\psi_{-}\right\rangle+e^{-\frac{iE_+t}{\hbar}}\sin\frac{\theta}{2}\left|\psi_{+}\right\rangle\\&=e^{-\frac{iE_-t}{\hbar}}\left[\cos\frac{\theta}{2}\left|\psi_{-}\right\rangle+e^{-\frac{i(E_+-E_-)t}{\hbar}}\sin\frac{\theta}{2}\left|\psi_{+}\right\rangle\right]\end{aligned} \tag{130}$$

在 T 时刻刚好一个周期，有

$$\frac{(E_+-E_-)T}{\hbar}=2\pi \tag{131}$$

$$|\psi(T)\rangle=e^{-\frac{iE_-T}{\hbar}}\left[\cos\frac{\theta}{2}\left|\psi_{-}\right\rangle+\sin\frac{\theta}{2}\left|\psi_{+}\right\rangle\right]=e^{-\frac{iE_-T}{\hbar}}|\psi(0)\rangle \tag{132}$$

total phase

$$\phi=-\frac{E_-T}{\hbar} \tag{133}$$

Dynamic phase

$$\begin{aligned}\alpha&=-\frac{1}{\hbar}\int_0^T<\psi(t)|H(t)|\psi(t)>\mathrm{d}t\\&=-\frac{1}{\hbar}\int_0^T\left[\cos\frac{\theta}{2}\left\langle\psi_{-}\right|+e^{\frac{i(E_+-E_-)t}{\hbar}}\sin\frac{\theta}{2}\left\langle\psi_{+}\right|\right]H(t)\left[\cos\frac{\theta}{2}\left|\psi_{-}\right\rangle+e^{-\frac{i(E_+-E_-)t}{\hbar}}\sin\frac{\theta}{2}\left|\psi_{+}\right\rangle\right]\mathrm{d}t\\&=-\frac{1}{\hbar}\int_0^T\left(\cos^2\frac{\theta}{2}E_-+\sin^2\frac{\theta}{2}E_+\right)\mathrm{d}t\\&=-\frac{1}{\hbar}\left(\cos^2\frac{\theta}{2}E_-+\sin^2\frac{\theta}{2}E_+\right)T\end{aligned} \tag{134}$$

A-A phase

$$\begin{aligned}\gamma&=\phi-\alpha\\&=-\frac{E_-T}{\hbar}+\frac{1}{\hbar}\left(\cos^2\frac{\theta}{2}E_-+\sin^2\frac{\theta}{2}E_+\right)T\\&=\frac{1}{\hbar}(E_+-E_-)T\left(\frac{1-\cos\theta}{2}\right)=\pi(1-\cos\theta)\neq0\end{aligned} \tag{135}$$

当 $|\psi(t)\rangle$ 在一个态上演化时，即 $\theta=0$ 或 $\theta=\pi$ 时

$$\gamma=\begin{cases}0 & \theta=0\\2\pi & \theta=\pi\end{cases} \tag{136}$$

因此在一般情况下，$\gamma\neq0$。

Example: Quantum Harmonic Oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{137}$$

$$E_n = (n + \frac{1}{2})\hbar\omega \tag{138}$$

$$|\psi(t=0)\rangle = \cos\frac{\theta}{2}|\psi_0\rangle + \sin\frac{\theta}{2}|\psi_1\rangle \tag{139}$$

$$\begin{aligned} |\psi(t)\rangle &= e^{-\frac{i\omega t}{2}}\cos\frac{\theta}{2}|\psi_0\rangle + e^{-\frac{i3\omega t}{2}}\sin\frac{\theta}{2}|\psi_1\rangle \\ &= e^{-\frac{i\omega t}{2}}\left(\cos\frac{\theta}{2}|\psi_0\rangle + e^{-i\omega t}\sin\frac{\theta}{2}|\psi_1\rangle\right) \end{aligned} \tag{140}$$

又

$$T = \frac{2\pi}{\omega} \tag{141}$$

因此

$$|\psi(T)\rangle = e^{-i\pi}\left(\cos\frac{\theta}{2}|\psi_0\rangle + \sin\frac{\theta}{2}|\psi_1\rangle\right) = e^{-i\pi}|\psi(0)\rangle \tag{142}$$

Total phase

$$\phi = -\pi \tag{143}$$

Dynamic phase

$$\begin{aligned} \alpha &= -\frac{1}{\hbar}\int_0^T <\psi(t)|H(t)|\psi(t)> \mathrm{d}t \\ &= -\frac{1}{\hbar}\int_0^T \left[\cos\frac{\theta}{2}\langle\psi_0| + e^{\frac{i\omega t}{2}}\sin\frac{\theta}{2}\langle\psi_1|\right] H(t) \left[\cos\frac{\theta}{2}|\psi_0\rangle + e^{-\frac{i\omega t}{2}}\sin\frac{\theta}{2}|\psi_1\rangle\right] \mathrm{d}t \\ &= -\frac{1}{2}\left(\cos^2\frac{\theta}{2} + 3\sin^2\frac{\theta}{2}\right)\omega T \\ &= -\pi(2-\cos\theta) \end{aligned} \tag{144}$$

A-A phase

$$\gamma = \phi - \alpha = -\pi + \pi(2-\cos\theta) = \pi(1-\cos\theta) \neq 0 \tag{145}$$

当 $|\psi(t)\rangle$ 在一个态上演化时，即 $\theta = 0$ 或 $\theta = \pi$ 时

$$\gamma = \begin{cases} 0 & \theta = 0 \\ 2\pi & \theta = \pi \end{cases} \tag{146}$$

5 Gauge Invariance of Quantum Mechanics 量子力学中的规范不变性

我们首先来回顾电动力学中的规范不变性。在电动力学中

$$\vec{E} = -\nabla V - \frac{1}{c}\frac{\partial \vec{A}}{\partial t} \tag{147}$$

$$\vec{B} = \nabla \times \vec{A} \tag{148}$$

通过规范变化 (gauge transformation)

$$V \to V' = V - \frac{1}{c}\frac{\partial}{\partial t}\chi \tag{149}$$

$$\vec{A} \to \vec{A}' = \vec{A} + \nabla\chi \tag{150}$$

我们得到

$$\vec{E} \to \vec{E} \qquad \vec{B} \to \vec{B} \tag{151}$$

接下来我们来说明量子力学中的规范不变性。量子力学中的规范不变性指薛定谔方程在规范变化下形式不变。

$$\left[\frac{\vec{p}^2}{2m} + V(\vec{r},t)\right]\psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) \tag{152}$$

考虑电场与磁场，薛定谔方程写成

$$\left[\frac{1}{2m}\left(\vec{p} - q\frac{\vec{A}}{c}\right)^2 + V(\vec{r},t)\right]\psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) \tag{153}$$

其中算符 $\vec{p}$ 为正则动量 (canonical momentum)，$\vec{p} - q\frac{\vec{A}}{c}$ 为运动动量 (kinetic momentum)。进行规范变化

$$V \to V' = V - \frac{q}{c}\frac{\partial}{\partial t}\chi \tag{154}$$

$$\vec{A} \to \vec{A}' = \vec{A} + \nabla\chi \tag{155}$$

在规范变化下，波函数多了一个相位因子

$$\psi \to \psi' = e^{\frac{iq\chi}{\hbar c}}\psi \tag{156}$$

$$\left[\frac{1}{2m}\left(\vec{p} - q\frac{\vec{A}'}{c}\right)^2 + V'(\vec{r},t)\right]\psi'(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi'(\vec{r},t) \tag{157}$$

接下来证明规范变化后的薛定谔方程与变化前的薛定谔方程等价。

$$\begin{aligned}
&\left(\vec{p} - q\frac{\vec{A}'}{c}\right) f(\vec{r},t)e^{\frac{iq\chi(\vec{r},t)}{\hbar c}} \\
=&\left(\frac{\hbar}{i}\nabla - q\frac{\vec{A}+\nabla\chi}{c}\right) f(\vec{r},t)e^{\frac{iq\chi(\vec{r},t)}{\hbar c}} \\
=&\left[\frac{\hbar}{i}\nabla f(\vec{r},t)\right]e^{\frac{iq\chi(\vec{r},t)}{\hbar c}} + \frac{q}{c}\nabla\chi f(\vec{r},t)e^{\frac{iq\chi(\vec{r},t)}{\hbar c}} - q\frac{\vec{A}}{c}f(\vec{r},t)e^{\frac{iq\chi(\vec{r},t)}{\hbar c}} - \frac{q}{c}\nabla\chi f(\vec{r},t)e^{\frac{iq\chi(\vec{r},t)}{\hbar c}} \\
=&\left[\left(\vec{p} - q\frac{\vec{A}}{c}\right) f(\vec{r},t)\right]e^{\frac{iq\chi(\vec{r},t)}{\hbar c}}
\end{aligned} \tag{158}$$

$f(\vec{r},t)$ 为任一函数。用该关系作用 $\psi'(\vec{r},t)$ 两次，得

$$\left(\vec{p} - q\frac{\vec{A}'}{c}\right)^2\psi'(\vec{r},t) = \left[\left(\vec{p} - q\frac{\vec{A}}{c}\right)^2\psi(\vec{r},t)\right]e^{\frac{iq\chi}{\hbar c}} \tag{159}$$

$$i\hbar\frac{\partial}{\partial t}\psi'(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\left[e^{\frac{iq\chi}{\hbar c}}\psi(\vec{r},t)\right] = \left(-\frac{q}{c}\frac{\partial}{\partial t}\chi\right)\psi'(\vec{r},t) + e^{\frac{iq\chi}{\hbar c}}i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) \tag{160}$$

代入 Eq.(157)，得

$$\left[\frac{1}{2m}\left(\vec{p} - q\frac{\vec{A}}{c}\right)^2 + V(\vec{r},t) - \frac{q}{c}\frac{\partial}{\partial t}\chi\right]\psi'(\vec{r},t) = \left(-\frac{q}{c}\frac{\partial}{\partial t}\chi\right)\psi'(\vec{r},t) + e^{\frac{iq\chi}{\hbar c}}i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) \tag{161}$$

$$\left[\frac{1}{2m}\left(\vec{p}-q\frac{\vec{A}}{c}\right)^2+V(\vec{r},t)\right]e^{\frac{iq\chi}{\hbar c}}\psi(\vec{r},t)=e^{\frac{iq\chi}{\hbar c}}i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) \tag{162}$$

即

$$\left[\frac{1}{2m}\left(\vec{p}-q\frac{\vec{A}}{c}\right)^2+V(\vec{r},t)\right]\psi(\vec{r},t)=i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) \tag{163}$$

证毕。

$$\vec{p}f(\vec{r},t)e^{-\frac{iS(\vec{r},t)}{\hbar}}=(\vec{p}-\nabla S)f(\vec{r},t)e^{\frac{iS(\vec{r},t)}{\hbar}} \tag{164}$$

6 Phase Change due to Scalar Potential $V(t)$ and Vector Potential $\vec{A}(\vec{r})$

在考虑标量势 $V(t)$ 和矢势 $\vec{A}(\vec{r})$ 之前

$$H(t)=H_0(t) \tag{165}$$

$$i\hbar\frac{\partial}{\partial t}\psi_0(\vec{r},t)=H_0(t)\psi_0(\vec{r,t}) \tag{166}$$

将标量势 $V(t)$ 和矢势 $\vec{A}(\vec{r})$ 分开讨论。

Scalar Potential $V(t)$

$$H(t)=H_0(t)+V(t) \tag{167}$$

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)=H(t)\psi(\vec{r,t}) \tag{168}$$

$\psi(\vec{r},t)$ 和 $\psi_0(\vec{r},t)$ 的关系

$$\psi(\vec{r},t)=\psi_0(\vec{r},t)e^{-\frac{iS(t)}{\hbar}} \tag{169}$$

其中

$$S(t)=\int_{t_0}^{t}V(t')\mathrm{d}t' \tag{170}$$

接下来证明这一关系。

将 $\psi(\vec{r},t)$ 代入薛定谔方程

$$\begin{aligned}\mathrm{LHS}&=i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)=i\hbar\frac{\partial}{\partial t}\left[\psi_0(\vec{r},t)e^{-\frac{iS(t)}{\hbar}}\right]\\&=i\hbar\frac{\partial}{\partial t}\psi_0(\vec{r},t)e^{-\frac{iS(t)}{\hbar}}+\psi_0(\vec{r},t)e^{-\frac{iS(t)}{\hbar}}\frac{\partial}{\partial t}S(t)\\&=\left[H_0(t)+V(t)\right]\psi_0(\vec{r},t)e^{-\frac{iS(t)}{\hbar}}\\&=H\psi(\vec{r},t)=\mathrm{RHS}\end{aligned} \tag{171}$$

证毕。

Vector Potential $\vec{A}(\vec{r})$

$$H_0(t) \sim \psi_0(\vec{r},t) \qquad i\hbar\frac{\partial}{\partial t}\psi_0(\vec{r},t) = H_0(t)\psi_0(\vec{r,t}) \tag{172}$$

考虑 $\vec{A}(\vec{r})$

$$H(t) \sim \psi(\vec{r},t) \qquad i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = H(t)\psi(\vec{r,t}) \tag{173}$$

$\psi(\vec{r},t)$ 和 $\psi_0(\vec{r},t)$ 的关系

$$\psi(\vec{r},t) = \psi_0(\vec{r},t)e^{-\frac{iS(\vec{r})}{\hbar}} \tag{174}$$

其中 Dirac factor

$$S(\vec{r}) = -\frac{q}{c}\int_{\vec{r}_0}^{\vec{r}} \vec{A}(\vec{r}')\cdot \mathrm{d}\vec{r}' \tag{175}$$

接下来证明这一关系。

$$H_0 = \frac{\vec{p}^2}{2m} \tag{176}$$

$$\vec{p}e^{-\frac{iS(\vec{r})}{\hbar}} = e^{-\frac{iS(\vec{r})}{\hbar}}(-i\hbar)\nabla\left[-\frac{iS(\vec{r})}{\hbar}\right] = e^{-\frac{iS(\vec{r})}{\hbar}}\frac{q}{c}\nabla\int_{\vec{r}_0}^{\vec{r}}\vec{A}(\vec{r}')\cdot\mathrm{d}\vec{r}' = e^{-\frac{iS(\vec{r})}{\hbar}}\frac{q}{c}\vec{A}(\vec{r}) \tag{177}$$

由 Eq.(164) 可得

$$\left[\vec{p}-\frac{q}{c}\vec{A}(\vec{r})\right]f(\vec{r},t)e^{-\frac{iS(\vec{r})}{\hbar}} = \left[\vec{p}f(\vec{r},t)\right]e^{-\frac{iS(\vec{r})}{\hbar}} \tag{178}$$

作用两次

$$\frac{1}{2m}\left[\vec{p}-\frac{q}{c}\vec{A}(\vec{r})\right]^2\psi_0(\vec{r},t)e^{-\frac{iS(\vec{r})}{\hbar}} = \frac{1}{2m}\left[\vec{p}^2\psi_0(\vec{r},t)\right]e^{-\frac{iS(\vec{r})}{\hbar}} \tag{179}$$

代入薛定谔方程

$$\mathrm{LHS} = i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\left[\psi_0(\vec{r},t)e^{-\frac{iS(\vec{r})}{\hbar}}\right] = i\hbar\left[\frac{\partial}{\partial t}\psi_0(\vec{r},t)\right]e^{-\frac{iS(\vec{r})}{\hbar}} \tag{180}$$

$$\mathrm{RHS} = H\psi(\vec{r},t) = \frac{1}{2m}\left[\vec{p}-\frac{q}{c}\vec{A}(\vec{r})\right]^2\psi_0(\vec{r},t)e^{-\frac{iS(\vec{r})}{\hbar}} = \frac{1}{2m}\left[\vec{p}^2\psi_0(\vec{r},t)\right]e^{-\frac{iS(\vec{r})}{\hbar}} \tag{181}$$

由 LHS = RHS 得

$$i\hbar\frac{\partial}{\partial t}\psi_0(\vec{r},t) = \frac{\vec{p}^2}{2m}\psi_0(\vec{r},t) \tag{182}$$

证毕。

General Case

$$H_0(t) \sim \psi_0(\vec{r},t) \tag{183}$$

将两种情况结合起来

$$H(t) \sim \psi(\vec{r},t) \tag{184}$$

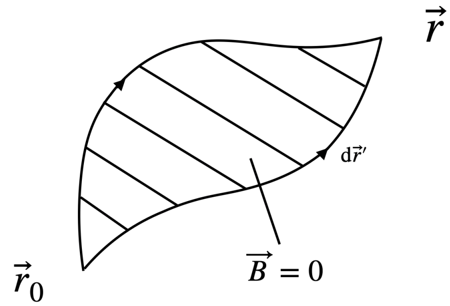
$$\psi(\vec{r},t) = \psi_0(\vec{r},t)e^{-\frac{iS(\vec{r},t)}{\hbar}} \tag{185}$$

其中

$$S(\vec{r},t) = \int_{t_0}^{t} V(t')\mathrm{d}t' - \frac{q}{c}\int_{\vec{r}_0}^{\vec{r}}\vec{A}(\vec{r}')\cdot\mathrm{d}\vec{r}' \tag{186}$$

$\int_{\vec{r}_0}^{\vec{r}}\vec{A}(\vec{r}')\cdot\mathrm{d}\vec{r}'$ 可能依赖路径，接下来我们来研究什么情况下 $\int_{\vec{r}_0}^{\vec{r}}\vec{A}(\vec{r}')\cdot\mathrm{d}\vec{r}'$ 与路径有关。

(1）图中区域 $\vec{B}(\vec{r}) = 0$



$$\nabla \times \vec{A}(\vec{r}) = \vec{B}(\vec{r}) = 0 \tag{187}$$

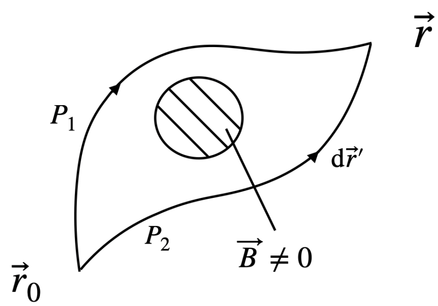
因此 $\vec{A}$ 可以写成

$$\vec{A}(\vec{r}) = \nabla\chi(\vec{r}) \tag{188}$$

$$\int_{\vec{r}_0}^{\vec{r}} \vec{A}(\vec{r}') \cdot \mathrm{d}\vec{r}' = \int_{\vec{r}_0}^{\vec{r}} \nabla\chi(\vec{r}) \cdot \mathrm{d}\vec{r}' = 0 \tag{189}$$

与路径无关

(2）图中区域 $\vec{B}(\vec{r}) \neq 0$



$$\begin{aligned} &\int_{\vec{r}_0(P_1)}^{\vec{r}} \vec{A}(\vec{r}') \cdot \mathrm{d}\vec{r}' + \int_{\vec{r}(P_2)}^{\vec{r}_0} \vec{A}(\vec{r}') \cdot \mathrm{d}\vec{r}' = \oint \vec{A}(\vec{r}') \cdot \mathrm{d}\vec{r}' \\ &= \iint_S \left[\nabla \times \vec{A}(\vec{r}')\right] \cdot \mathrm{d}\vec{S} = \iint_S \vec{B}(\vec{r}') \cdot \mathrm{d}\vec{S} = \Phi \neq 0 \end{aligned} \tag{190}$$

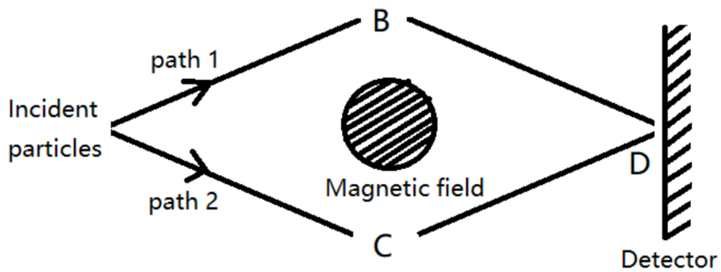
故

$$\int_{\vec{r}_0(P_1)}^{\vec{r}} \vec{A}(\vec{r}') \cdot \mathrm{d}\vec{r}' \neq \int_{\vec{r}_0(P_2)}^{\vec{r}} \vec{A}(\vec{r}') \cdot \mathrm{d}\vec{r}' \tag{191}$$

积分与路径有关。

7 Aharanov-Bohm Effect

Magnetic A-B Effect Experiment(1959)



设在路径 A-B-D 中，$|\psi_2| \ll |\psi_1|$；在路径 A-C-D 中，$|\psi_1| \ll |\psi_2|$。

当 $\vec{B} = 0$ 时

$$\psi_0(\vec{r}, t) \sim \psi_1(\vec{r}, t) + \psi_2(\vec{r}, t) \tag{192}$$

当 $\vec{B} \neq 0$ 时

$$\begin{aligned}
\psi(\vec{r}, t) \sim & \exp\left[\frac{iq}{\hbar c}\int_{\vec{r}_0}^{\vec{r}} \vec{A}(\vec{r}') \cdot \mathrm{d}\vec{r}'\right]\psi_0(\vec{r}, t) \\
&= \exp\left[\frac{iq}{\hbar c}\int_{\vec{r}_0(P_1)}^{\vec{r}} \vec{A}(\vec{r}') \cdot \mathrm{d}\vec{r}'\right]\psi_1(\vec{r}, t) + \exp\left[\frac{iq}{\hbar c}\int_{\vec{r}_0(P_2)}^{\vec{r}} \vec{A}(\vec{r}') \cdot \mathrm{d}\vec{r}'\right]\psi_2(\vec{r}, t) \\
&= \exp\left[\frac{iq}{\hbar c}\int_{\vec{r}_0(P_1)}^{\vec{r}} \vec{A}(\vec{r}') \cdot \mathrm{d}\vec{r}'\right]\left\{\psi_1(\vec{r}, t) + \psi_2(\vec{r}, t)\exp\left[\frac{iq}{\hbar c}\left(\int_{\vec{r}_0(P_2)}^{\vec{r}} - \int_{\vec{r}_0(P_1)}^{\vec{r}}\right)\vec{A}(\vec{r}') \cdot \mathrm{d}\vec{r}'\right]\right\} \\
&= \exp\left[\frac{iq}{\hbar c}\int_{\vec{r}_0(P_1)}^{\vec{r}} \vec{A}(\vec{r}') \cdot \mathrm{d}\vec{r}'\right]\left\{\psi_1(\vec{r}, t) + \psi_2(\vec{r}, t)\exp\left[-\frac{iq}{\hbar c}\oint \vec{A}(\vec{r}') \cdot \mathrm{d}\vec{r}'\right]\right\} \\
&\sim \psi_1(\vec{r}, t) + \psi_2(\vec{r}, t)\exp\left(-\frac{iq}{\hbar c}\Phi\right)
\end{aligned} \tag{193}$$

$$\begin{aligned}
|\psi(\vec{r}, t)|^2 &= \left[\psi_1^\dagger(\vec{r}, t) + \psi_2^\dagger(\vec{r}, t)e^{\frac{iq}{\hbar c}\Phi}\right]\left[\psi_1(\vec{r}, t) + \psi_2(\vec{r}, t)e^{-\frac{iq}{\hbar c}\Phi}\right] \\
&= |\psi_1|^2 + |\psi_2|^2 + \psi_1^\dagger\psi_2 e^{-\frac{iq}{\hbar c}\Phi} + \psi_1\psi_2^\dagger e^{\frac{iq}{\hbar c}\Phi} \\
&= |\psi_1|^2 + |\psi_2|^2 + 2|\psi_1\psi_2|\cos\left(\phi_1 - \phi_2 + \frac{q\Phi}{\hbar c}\right)
\end{aligned} \tag{194}$$

Φ 和 $\vec{B}$ 有关

$$\delta\phi = \frac{q\Phi}{\hbar c} \tag{195}$$

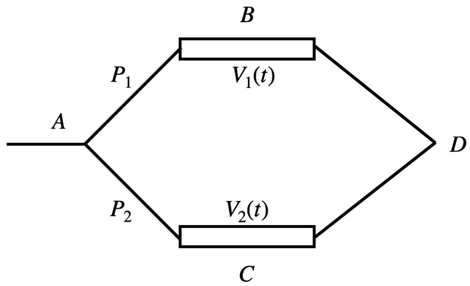
当经过一个周期即

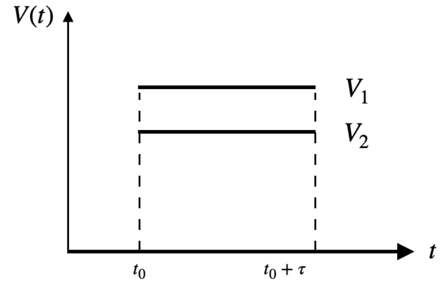
$$\frac{q\Delta\Phi}{\hbar c} = 2\pi \tag{196}$$

$$\Delta\Phi = \frac{2\pi\hbar c}{q} \tag{197}$$

在经典电动力学中，$\vec{A}$ 无物理意义，而在量子力学中 $\vec{A}$ 能够显现出来，即 A-B 效应。

Electric Aharonov–Bohm Effect





设在路径 A-B-D 中，$|\psi_2| \ll |\psi_1|$；在路径 A-C-D 中，$|\psi_1| \ll |\psi_2|$。

当 $V_1(t) = 0, V_2(t) = 0$ 时

$$\psi_0(\vec{r},t) \sim \psi_1(\vec{r},t) + \psi_2(\vec{r},t) \tag{198}$$

当 $V_1(t) \neq 0, V_2(t) \neq 0$ 时

$$\begin{aligned}\psi(\vec{r},t) \sim& \exp\left[\frac{i}{\hbar}\int_{(P_1)}^{t} V(t')\cdot \mathrm{d}t'\right]\psi_1(\vec{r},t) + \exp\left[\frac{i}{\hbar}\int_{(P_1)}^{t} V(t')\cdot \mathrm{d}t'\right]\psi_2(\vec{r},t) \\ \sim& \psi_1(\vec{r},t) + \psi_2(\vec{r},t)\exp\left\{i\left[\int_{(P_2)}^{t} V(t')\cdot \mathrm{d}t' - \int_{(P_1)}^{t} V(t')\cdot \mathrm{d}t'\right]\frac{1}{\hbar}\right\}\end{aligned} \tag{199}$$

设 $V_1(t), V_2(t)$ 是如上图的函数

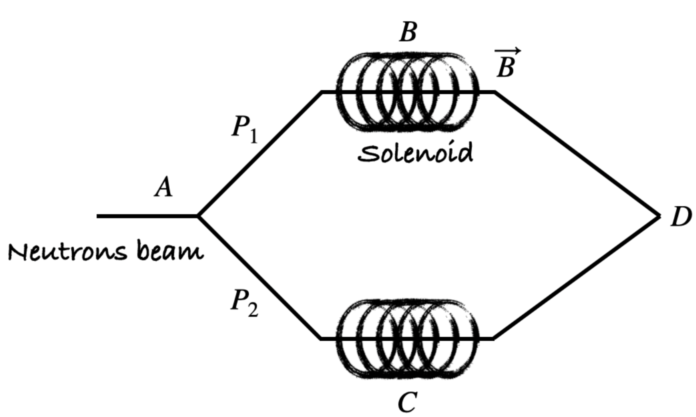
$$\begin{aligned}\psi(\vec{r},t) \sim& \psi_1(\vec{r},t) + \psi_2(\vec{r},t)\exp\left[i\left(V_2 - V_1\right)\frac{\tau}{\hbar}\right] \\ =& \psi_1(\vec{r},t) + \psi_2(\vec{r},t)e^{-\frac{i\Delta V\tau}{\hbar}} \qquad (\Delta V = V_1 - V_2)\end{aligned} \tag{200}$$

$$\begin{aligned}|\psi(\vec{r},t)|^2 &= \left[\psi_1^\dagger(\vec{r},t) + \psi_2^\dagger(\vec{r},t)e^{\frac{i\Delta V\tau}{\hbar}}\right]\left[\psi_1(\vec{r},t) + \psi_2(\vec{r},t)e^{-\frac{i\Delta V\tau}{\hbar}}\right] \\ &= |\psi_1|^2 + |\psi_2|^2 + \psi_1^\dagger\psi_2 e^{-\frac{i\Delta V\tau}{\hbar}} + \psi_1\psi_2^\dagger e^{\frac{i\Delta V\tau}{\hbar}} \\ &= |\psi_1|^2 + |\psi_2|^2 + 2|\psi_1\psi_2|\cos\left(\phi_1 - \phi_2 + \frac{\Delta V\tau}{\hbar}\right)\end{aligned} \tag{201}$$

$$\Delta\phi = \frac{\Delta V\tau}{\hbar} \tag{202}$$

由于存在技术上的困难，目前在实验中还未观察到这一现象。

Scalar Aharanov-Bohm Effect Experiment(1992)



$$H = \frac{\vec{p}^2}{2m} - \vec{\mu}\cdot\vec{B} = \frac{p^2}{2m} - \mu_B\vec{\sigma}\cdot\vec{B} \tag{203}$$

$$V = \mu_B\vec{\sigma}\cdot\vec{B} \tag{204}$$

假设

$$\vec{B}_1 = \hat{e}_z B \qquad \vec{B}_2 = 0 \tag{205}$$

则

$$\Delta V = \mu_B B\sigma \tag{206}$$

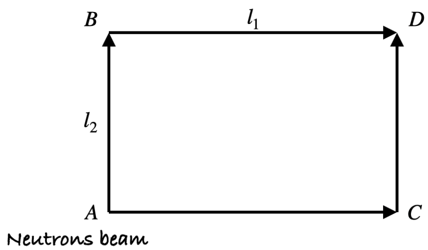
在 $t_0 \to t_0+\tau$ 加磁场 $\vec{B}$，观察到

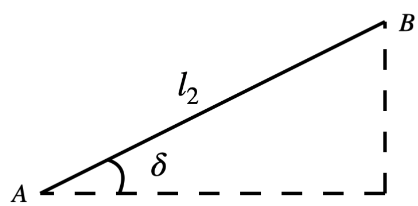
$$\Delta\phi = \frac{\Delta V\tau}{\hbar} \tag{207}$$

8 Gravitationally Induced Phase

Experiment(1975)

引力和量子力学是相洽的吗？我们来设计一个实验观察引力在量子力学中的表现。





将 BD 边抬高

$$\Delta V = m_n g l_2 \sin\delta \tag{208}$$

如果这个势能能够在量子力学中表现出来且被观察到，那么会引起的相位变化

$$\Delta\phi = \frac{\Delta VT}{\hbar} \tag{209}$$

设中子速度 $\vec{v}$

$$T = \frac{l_1}{v} = \frac{l_1}{\hbar/m_n\lambda} = \frac{l_1 m_n\lambda}{\hbar} \tag{210}$$

则

$$\Delta\phi = \frac{\Delta VT}{\hbar} = \frac{m_n^2 g l_1 l_2 \lambda\sin\delta}{\hbar^2} \tag{211}$$

若 $\hbar \to 0$，则 $\Delta\phi \to \infty$，无任何效应。因此这是纯粹的量子力学效应。

实验中 $l_1 l_2 = 10cm^2, \lambda = 1.42\mathring{A}$, 实验结果证实了引力效应可以在量子力学中观察到。