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绝热近似、动力学相位与几何相位

本文采用自然单位制 $c=\hbar=k_B=1$。

一. 绝热近似

考虑体系哈密顿量是d维含时变量 $R_i(t)$ 的函数

$$H(R_i(t)), \quad i=1,2,\cdots,d$$

$R_i(t)$ 构成d维参数空间。哈密顿量变化频率 $\omega=\left|\frac{d\vec{R}}{dt}\right|/|\vec{R}|$。

如果体系满足

$$\omega \ll \omega_{nm}=E_n-E_m \tag{1}$$

那就可以忽略从m态到n态的跃迁。这样，若t_1时刻体系处在瞬时本征态 $\psi_m(\vec{r},t_1)$，则在t_2时刻，体系仍处在本征态 $\psi_m(\vec{r},t_2)$。

(也就是说体系哈密顿量要变化得足够缓慢，且不同能级之间能量差足够大。物理上还可以这样理解：体系能级跃迁需要吸收 $E_n-E_m=\omega_{nm}$ 的能量，但只吸收了 $\omega\ll\omega_{nm}$ 的能量，体系状态近似不变。)

此即绝热定理：如果一个体系的哈密顿量缓慢变化，并且体系一开始处于能量本征态，那么体系将在整个演化过程中继续保持在该能量本征态。(1)式称绝热近似条件。(本文只考虑非简并情况)

二. 动力学相位

含时Schrödinger方程

$$i\frac{\partial}{\partial t}|\Psi(t)\rangle = H(\vec{R}(t))|\Psi(t)\rangle \tag{2}$$

当$\vec{R}(t)$缓变使得绝热近似成立，且体系初始状态为某本征态时，对于某一瞬间t，可写出瞬时本征方程

$$H(\vec{R}(t))\,|n(\vec{R}(t))\rangle = E_n(\vec{R}(t))\,|n(\vec{R}(t))\rangle \quad (3)$$

基矢满足正交归一条件

$$\langle n(\vec{R}(t))\,|\,m(\vec{R}(t))\rangle = \delta_{m,n} \quad (4)$$

※现在定义简记符号

$$|n_t\rangle \equiv |n(\vec{R}(t))\rangle, \quad |n_0\rangle \equiv |n(\vec{R}(0))\rangle$$

$$|\Psi_t\rangle \equiv |\Psi(t)\rangle, \quad |\Psi_0\rangle \equiv |\Psi(0)\rangle$$

$$H_t \equiv H(\vec{R}(t)), \quad H_0 \equiv H(\vec{R}(0))$$

定义幺正算符

$$Q_t \equiv Q(\vec{R}(t)) \equiv \sum_n |n_t\rangle\langle n_0| \quad (5)$$

则

$$|n_t\rangle = Q_t\,|n_0\rangle \quad (6)$$

这表明任一时刻本征态可通过初态幺正变换而来。

定义

$$|\Psi_t\rangle \equiv Q_t\,|\psi_t\rangle \quad (7)$$

显然 $|\Psi_0\rangle = Q_0|\psi_0\rangle = |\psi_0\rangle$，将(7)代入(2)，得

$$i\frac{\partial}{\partial t}|\psi_t\rangle = (H_0' + H_t')\,|\psi_t\rangle \quad (8)$$

推导：$i\frac{\partial}{\partial t}(Q_t|\psi_t\rangle) = H_t Q_t|\psi_t\rangle$

$$i\frac{\partial Q_t}{\partial t}|\psi_t\rangle + iQ_t\frac{\partial}{\partial t}|\psi_t\rangle = H_t Q_t|\psi_t\rangle$$

$$iQ_t^\dagger\frac{\partial Q_t}{\partial t}|\psi_t\rangle + i\frac{\partial}{\partial t}|\psi_t\rangle = Q_t^\dagger H_t Q_t|\psi_t\rangle$$

$$i\frac{\partial}{\partial t}|\psi_t\rangle = \left(Q_t^\dagger H_t Q_t - iQ_t^\dagger\frac{\partial}{\partial t}Q_t\right)|\psi_t\rangle$$

$$i\frac{\partial}{\partial t}|\psi_t\rangle = (H_0' + H_t')\,|\psi_t\rangle$$

其中 $H_0' \equiv Q_t^\dagger H_t Q$，$H_t' \equiv -iQ_t^\dagger\frac{\partial}{\partial t}Q_t$ (i)

且 $|n_0\rangle$ 是 H_0' 的本征态。

推导：$H_0'|n_0\rangle = Q_t^\dagger H_t Q_t|n_0\rangle = Q_t^\dagger H_t|n_t\rangle$

$$= E_n(\vec{R}(t))\,Q_t^\dagger|n_t\rangle = E_n(\vec{R}(t))\,|n_0\rangle$$

注意区别 $H_0|n_0\rangle = E_n(\vec{R}(0))\,|n_0\rangle$

定义演化算符 $V_t \equiv V(t)$ 满足

$$i\frac{\partial}{\partial t}V(t) = H_0' V(t), \quad V_0 = V(0) = 1 \tag{9}$$

采用 H_0 表象，也即以 $|n_0\rangle$ 为基矢，将 $\langle m_0|$ 和 $|n_0\rangle$ 分别向左向右作用于 (9) 得

$$i\frac{\partial}{\partial t}\langle m_0|V(t)|n_0\rangle = \langle m_0|H_0' V(t)|n_0\rangle$$

$$i\frac{\partial}{\partial t}V_{mn}(t) = E_m(\vec{R}(t))\, V_{mn}(t)$$

和 $V_{mn}(0) = \delta_{mn}$，解得

$$V(t) = \sum_n e^{i\phi_n(t)}|n_0\rangle\langle n_0| \tag{10}$$

推导：$i\frac{\partial}{\partial t}V_{mn}(t) = E_m(\vec{R}(t))\, V_{mn}(t)$

$$\frac{1}{V_{mn}(t)}\partial V_{mn}(t) = -i\, E_m(\vec{R}(t))\, \partial t$$

$$V_{mn}(t) = V_{mn}(0)\exp^{-i\int_0^t E_m(\vec{R}(\tau))d\tau}$$

$$V_{mn}(t) = e^{i\phi_m(t)}\delta_{mn}$$

其中 $\phi_m(t) \equiv -\int_0^t E_m(\vec{R}(\tau))\,d\tau$

$$V(t) = \sum_{mn}|m_0\rangle\langle m_0|V(t)|n_0\rangle\langle n_0|$$

$$= \sum_{mn}|m_0\rangle\langle n_0|\, V_{mn}(t)$$

$$= \sum_n e^{i\phi_n(t)}|n_0\rangle\langle n_0|$$

$e^{i\phi_n(t)}$ 称为动力学相位因子，$\phi_n(t)$ 就是动力学相位，由定义发现动力学相位是动力学系统的瞬时本征能量积累的结果，这就是其名称来由。

三. 绝热近似解

由 $V_t^\dagger V_t = \sum_{mn} e^{i(\phi_m(t)-\phi_n(t))}|m_0\rangle\langle m_0|n_0\rangle\langle n_0| = \sum_n |n_0\rangle\langle n_0| = 1$ 知 V_t 是幺正的，再做幺正变换

$$|\psi_t\rangle = V_t\,|\varphi_t\rangle \tag{11}$$

代入 (8)，得

$$i\frac{\partial}{\partial t}|\varphi_t\rangle = H_t''|\varphi_t\rangle \tag{12}$$

推导：$i\frac{\partial}{\partial t}(V_t|\varphi_t\rangle) = (H_0' + H_t')V_t|\varphi_t\rangle$

$$iV_t\frac{\partial}{\partial t}|\varphi_t\rangle + H_0'V_t|\varphi_t\rangle = (H_0' + H_t')V_t|\varphi_t\rangle$$

$$i\frac{\partial}{\partial t}|\varphi_t\rangle = V_t^\dagger H_t' V_t|\varphi_t\rangle$$

$$i\frac{\partial}{\partial t}|\varphi_t\rangle = H_t''|\varphi_t\rangle$$

其中 $H_t'' \equiv V_t^\dagger H_t' V_t$

将 $|\varphi_t\rangle$ 用 $|n_0\rangle$ 展开

$$|\varphi_t\rangle = \sum_n \alpha_n(t)|n_0\rangle \tag{13}$$

代入(12)得

$$\dot{\alpha}_m(t) = -\sum_n \alpha_n(t) e^{i(\phi_n(t)-\phi_m(t))}\langle m_t|\frac{\partial}{\partial t}|n_t\rangle \tag{14}$$

推导：$i\frac{\partial}{\partial t}\left(\sum_m \alpha_m(t)|m_0\rangle\right) = H''\sum_n \alpha_n(t)|n_0\rangle$

$$i\frac{d}{dt}\alpha_m(t) = \sum_n \alpha_n(t)\langle m_0|H_t''|n_0\rangle \tag{ii}$$

$\langle m_0|H_t''|n_0\rangle$

$= \langle m_0|V^\dagger H_t' V|n_0\rangle$

$\overset{代入(10)}{=} \sum_{sl}\langle m_0|s_0\rangle\langle s_0|H_t'|l_0\rangle\langle l_0|n_0\rangle e^{i(\phi_l(t)-\phi_s(t))}$

$= e^{i(\phi_n(t)-\phi_m(t))}\langle m_0|H_t'|n_0\rangle$

$$\overset{代入(i)}{=} -ie^{i(\phi_n(t)-\phi_m(t))}\langle m_t|\frac{\partial}{\partial t}|n_t\rangle \tag{iii}$$

(iii) 代入 (ii) 得 $\dot{\alpha}_m(t) = -\sum_n \alpha_n(t) e^{i(\phi_n(t)-\phi_m(t))}\langle m_t|\frac{\partial}{\partial t}|n_t\rangle$

采用绝热近似

$$\langle m_t|\frac{\partial}{\partial t}|n_t\rangle = 0 \quad (m\neq n) \tag{15}$$

(15) 物理上是很好理解的，绝热定理表明体系在整个演化过程中保持在同一个能量本征态，$\frac{\partial}{\partial t}|n_t\rangle$ 表示态的演化，因为还是在同一个能量本征态，故与 $|m_t\rangle$ 是正交的。

(14) 简化为

$$\dot{\alpha}_n(t) = -\alpha_n(t)\langle n_t|\frac{\partial}{\partial t}|n_t\rangle \tag{16}$$

取 $\alpha_n(0)=1$，对 (16) 积分得

$$\alpha_n(t) = e^{-\int_0^t \langle n_\tau|\frac{\partial}{\partial\tau}|n_\tau\rangle d\tau} \tag{17}$$

$\langle n_t|\frac{\partial}{\partial t}|n_t\rangle$ 是纯虚数，定义

$$\gamma_n(t) \equiv i\int_0^t \langle n_\tau|\frac{\partial}{\partial\tau}|n_\tau\rangle d\tau \tag{18}$$

则

$$\alpha_n(t) = e^{i\gamma_n(t)} \tag{19}$$

推导：$\langle n_t|n_t\rangle = 1$

$$\frac{\partial}{\partial t}(\langle n_t|n_t\rangle) = 0$$

$$\left(\frac{\partial}{\partial t}\langle n_t|\right)|n_t\rangle + \langle n_t|\frac{\partial}{\partial t}|n_t\rangle = 0$$

$$-\langle n_t|\frac{\partial}{\partial t}|n_t\rangle = \left(\langle n_t|\frac{\partial}{\partial t}|n_t\rangle\right)^\dagger$$

$$\Rightarrow \quad Re\left(\langle n_t|\frac{\partial}{\partial t}|n_t\rangle\right) = 0$$

由(5)(6)(7)(11)(13)及初始条件$|\Psi_0\rangle = |n_0\rangle$，推出$t$时刻波函数绝热近似解的最终形式

$$|\Psi_t\rangle = e^{i\gamma_n(t)} e^{i\phi_n(t)} |n_t\rangle \tag{20}$$

推导：
$$\begin{aligned}
|\Psi_t\rangle &= Q_t|\psi_t\rangle \\
&= Q_t V_t |\varphi_t\rangle \\
&= Q_t V_t \sum_n \alpha_n(t) |n_0\rangle \\
&= Q_t \sum_n \alpha_n(t) V_t |n_0\rangle \\
&= Q_t \sum_{mn} e^{i\gamma_n(t)} e^{i\phi_m(t)} |m_0\rangle\langle m_0|n_0\rangle \\
&= \sum_n e^{i\gamma_n(t)} e^{i\phi_n(t)} |n_t\rangle
\end{aligned}$$

由初始条件 $Q_0 = V_0 = \alpha_n(0) = 1$，推出 $|\Psi_0\rangle = |n_0\rangle$

四. 几何相位

1. $\gamma_n(t)$ 称为几何相位，因为它是几何的。

$$\gamma_n(t) = i\int_0^t \langle n(\vec{R}(\tau))|\frac{\partial}{\partial\tau}|n(\vec{R}(\tau))\rangle\, d\tau$$
$$= i\int_0^t \langle n(\vec{R}(\tau))|\frac{\partial\vec{R}}{\partial\tau}\frac{\partial}{\partial\vec{R}}|n(\vec{R}(\tau))\rangle\, d\tau$$
$$= i\int_{\vec{R}(0)}^{\vec{R}(t)} \langle n(\vec{R})|\nabla_{\vec{R}}|n(\vec{R})\rangle\, d\vec{R} \tag{21}$$

它实际上是由量子绝热过程在参数空间的路径决定的，和这个体系变化的快慢无关。

2. 定义 $\vec{A}_n(\vec{R}) = i\langle n(\vec{R})|\frac{\partial}{\partial\vec{R}}|n(\vec{R})\rangle$，对其矢作规范变换

$$|n(\vec{R})\rangle \longrightarrow e^{-i\alpha(\vec{R})}|n(\vec{R})\rangle \tag{22}$$

则有

$$\vec{A}_n(\vec{R}) \longrightarrow \vec{A}_n(\vec{R}) + \nabla\alpha(\vec{R}) \tag{23}$$

$$\gamma_n(t) \longrightarrow \gamma_n(t) + \alpha(\vec{R}(t)) - \alpha(\vec{R}(0)) \tag{24}$$

推导：$\tilde{\vec{A}}_n(\vec{R}) = i\langle\tilde{n}(\vec{R})|\frac{\partial}{\partial\vec{R}}|\tilde{n}(\vec{R})\rangle$

$$= i\langle n(\vec{R})|e^{i\alpha(\vec{R})}\frac{\partial}{\partial\vec{R}}\left[e^{-i\alpha(\vec{R})}|n(\vec{R})\rangle\right]$$
$$= \vec{A}_n(\vec{R}) + \nabla\alpha(\vec{R})$$
$$\tilde{\gamma}_n(t) = \int_{\vec{R}(0)}^{\vec{R}(t)} \vec{A}_n(\vec{R})\cdot d\vec{R}$$
$$= \gamma_n(t) + \alpha(\vec{R}(t)) - \alpha(\vec{R}(0))$$

此时我们总可以选取一个规范使得新的 $\gamma_n(t)$ 是零。

3. 若哈密顿量在参数空间的演化是个闭合回路，且具有周期性，即满足 $\vec{R}(T) = \vec{R}(0)$，那么此时

$$\gamma_n = \oint_C d\vec{R}\cdot\vec{A}_n(\vec{R}) \tag{25}$$

是规范不变的，称为 Berry 相位。

4. 事实上，由于其几何性，我们完全可以不通过演化而直接在参数空间下推得 Berry 相位。

定义参数空间中两个量子态的距离

$$D_{12}^2 \equiv -\ln |\langle \psi(\vec{R}_1) | \psi(\vec{R}_2) \rangle|^2 \tag{26}$$

记

$$\langle \psi(\vec{R}_1) | \psi(\vec{R}_2) \rangle = |\langle \psi(\vec{R}_1) | \psi(\vec{R}_2) \rangle| e^{i\Delta\varphi_{21}} \tag{27}$$

可推出

$$\mathrm{Im} \ln \langle \psi_1 | \psi_2 \rangle = \Delta\varphi_{21} = -\Delta\varphi_{12} \tag{28}$$

那么 Berry 相位写为

$$\begin{aligned}
\gamma_c &= \Delta\varphi_{01} + \Delta\varphi_{12} + \cdots + \Delta\varphi_{N-1,N} \\
&= -\sum_{j=0}^{N-1} \mathrm{Im} \ln \langle \psi(\vec{R}_j) | \psi(\vec{R}_{j+1}) \rangle \\
&= -\mathrm{Im} \oint d\vec{R} \langle \psi(\vec{R}) | \nabla_{\vec{R}} | \psi(\vec{R}) \rangle \\
&= i \oint d\vec{R} \langle \psi(\vec{R}) | \nabla_{\vec{R}} | \psi(\vec{R}) \rangle \\
&= \oint \vec{A} \cdot d\vec{R}
\end{aligned} \tag{29}$$

取连续参数，作2次一阶Taylor展开

由于每个 $|\psi(\vec{R}_j)\rangle$ 和它的复共轭在(29)式中成对出现，故这里也能看出 Berry 相位是规范不变的。

五. 可解模型

题：$H(\vec{R}) = \vec{S} \cdot \vec{R}(t)$，$[S_i, S_j] = i\epsilon_{ijk} S_k$，$\vec{S}^2 = s(s+1)$

$\vec{R}(t) = R\,\vec{n}(t)$，$\vec{n}(t) = (\sin\theta\cos\omega t, \sin\theta\sin\omega t, \cos\theta)$

解：$H(t) = R S_x \sin\theta\cos\omega t + R S_y \sin\theta\sin\omega t + R S_z \cos\theta$

$S_i = \frac{1}{2}\sigma_i$，$\sigma_i$ 为 Pauli 矩阵

$S_x=\frac{1}{2}\begin{bmatrix} & 1\\ 1 & \end{bmatrix}$, $S_y=\frac{1}{2}\begin{bmatrix} & -i\\ i & \end{bmatrix}$, $S_z=\frac{1}{2}\begin{bmatrix}1 & \\ & -1\end{bmatrix}$

写出 Hamiltonian 的矩阵：

$$H(t)=\frac{R}{2}\begin{bmatrix}\cos\theta & \sin\theta(\cos\omega t-i\sin\omega t)\\ \sin\theta(\cos\omega t+i\sin\omega t) & -\cos\theta\end{bmatrix}=\frac{R}{2}\begin{bmatrix}\cos\theta & \sin\theta e^{-i\omega t}\\ \sin\theta e^{i\omega t} & -\cos\theta\end{bmatrix}$$

求本征值，解久期方程

$$\begin{vmatrix}\cos\theta-\frac{2E}{R} & \sin\theta e^{-i\omega t}\\ \sin\theta e^{i\omega t} & -\cos\theta-\frac{2E}{R}\end{vmatrix}=0$$

$$E^2=\frac{R^2}{4}$$

$$E_\pm=\pm\frac{R}{2}\Rightarrow\begin{cases}E_+=\frac{R}{2}\\ E_-=-\frac{R}{2}\end{cases}$$

这是个非简并二能级系统，且能级能量不随时间改变。

考虑基态，即 E_- 对应的本征态 $|\psi_-(t)\rangle$

设 $|\psi_-(t)\rangle=\begin{bmatrix}x\\ y\end{bmatrix}$，由本征方程 $H(t)|\psi_-(t)\rangle=E_-|\psi_-(t)\rangle$

得 $\begin{cases}\cos\theta x+\sin\theta e^{-i\omega t}y=-x\\ \sin\theta e^{i\omega t}x-\cos\theta y=-y\end{cases}\Rightarrow\frac{\sin\theta e^{i\omega t}}{\cos\theta-1}x=y$

$$\Rightarrow|\psi_-(t)\rangle=\begin{bmatrix}x\\ \frac{\sin\theta e^{i\omega t}}{\cos\theta-1}x\end{bmatrix}$$

归一化. $x^2\left(1+\frac{\sin^2\theta}{(\cos\theta-1)^2}\right)=1$

$$x=\frac{\cos\theta-1}{\sqrt{2-2\cos\theta}}=-\sqrt{\frac{1-\cos\theta}{2}}$$

$$\Rightarrow|\psi_-(t)\rangle=\begin{bmatrix}-\sqrt{\frac{1-\cos\theta}{2}}\\ \frac{\sin\theta e^{i\omega t}}{\sqrt{2-2\cos\theta}}\end{bmatrix}$$

可见该系统能量本征值不随时间改变（当然，期望值是可变的），本征态随时间周期性改变（$T=\frac{2\pi}{\omega}$）。

① 绝热近似解

绝热近似条件(1)要求

$$\left|\frac{d\vec{R}}{dt}\right| / |\vec{R}| \ll E_{gap} = R$$

$$\sqrt{\omega^2\sin^2\theta+\cos^2\theta} \ll R$$

假定满足绝热近似条件，考虑绝热近似解(20)，初态为基态 $|\psi_-(0)\rangle$，则

$$|\Psi(t)\rangle = e^{i\gamma_-(t)} e^{i\phi_-(t)} |\psi_-(t)\rangle$$

动力学相位 $\phi_-(t) = -\int_0^t E_- \, d\tau = \frac{R}{2} t$

几何相位 $\gamma_-(t) = i\int_0^t \langle\psi_-(\tau)|\frac{\partial}{\partial\tau}|\psi_-(\tau)\rangle \, d\tau$

$$= i\int_0^t \left(-\sqrt{\frac{1-\cos\theta}{2}}, \frac{\sin\theta e^{-i\omega\tau}}{\sqrt{2-2\cos\theta}}\right) \begin{pmatrix} 0 \\ \frac{i\omega\sin\theta e^{i\omega\tau}}{\sqrt{2-2\cos\theta}} \end{pmatrix} d\tau$$

$$= -\frac{\omega}{2}(1+\cos\theta)\, t$$

得到 $|\Psi(t)\rangle = e^{-i\frac{\omega}{2}(1+\cos\theta)t} e^{i\frac{R}{2}t} \begin{bmatrix} -\sqrt{\frac{1-\cos\theta}{2}} \\ \frac{\sin\theta e^{i\omega t}}{\sqrt{2-2\cos\theta}} \end{bmatrix}$，

初始条件为 $|\Psi(0)\rangle = \begin{bmatrix} -\sqrt{\frac{1-\cos\theta}{2}} \\ \frac{\sin\theta}{\sqrt{2-2\cos\theta}} \end{bmatrix}$

② 精确解

若不同时刻的 $H(t)$ 对易，则可以有

$$i\frac{\partial}{\partial t}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle$$

$$|\Psi(t)\rangle = e^{-i\int_0^t H(\tau)d\tau}|\Psi(0)\rangle$$

然而这里 $[H(t), H(\tau)] \neq 0$，不再求精确解。