含时微扰论（Time-Dependent Perturbation Theory）

$$|\Psi(t)\rangle = \hat{U}(t,t_0)\,|\Psi(t_0)\rangle \qquad i\hbar\frac{\partial \hat{U}(t,t_0)}{\partial t} = \hat{H}\hat{U}(t,t_0)$$

H不显含t

$$\hat{U}(t,t_0) = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}$$

H显含t

角度一：迭代形式

$$\hat{U}(t,t_0) = \mathbf{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{H}(t')\hat{U}(t',t_0)$$

角度二

$$\begin{aligned}\hat{U}(t,t_0) &= \lim_{N\to\infty} e^{-\frac{i}{\hbar}\hat{H}(t)\frac{t-t_0}{N}}\, e^{-\frac{i}{\hbar}\hat{H}(t_{N-1})\frac{t-t_0}{N}} \cdots e^{-\frac{i}{\hbar}\hat{H}(t_0)\frac{t-t_0}{N}} \\ &= \lim_{N\to\infty} e^{-\frac{i}{\hbar}\left[\hat{H}(t)+\hat{H}(t_{N-1})+\hat{H}(t_0)\right]\frac{t-t_0}{N}} \\ &= \hat{\mathcal{T}} e^{\int_{t_0}^{t} -\frac{i}{\hbar}\hat{H}(t')dt'}\end{aligned}$$

$\hat{\mathcal{T}}$ 是编时算符 作用是将被积算符微元对应的指数项按时间顺序排列

相互作用绘景

不含时H0给出U0表达式如上所示

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t) \qquad \hat{U}(t,t_0) = \hat{U}_0(t,t_0)\hat{U}_{\mathcal{I}}(t,t_0)$$

$$\langle\Psi(t)|\,\hat{O}\,|\Psi(t)\rangle = \langle\Psi(t_0)|\,\hat{U}_{\mathcal{I}}^{\dagger}(t,t_0)U_0^{\dagger}(t,t_0)\hat{O}\hat{U}_0(t,t_0)\hat{U}_{\mathcal{I}}(t,t_0)\,|\Psi(t_0)\rangle$$

$$\boxed{\begin{aligned}\hat{O}_{\mathcal{I}}(t) &= U_0^{\dagger}(t,t_0)\hat{O}\hat{U}_0(t,t_0) \\ |\Psi_{\mathcal{I}}(t)\rangle &= \hat{U}_{\mathcal{I}}(t,t_0)\,|\Psi(t_0)\rangle\end{aligned}}$$

含时微扰论

到这里你可能会有疑问，因为我们知道 $\hat{U}_0(t,t_0)$ 的形式，所以相互作用绘景下的算符 $\hat{O}_{\mathcal{I}}$ 我们可以直接写出来。但 $\hat{U}_{\mathcal{I}}(t,t_0)$ 该怎么确认呢？现在回忆一下前面 (4) 式 $i\hbar\frac{\partial\hat{U}(t,t_0)}{\partial t} = \hat{H}\hat{U}(t,t_0)$，现在我们把相互作用绘景下的时间演化算符代入并计算

$$i\hbar\frac{\partial \hat{U}_{\mathcal{I}}(t,t_0)}{\partial t} = \hat{V}_{\mathcal{I}}(t)\hat{U}_{\mathcal{I}}(t,t_0) \qquad \hat{V}_{\mathcal{I}}(t) = \hat{U}_0^{\dagger}(t,t_0)\hat{V}(t)\hat{U}_0(t,t_0)$$

$$\hat{U}_{\mathcal{I}}(t,t_0) = \mathbf{1} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,\hat{V}_{\mathcal{I}}(t')\hat{U}_{\mathcal{I}}(t',t_0)$$

展开到一阶（VI很小时）

$$\hat{U}_{\mathcal{I}} \approx \mathbf{1} + \frac{1}{i\hbar}\int_{t_0}^{t}\hat{V}_{\mathcal{I}}(t_1)dt_1$$

将这个式子反复迭代，得到戴森级数

$$\boxed{\hat{U}_{\mathcal{I}} = \sum_{n=0}^{\infty}\left(\frac{1}{i\hbar}\right)^{n}\int_{t_0}^{t}dt_1\int_{t_0}^{t_1}dt_2\cdots\int_{t_0}^{t_{n-1}}dt_n\,\hat{V}_{\mathcal{I}}(t_1)\hat{V}_{\mathcal{I}}(t_2)\cdots\hat{V}_{\mathcal{I}}(t_n)}$$

经过时间演化后系统向各个态跃迁的概率

$$P_{n\leftarrow m} = \left|\left\langle\psi_n^0\left|\hat{U}(t,t_0)\right|\psi_m^0\right\rangle\right|^2$$

$$\begin{aligned}\left\langle\psi_n^0\left|\hat{U}(t,t_0)\right|\psi_m^0\right\rangle &= \left\langle\psi_n^0\left|\hat{U}_0(t,t_0)\hat{U}_{\mathcal{I}}(t,t_0)\right|\psi_m^0\right\rangle \\ &= e^{-\frac{i}{\hbar}\hat{H}_0(t-t_0)}\left\langle\psi_n^0\left|\hat{U}_{\mathcal{I}}(t,t_0)\right|\psi_m^0\right\rangle\end{aligned}$$

$$\begin{aligned}\left\langle\psi_n^0\left|\hat{U}_{\mathcal{I}}(t,t_0)\right|\psi_m^0\right\rangle &= \delta_{mn} + \frac{1}{i\hbar}\int_{t_0}^{t}dt_1\left\langle\psi_n^0\left|\hat{U}_0^{\dagger}(t_1,t_0)\hat{V}(t_1)\hat{U}_0(t_1,t_0)\right|\psi_m^0\right\rangle \\ &= \delta_{mn} + \frac{1}{i\hbar}\int_{t_0}^{t}dt_1\left\langle\psi_n^0\left|\hat{V}(t_1)\right|\psi_m^0\right\rangle e^{-\frac{i}{\hbar}(E_m^0-E_n^0)(t_1-t_0)}\end{aligned}$$

$$P_{n\leftarrow m} = \left(\frac{1}{\hbar}\right)^2\left|\int_{t_0}^{t}\left\langle\psi_n^0\left|\hat{V}(t_1)\right|\psi_m^0\right\rangle e^{-\frac{i}{\hbar}(E_m^0-E_n^0)(t_1-t_0)}dt_1\right|^2$$

绝热近似（Adiabatic Approximation）

缓慢变化的系统

$$\hat{H}=\hat{H}_0+\hat{V}[\vec{\lambda}(t)]$$

$$\vec{\lambda}(t)\equiv[\lambda_1(t),\lambda_2(t),\cdots,\lambda_n(t)]$$

$$\lambda_1(t)=B_x(t),\lambda_2(t)=E_z(t),\cdots$$

慢变微扰 V

$$\hat{H}(\lambda)\left|\psi_n(\lambda)\right\rangle=E_n(\lambda)\left|\psi_n(\lambda)\right\rangle$$

瞬时本征方程

酉变换

$$\left|\Psi(t)\right\rangle=\hat{U}(t)\left|\psi(t)\right\rangle$$

$$i\hbar\frac{\partial\left[\hat{U}(t)\left|\psi(t)\right\rangle\right]}{\partial t}=\hat{H}[\vec{\lambda}(t)]\hat{U}(t)\left|\psi(t)\right\rangle$$

$$\hat{H}_{eff}=\hat{U}^{\dagger}(t)\hat{H}[\vec{\lambda}(t)]\hat{U}(t)-i\hbar\hat{U}^{\dagger}(t)\frac{\partial\hat{U}(t)}{\partial t}$$

$$i\hbar\frac{\partial\left|\psi(t)\right\rangle}{\partial t}=\hat{H}_{eff}\left|\psi(t)\right\rangle$$

应用一：U(t)=U(t, t0)为时间演化算子，则变换后的态给出Heisenberg绘景下的态

应用二：U(t)=U(t, t0)给出相互作用绘景

$$\begin{aligned}\hat{H}_{eff}(t)&=\hat{U}_0^{\dagger}(t,t_0)\hat{H}[\vec{\lambda}(t)]\hat{U}_0(t,t_0)-i\hbar\hat{U}_0^{\dagger}(t,t_0)\frac{\partial\hat{U}_0(t,t_0)}{\partial t}\\&=\hat{U}_0^{\dagger}(t,t_0)\hat{H}[\vec{\lambda}(t)]\hat{U}_0(t,t_0)-\hat{U}_0^{\dagger}(t,t_0)\hat{H}_0\hat{U}_0(t,t_0)\\&=\hat{U}_0^{\dagger}(t,t_0)\left[\hat{H}[\vec{\lambda}(t)]-\hat{H}_0\right]\hat{U}_0(t,t_0)\\&=\hat{U}_0^{\dagger}(t,t_0)\hat{V}[\vec{\lambda}(t)]\hat{U}_0(t,t_0)\\&=\hat{V}_{\mathcal{I}}[\vec{\lambda}(t)]\end{aligned}$$

绝热微扰

考虑酉变换 $\boxed{\hat{U}(t)=\sum_n\left|\psi_n[\vec{\lambda}(t)]\right\rangle\left\langle\psi_n[\vec{\lambda}(0)]\right|}$ （H不显含t时退化为U(t, t0)）

$$i\hbar\frac{\partial\left|\psi(t)\right\rangle}{\partial t}=\sum_n E_n[\vec{\lambda}(t)]\left|\psi(t)\right\rangle-i\hbar\sum_{m,n}\left|\psi_n[\vec{\lambda}(0)]\right\rangle\left\langle\psi_m[\vec{\lambda}(0)]\right|\left\langle\psi_n[\vec{\lambda}(t)]\middle|\frac{\mathrm{d}\psi_m[\vec{\lambda}(t)]}{\mathrm{d}t}\right\rangle\left|\psi(t)\right\rangle$$

用初始时刻m本征态左作用

$$i\hbar\frac{\mathrm{d}D_m}{\mathrm{d}t}=E_m[\vec{\lambda}(t)]D_m-i\hbar\sum_n\left\langle\psi_m[\vec{\lambda}(t)]\middle|\frac{\mathrm{d}\psi_n[\vec{\lambda}(t)]}{\mathrm{d}t}\right\rangle D_n$$

$$D_n(t)=\left\langle\psi_n[\vec{\lambda}(0)]\middle|\psi(t)\right\rangle$$

$$\frac{\mathrm{d}y}{\mathrm{d}x}+P(x)y=Q(x)$$

$$D_n=C_ne^{i\theta_n}$$

常数变易法，Cn = Cn(t)

$$\boxed{\theta_n(t)=-\frac{1}{\hbar}\int_0^t E_n[\vec{\lambda}(t')]\mathrm{d}t'}$$

动力学项
瞬时本征能量积累的结果

$$\dot{C}_m=-\sum_n C_n\left\langle\psi_m[\vec{\lambda}(t)]\middle|\frac{\mathrm{d}\psi_n[\vec{\lambda}(t)]}{\mathrm{d}t}\right\rangle e^{i(\theta_n-\theta_m)}$$

$$\int_0^T\dot{C}_m\mathrm{d}t=\int_0^T-C_m\left\langle\psi_m[\vec{\lambda}(t)]\middle|\frac{\mathrm{d}\psi_m[\vec{\lambda}(t)]}{\mathrm{d}t}\right\rangle\mathrm{d}t-\int_0^T\sum_{n\neq m}C_n\left\langle\psi_m[\vec{\lambda}(t)]\middle|\frac{\mathrm{d}\psi_n[\vec{\lambda}(t)]}{\mathrm{d}t}\right\rangle e^{i(\theta_n-\theta_m)}\mathrm{d}t$$

从这里开始有近似，注意到等式右边第二项可化为

$$\left\langle\psi_m[\vec{\lambda}(t)]\middle|\frac{\mathrm{d}\psi_n[\vec{\lambda}(t)]}{\mathrm{d}t}\right\rangle=\frac{\left\langle\psi_m[\vec{\lambda}(t)]\right|\frac{\mathrm{d}\hat{H}[\lambda(t)]}{\mathrm{d}t}\left|\psi_n[\vec{\lambda}(t)]\right\rangle}{E_n-E_m}$$

由于是慢变系统，dH/dt 很小，且存在指数振荡，因此较大时间尺度下这一项可忽略，即

$$\dot{C}_m\approx-C_m\left\langle\psi_m[\vec{\lambda}(t)]\middle|\frac{\mathrm{d}\psi_m[\vec{\lambda}(t)]}{\mathrm{d}t}\right\rangle$$

$$C_m(t)=C_m(0)e^{i\gamma_m}$$

$$\boxed{\gamma_m(t)=i\int_0^t\left\langle\psi_m[\vec{\lambda}(t')]\middle|\frac{\mathrm{d}\psi_m[\vec{\lambda}(t')]}{\mathrm{d}t'}\right\rangle\mathrm{d}t'}$$

$$D_n(t)=\left\langle\psi_n[\vec{\lambda}(0)]\middle|\psi(t)\right\rangle=C_n(0)e^{i\gamma_n}e^{i\theta_n}$$

$$\left|\Psi(t)\right\rangle=\sum_n\left|\psi_n[\vec{\lambda}(t)]\right\rangle\left\langle\psi_n[\vec{\lambda}(0)]\middle|\psi(t)\right\rangle$$

几何项

几何相位实际上是由量子绝热过程在参数空间里的路径决定的，和这个系统变化的多快多慢没什么关系，所以叫几何相。

$$\begin{aligned}\gamma_m(t)&=i\int_0^t\left\langle\psi_m[\vec{\lambda}(t')]\middle|\sum_i\frac{\partial\psi_m[\vec{\lambda}(t')]}{\partial\lambda_i}\right\rangle\frac{\mathrm{d}\lambda_i}{\mathrm{d}t'}\mathrm{d}t'\\&=i\int_{\lambda(0)}^{\lambda(t)}\left\langle\psi_m[\vec{\lambda}(t')]\middle|\sum_i\frac{\partial\psi_m[\vec{\lambda}(t')]}{\partial\lambda_i}\right\rangle\mathrm{d}\lambda_i\end{aligned}$$

假定一开始系统处在初始时刻的第m个瞬时本征态上

$$\left|\Psi(0)\right\rangle=\left|\psi_m[\vec{\lambda}(0)]\right\rangle$$

$$C_n(0)=\delta_{mn}$$

$$\boxed{\begin{aligned}\left|\Psi(t)\right\rangle&=\delta_{mn}e^{i\theta_n(t)}e^{i\gamma_n(t)}\sum_m\left|\psi_m[\vec{\lambda}(t)]\right\rangle\\&=e^{i\theta_m(t)}e^{i\gamma_m(t)}\left|\psi_m[\vec{\lambda}(t)]\right\rangle\end{aligned}}$$

系统在t时刻的第m个瞬时本征态上！只不过前面叠加了一个相位因子，总的相位变化是动力学相和几何相的叠加。

这就是绝热近似的内容，对于一个缓慢变化的系统，如果初始时刻系统处在第m个本征态，那么在经过一段时间后系统还是处在第m个本征态。

费曼路径积分表述（Feynman Path Integral Formulation）

作用量 $S = \int dtL$ 　 Feynman-Dirac解释 $\phi[x(t)] = Ce^{\frac{i}{\hbar}S[x(t)]}$

在量子力学中，粒子从 (a, t_a) 运动到 (b, t_b) 有无穷多可能的轨迹，这些轨迹弥漫整个空间，每个轨迹都有一定的概率。如果粒子沿着每一条轨迹运动的概率幅为：

Feynman路径积分

$$\boxed{K(b,a) = \int \mathcal{D}x(t) e^{\frac{i}{\hbar}S(b,a)}}$$

$$\langle x_N, t_N | x_1, t_1 \rangle = \int_{x_1}^{x_N} \mathcal{D}[x(t)] \exp\left[i \int_{t_1}^{t_N} dt \frac{L_{\text{经典}}(x, \dot{x})}{\hbar} \right]$$

传播子

$$K(\mathbf{x}'', t; \mathbf{x}', t_0) = \sum_{a'} \langle \mathbf{x}'' | a' \rangle \langle a' | \mathbf{x}' \rangle \exp\left[\frac{-iE_{a'}(t-t_0)}{\hbar} \right]$$

$$K(\mathbf{x}'', t; \mathbf{x}', t_0) = \langle \mathbf{x}'' | \exp\left[\frac{-iH(t-t_0)}{\hbar} \right] | \mathbf{x}' \rangle = \langle \mathbf{x}'', t | \mathbf{x}', t_0 \rangle$$

跃迁振幅 　 从 (a, t_a) 移动到 (b, t_b) 的**概率幅** 　 $P_{b \leftarrow a} = |K(b,a)|^2$

系起来．但首先回忆一下，波函数作为固定的位置左矢 $\langle \mathbf{x}' |$ 与运动的态右矢 $| \alpha, t_0; t \rangle$ 的内积，还可以看作是随时间“相反”运动的海森伯绘景的位置左矢 $\langle \mathbf{x}', t |$ 与海森伯绘景中时间固定的态右矢 $| \alpha, t_0 \rangle$ 的内积．同样地，传播子也可以写为

值 $\mathbf{x}'$ 的粒子将在稍后的 t 时刻在 $\mathbf{x}''$ 处被发现的概率振幅．粗略地讲，$\langle \mathbf{x}'', t | \mathbf{x}', t_0 \rangle$ 是粒子从时空点（$\mathbf{x}', t_0$）到另一个时空点（$\mathbf{x}'', t$）的振幅，因此，术语跃迁振幅对于这个表示式是

积分算子D[x(t)]给出该积分的测度（事实上是给出了该积分具体的形式）：

$$\boxed{\int_{x_1}^{x_N} \mathcal{D}[x(t)] \equiv \lim_{N \to} \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{(N-1)/2} \int dx_{N-1} \int dx_{N-2} \cdots \int dx_2}$$

路径积分表述与Schrodinger方程给出等价的时间演化：

$$\psi(x_2, t_2) = \int dx_1 K(x_2, t_2; x_1, t_1) \psi(x_1, t_1)$$

$$\psi(x_2, t+\epsilon) = \int d\eta \frac{1}{A} e^{\frac{im\eta^2}{2\hbar\epsilon}} e^{-\frac{i}{\hbar}\epsilon V(x_2 + \frac{\eta}{2}, t)} \psi(x_2 + \eta, t)$$

小时间变化，换元x1 = x2 + η

$$\begin{aligned} \psi(x_2, t) + \varepsilon \frac{\partial \psi(x_2, t)}{\partial t} = & \frac{\left[1 - \frac{i\varepsilon}{\hbar} V(x_2, t)\right] \psi(x_2, t)}{A} \int d\eta e^{\frac{im\eta^2}{2\hbar\varepsilon}} \\ & + \frac{\left[1 - \frac{i\varepsilon}{\hbar} V(x_2, t)\right]}{A} \frac{\partial \psi(x_2, t)}{\partial x_2} \int d\eta e^{\frac{im\eta^2}{2\hbar\varepsilon}} \eta \\ & + \frac{\left[1 - \frac{i\varepsilon}{\hbar} V(x_2, t)\right]}{A} \frac{\partial^2 \psi(x_2, t)}{\partial x_2^2} \int d\eta e^{\frac{im\eta^2}{2\hbar\varepsilon}} \frac{\eta^2}{2} \end{aligned}$$

$$A = \sqrt{\frac{2\pi i \hbar \varepsilon}{m}}$$

$$\int d\eta e^{\frac{im\eta^2}{2\hbar\varepsilon}} \eta = 0$$

$$\int d\eta e^{\frac{im\eta^2}{2\hbar\varepsilon}} \frac{\eta^2}{2} = \frac{i\hbar\varepsilon}{2m}$$

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t)$$

实际上路径积分中的传播子就是坐标表象下的时间演化算符

$$\frac{\partial K(x_2, t_2; x_1, t_1)}{\partial t_2} = -\frac{\hbar^2}{2m} \frac{\partial^2 K(x_2, t_2; x_1, t_1)}{\partial x_2^2} + V(x_2, t_2) K(x_2, t_2; x_1, t_1)$$