

含时微扰论(Time-Dependent Perturbation Theory)

$$|\Psi(t)
angle = \hat{U}(t,t_0) \ket{\Psi(t_0)}$$

$$i\hbarrac{\partial \hat{U}(t,t_0)}{\partial t}=\hat{H}\hat{U}(t,t_0)$$



H不显含t

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

H显含t

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

角度二

角度一: 迭代形式

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

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

$$\hat{H}(t) = \hat{H}_0 + \hat{V}(t)$$

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



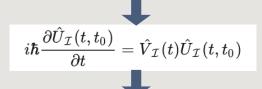
 $ra{\langle \Psi(t) | \hat{\mathcal{O}} | \Psi(t)
angle} = ra{\langle \Psi(t_0) | \hat{U}_{\mathcal{I}}^\dagger(t,t_0) U_0^\dagger(t,t_0) \hat{\mathcal{O}} \hat{U}_0(t,t_0) \hat{U}_{\mathcal{I}}(t,t_0) | \Psi(t_0)
angle}$



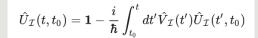
$$egin{aligned} \hat{\mathcal{O}}_{\mathcal{I}}(t) &= U_0^\dagger(t,t_0) \hat{\mathcal{O}} \hat{U}_0(t,t_0) \ |\Psi_{\mathcal{I}}(t)
angle &= \hat{U}_{\mathcal{I}}(t,t_0) \, |\Psi(t_0)
angle \end{aligned}$$

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 $\hat{\mathcal{O}}_{\mathcal{I}}$ 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 $i\hbarrac{\partial \hat{U}(t,t_0)}{\partial t}=\hat{H}\hat{U}(t,t_0)$,现在我们把相互作用绘景下的时间演化算符代入并计算



$$\hat{V}_{\mathcal{I}}(t) = \hat{U}_0^{\dagger}(t,t_0)\hat{V}(t)\hat{U}_0(t,t_0)$$



展开到一阶(VI很小时)
$$\hat{U}_{\mathcal{I}}pprox \mathbf{1} + rac{1}{i\hbar}\int_{t_0}^t \hat{V}_{\mathcal{I}}(t_1)dt_1$$

将这个式子反复迭代,得到戴森级数
$$\hat{U}_{\mathcal{I}} = \sum_{n=0}^{\infty} \left(\frac{1}{i\hbar}\right)^n \int_{t_0}^t dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \hat{V}_{\mathcal{I}}(t_1) \hat{V}_{\mathcal{I}}(t_2) \cdots \hat{V}_{\mathcal{I}}(t_n)$$

经过时间演化后系统向各个态跃迁的概率 $P_{n\leftarrow m} = \left|\left\langle \psi_n^0 \left| \hat{U}(t,t_0) \right| \psi_m^0 \right\rangle \right|^2$

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

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

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

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



绝热近似(Adiabatic Approximation)

缓慢变化的系统

$$\hat{H}=\hat{H}_0+\hat{V}[ec{\lambda}(t)] egin{aligned} ec{\lambda}(t) \equiv [\lambda_1(t),\lambda_2(t),\cdots,\lambda_n(t)] \ \hline \lambda_1(t) = B_x(t),\lambda_2(t) = E_z(t),\cdots \end{aligned}$$

$$\hat{H}(\lambda)\ket{\psi_n(\lambda)} = E_n(\lambda)\ket{\psi_n(\lambda)}$$

慢变微扰 V

瞬时本征方程

酉变换

$$\ket{\Psi(t)} = \hat{U}(t)\ket{\psi(t)}$$

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

$$i\hbarrac{\partial\left[\hat{U}(t)\left|\psi(t)
ight
angle
ight]}{\partial t}=\hat{H}[ec{\lambda}(t)]\hat{U}(t)\left|\psi(t)
ight
angle$$

$$i\hbarrac{\partial\left|\psi(t)
ight
angle}{\partial t}=\hat{H}_{eff}\left|\psi(t)
ight
angle$$

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

$$\begin{split} \hat{H}_{eff}(t) &= \hat{U}_{0}^{\dagger}(t,t_{0}) \hat{H}[\vec{\lambda}(t)] \hat{U}_{0}(t,t_{0}) - i\hbar \hat{U}_{0}^{\dagger}(t,t_{0}) \frac{\partial \hat{U}_{0}(t,t_{0})}{\partial t} \\ &= \hat{U}_{0}^{\dagger}(t,t_{0}) \hat{H}[\vec{\lambda}(t)] \hat{U}_{0}(t,t_{0}) - \hat{U}_{0}^{\dagger}(t,t_{0}) \hat{H}_{0} \hat{U}_{0}(t,t_{0}) \\ &= \hat{U}_{0}^{\dagger}(t,t_{0}) \left[\hat{H}[\vec{\lambda}(t)] - \hat{H}_{0} \right] \hat{U}_{0}(t,t_{0}) \\ &= \hat{U}_{0}^{\dagger}(t,t_{0}) \hat{V}[\vec{\lambda}(t)] \hat{U}_{0}(t,t_{0}) \\ &= \hat{V}_{\mathcal{I}}[\vec{\lambda}(t)] \end{split}$$

绝热微扰

考虑酉变换
$$\hat{U}(t) = \sum_{n} \left| \psi_n[\vec{\lambda}(t)] \right\rangle \left\langle \psi_n[\vec{\lambda}(0)] \right|$$

(H不显含t时退化为U(t, t0))

$$i\hbarrac{\partial\ket{\psi(t)}}{\partial t} = \sum_n E_n[ec{\lambda}(t)]\ket{\psi(t)} - i\hbar\sum_{m,n}\left|\psi_n[ec{\lambda}(0)]
ight>\left<\psi_m[ec{\lambda}(0)]\left|\left<\psi_n[ec{\lambda}(t)]
ight| rac{\mathrm{d}\psi_m[ec{\lambda}(t)]}{\mathrm{d}t}
ight>\ket{\psi(t)}$$

用初始时刻m本征态左作用
$$i\hbar \frac{\mathrm{d}D_m}{\mathrm{d}t} = E_m[\vec{\lambda}(t)]D_m - i\hbar \sum_n \left\langle \psi_m[\vec{\lambda}(t)] \left| \frac{\mathrm{d}\psi_n[\vec{\lambda}(t)]}{\mathrm{d}t} \right\rangle D_n$$
 $D_n(t) = \left\langle \psi_n[\vec{\lambda}(0)]|\psi(t) \right\rangle$

瞬时本征 能量积累

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



 $D_n=C_ne^{i heta_n}$ 常数变易法,Cn = Cn(t) $heta_n(t)=-rac{1}{\hbar}\int_0^t E_n[ec{\lambda}(t')]\mathrm{d}t'$



$$\dot{C}_m = -\sum_n C_n \left< \psi_m[ec{\lambda}(t)]
ight| rac{\mathrm{d}\psi_n[ec{\lambda}(t)]}{\mathrm{d}t}
ight> e^{i(heta_n - heta_m)} \ .$$



$$\left[\dot{C}_m = -\sum_n C_n \left\langle \psi_m[ec{\lambda}(t)] \middle| rac{\mathrm{d}\psi_n[ec{\lambda}(t)]}{\mathrm{d}t}
ight
angle e^{i(heta_n - heta_m)}
ight] = \int_0^T \dot{C}_m \mathrm{d}t = \int_0^T -C_m \left\langle \psi_m[ec{\lambda}(t)] \middle| rac{\mathrm{d}\psi_m[ec{\lambda}(t)]}{\mathrm{d}t}
ight
angle \mathrm{d}t - \int_0^T \sum_{n
eq m} C_n \left\langle \psi_m[ec{\lambda}(t)] \middle| rac{\mathrm{d}\psi_m[ec{\lambda}(t)]}{\mathrm{d}t}
ight
angle e^{i(heta_n - heta_m)} \mathrm{d}t$$

从这里开始有近似,注意到等式右边第二项可化为
$$\left\langle \psi_m[\vec{\lambda}(t)] \right| \frac{\mathrm{d}\psi_n[\vec{\lambda}(t)]}{\mathrm{d}t} \right\rangle = \frac{\left\langle \psi_m[\vec{\lambda}(t)] \right| \frac{\mathrm{d}\vec{\mu}[\lambda(t)]}{\mathrm{d}t} \left| \psi_n[\vec{\lambda}(t)] \right\rangle}{E_n - E_m}$$

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

$$\dot{C}_m pprox - C_m \left< \psi_m[ec{\lambda}(t)] \middle| rac{\mathrm{d}\psi_m[ec{\lambda}(t)]}{\mathrm{d}t}
ight> lacksquare$$

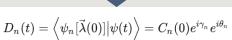


空间里的路径决定的

和这个系统变化的多 快多慢没什么关系,

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

 $\left| \gamma_m(t) = i \int_0^t \left\langle \psi_m[ec{\lambda}(t')] \left| rac{\mathrm{d} \psi_m[ec{\lambda}(t')]}{\mathrm{d} t'}
ight
angle \mathrm{d} t'
ight|$

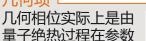


$$\left|\Psi(t)\right\rangle = \sum_{n} \left|\psi_{n}[\vec{\lambda}(t)]\right\rangle \left\langle \psi_{n}[\vec{\lambda}(0)] \right| \psi(t) \rangle$$

假定一开始系 统处在初始时 刻的第m个瞬时 本征态上

$$\ket{\Psi(0)} = \ket{\psi_m[ec{\lambda}(0)]}$$

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



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



所以叫几何相。

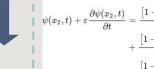
几何项

$$oxed{ \ket{\Psi(t)} = \delta_{mn} e^{i heta_n(t)} e^{i\gamma_n(t)} \sum_m \left|\psi_m[ec{\lambda}(t)]
ight>} \ = e^{i heta_m(t)} e^{i\gamma_m(t)} \left|\psi_m[ec{\lambda}(t)]
ight>}$$

系统在时刻的第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)

$$S=\int dt L$$

Feynman-Dirac解释 $\phi[x(t)] = Ce^{rac{i}{\hbar}S[x(t)]}$

$$\phi[x(t)] = C e^{rac{i}{\hbar}S[x(t)]}$$

个轨迹都有一定的概率。 加里拉子沿着有一条轨迹运动的概率振为

Feynman路径积分

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

$$K(b,a) = \int \mathcal{D}x(t)e^{rac{i}{\hbar}S(b,a)} \hspace{1cm} \langle x_N, t_N | x_1, t_1
angle = \int_{x_1}^{x_1} \mathfrak{D}[x(t)] \exp [i \int_{t_1}^{x_1} dt \, rac{L_{\mathfrak{BR}}(x, \dot{x})}{\hbar}]$$

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

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

跃迁振幅

从
$$(a,t_a)$$
 移动到 (b,t_b) 的概率幅

从
$$(a,t_a)$$
 移动到 (b,t_b) 的概率幅 $\left. P_{b\leftarrow a} = \left| K(b,a)
ight|^2$

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, $\langle \mathbf{x}'', t \mid \mathbf{x}', t_0 \rangle$ 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):

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

路径积分表述与Schrodinger方程给出等价的时间演化:

$$\psi(x_2,t_2) = \int dx_1 K(x_2,t_2;x_1,t_1) \psi(x_1,t_1) \qquad \psi(x_2,t+\epsilon) = \int d\eta rac{1}{A} e^{rac{im\eta^2}{2\hbar\epsilon}} e^{-rac{i}{\hbar}\epsilon V(x_2+rac{\eta}{2},t)} \psi(x_2+\eta,t)$$

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

小时间变化,换元x1 = x2 + n



$$\int rac{A-\sqrt{rac{2\pi\imath\hbar kc}{m}}}{\int d\eta e^{rac{i\omega^2}{2m}}\eta^2-0} \int rac{i\hbar arepsilon}{2} rac{i\hbar arepsilon}{2} = rac{\hbar^2}{2m} rac{\partial^2 \psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t)$$

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

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