0.1 微扰论

0.1.1 不含时微扰

0.1.1.1 微扰论的一般想法

1. 不含时微扰: 给定 H_0 的 E_n 和 $|\psi_n\rangle$, 计算 $H = H_0 + \lambda V(\lambda \ll 1)$ 的能谱.
2. 含时微扰: 给定裸传播子 $U_0(t) = \exp[-iH_0 t]$, 计算传播子 $U(t) = \tau\exp\left[-i\int_0^t \mathrm{d}t' H(t')\right]$, 其中 $H(t) = H_0 + \lambda V(t)$.

0.1.1.2 非简并微扰论

$$
\begin{aligned}
H(\lambda) &= H_0 + \lambda V \\
H(0) &= H_0, \quad \frac{\partial H(0)}{\partial \lambda} = V, \quad \frac{\partial^2 H(0)}{\partial \lambda^2} = \frac{\partial^3 H}{\partial \lambda^3} = \cdots = 0 \\
H(\lambda)|n(\lambda)\rangle &= E_n(\lambda)|n(\lambda)\rangle, \quad |n(\lambda)\rangle = \sum_l \psi_{nl}(\lambda)|l\rangle
\end{aligned}
$$

0.1.1.2.1 HF 定理

$$
\begin{aligned}
&\frac{\partial}{\partial\lambda}(H|n\rangle) = \frac{\partial}{\partial\lambda}(E_n|n\rangle) \Rightarrow \frac{\partial H}{\partial \lambda}|n\rangle + H\frac{\partial|n\rangle}{\partial\lambda} = \frac{\partial E_n}{\partial\lambda}|n\rangle + E_n\frac{\partial|n\rangle}{\partial\lambda} \\
&\text{左乘}\langle m|: \quad \langle m|\frac{\partial H}{\partial\lambda}|n\rangle + \langle m|H\frac{\partial|n\rangle}{\partial\lambda} = \langle m|\frac{\partial E_n}{\partial\lambda}|n\rangle + \langle m|E_n\frac{\partial|n\rangle}{\partial\lambda} \\
&V_{mn} + \langle m|E_m\frac{\partial|n\rangle}{\partial\lambda} = \frac{\partial E_n}{\partial\lambda}\delta_{mn} + \langle m|E_n\frac{\partial|n\rangle}{\partial\lambda} \\
&V_{mn} = \frac{\partial E_n}{\partial\lambda}\delta_{mn} + (E_n - E_m)\langle m|\frac{\partial|n\rangle}{\partial\lambda} \\
&\begin{cases}
m = n: \quad \dfrac{\partial E_n}{\partial\lambda} = V_{nn} \\
m \neq n: \quad V_{mn} = (E_n - E_m)\langle m|\dfrac{\partial|n\rangle}{\partial\lambda} \Rightarrow \langle m|\dfrac{\partial|n\rangle}{\partial\lambda} = \dfrac{V_{mn}}{E_n - E_m}, \quad \dfrac{\partial\langle n|}{\partial\lambda}|m\rangle = \dfrac{V_{nm}}{E_n - E_m}
\end{cases}
\end{aligned}
$$

0.1.1.2.2 能量的微扰修正

$$
\begin{aligned}
E_n(\lambda) &= \sum_l^\infty \frac{1}{l!}\frac{\partial^l E_n}{\partial\lambda^l}\lambda^l = E_n + \frac{\partial E_n}{\partial\lambda}\lambda + \frac{1}{2}\frac{\partial^2 E_n}{\partial\lambda^2}\lambda^2 + \cdots \\
\frac{\partial E_n}{\partial\lambda} &= V_{nn} = \langle n|\frac{\partial H}{\partial\lambda}|n\rangle = \langle n|V|n\rangle \\
\frac{\partial^2 E_n}{\partial\lambda^2} &= \frac{\partial}{\partial\lambda}\langle n|\frac{\partial H}{\partial\lambda}|n\rangle = \frac{\partial\langle n|}{\partial\lambda}\frac{\partial H}{\partial\lambda}|n\rangle + \langle n|\frac{\partial^2 H}{\partial\lambda^2}|n\rangle + \langle n|\frac{\partial H}{\partial\lambda}\frac{\partial|n\rangle}{\partial\lambda} \\
\frac{\partial^2 H}{\partial\lambda^2} = 0: \quad &= \sum_m \frac{\partial\langle n|}{\partial\lambda}|m\rangle\langle m|\frac{\partial H}{\partial\lambda}|n\rangle + \sum_m \langle n|\frac{\partial H}{\partial\lambda}|m\rangle\langle m|\frac{\partial|n\rangle}{\partial\lambda} \\
&= \sum_{m\neq n}\left[\frac{V_{nm}}{E_n - E_m}V_{mn} + V_{nm}\frac{V_{mn}}{E_n - E_m}\right] + V_{nn}\frac{\partial\langle n|n\rangle}{\partial\lambda} \\
&= 2\sum_{m\neq n}\frac{|V_{mn}|^2}{E_n - E_m} \\
\Rightarrow E_n &= E_n + V_{nn}\lambda + \sum_{m\neq n}\frac{|V_{mn}|^2}{E_n - E_m}\lambda^2 + \cdots
\end{aligned}
$$

0.1.1.2.3 态的微扰修正

$$
\begin{aligned}
|n(\lambda)\rangle &= \sum_{k=0}^{\infty}\frac{1}{k!}\frac{\partial^k|n\rangle}{\partial\lambda^k}\lambda^k = |n\rangle + \frac{\partial|n\rangle}{\partial\lambda}\lambda + \frac{1}{2}\frac{\partial^2|n\rangle}{\partial\lambda^2}\lambda^2 + \cdots \\
\frac{\partial|n\rangle}{\partial\lambda} &= \sum_{m\neq n}|m\rangle\langle m|\frac{\partial|n\rangle}{\partial\lambda} = \sum_{m\neq n}|m\rangle\frac{V_{mn}}{E_n-E_m} \\
\frac{\partial^2|n\rangle}{\partial\lambda^2} &= \frac{\partial}{\partial\lambda}\sum_{m\neq n}|m\rangle\frac{1}{E_n-E_m}\langle m|\frac{\partial H}{\partial\lambda}|n\rangle \\
&= \sum_{m\neq n}\Bigg[\frac{\partial|m\rangle}{\partial\lambda}\langle m|\frac{1}{E_n-E_m}\frac{\partial H}{\partial\lambda}|n\rangle + |m\rangle\frac{\partial\langle m|}{\partial\lambda}\frac{1}{E_n-E_m}\frac{\partial H}{\partial\lambda}|n\rangle \\
&\quad -|m\rangle\langle m|\frac{\partial H}{\partial\lambda}|n\rangle\frac{1}{(E_n-E_m)^2}\left(\frac{\partial E_n}{\partial\lambda}-\frac{\partial E_m}{\partial\lambda}\right) + |m\rangle\langle m|\frac{1}{E_n-E_m}\frac{\partial H}{\partial\lambda}\frac{\partial|n\rangle}{\partial\lambda}\Bigg] \\
&= \sum_{m\neq n}\Bigg[\sum_{l\neq m}|l\rangle\frac{V_{lm}}{E_m-E_l}\frac{V_{mn}}{E_n-E_m} + \sum_{l\neq m}|m\rangle\frac{V_{ml}}{E_m-E_l}\frac{V_{ln}}{E_n-E_m} \\
&\quad -|m\rangle\frac{V_{mn}}{(E_n-E_m)}(V_{nn}-V_{mm}) + \sum_{l\neq n}\frac{V_{ml}}{E_n-E_m}\frac{V_{ln}}{E_n-E_l}\Bigg]
\end{aligned}
$$

0.1.1.2.4 非简并微扰的物理图像

0.1.1.3 简并微扰论

0.1.1.3.1 简并微扰论的一般思想　简并态张成的空间是简并子空间.

1. 利用非简并微扰论将哈密顿量块对角化.
2. 分别处理每个对角块.
   (a) 对角块的对角元已经没有简并, 使用非简并微扰;
   (b) 对角块的对角元还有简并, 使用严格对角化.

0.1.1.3.2 HF 定理的推广　增加一个量子数 α 来区分同一能级 E_n 的本征态, 如 $|n\alpha\rangle$. 那么本征方程化为 $H_0|n\alpha\rangle = E_n|n\alpha\rangle$, 本征态互相正交: $\langle n'\alpha'|n\alpha\rangle = \delta_{nn'}\delta_{\alpha\alpha'}$ 将微扰项 V 通过新基矢展开:

$$
\begin{aligned}
V &= \sum_{n'\alpha',n\alpha}|n'\alpha'\rangle\langle n'\alpha'|V|n\alpha\rangle\langle n\alpha| = \sum_{n'\alpha',n\alpha}|n'\alpha'\rangle V_{n'\alpha',n\alpha}\langle n\alpha| \\
H(\lambda)|n\alpha(\lambda)\rangle &= \sum_{\alpha'}|n\alpha'(\lambda)\rangle\langle n\alpha'(\lambda)|H(\lambda)|n\alpha(\lambda)\rangle = \sum_{\alpha'}|n\alpha'(\lambda)\rangle E_{n\alpha',n\alpha} \\
&= \sum_{\alpha'}|n\alpha'(\lambda)\rangle E^{(n)}_{\alpha',\alpha}(\lambda) \\
\Rightarrow \langle m\beta(\lambda)|H(\lambda) &= \sum_{\beta'}\langle m\beta'|E^*_{m\beta',m\beta}(\lambda) = \sum_{\beta'}\langle m\beta'(\lambda)|[E^{(m)}_{\beta',\beta}]^*(\lambda) = \sum_{\beta'}E^{(m)}_{\beta,\beta'}(\lambda)\langle m\beta'(\lambda)|
\end{aligned}
$$

$E^{(n)}_{\alpha',\alpha}$ 是第 n 个能级的简并子空间内哈密顿量的矩阵元. 左乘 $\langle m\beta|\frac{\partial}{\partial\lambda}$:

$$\langle m\beta|\frac{\partial}{\partial\lambda}\Big[H(\lambda)|n\alpha(\lambda)\rangle\Big] = \langle m\beta|\frac{\partial}{\partial\lambda}\Big[\sum_{\alpha'}|n\alpha'(\lambda)\rangle E^{(n)}_{\alpha',\alpha}(\lambda)\Big]$$

$$\langle m\beta|\frac{\partial H}{\partial\lambda}|n\alpha\rangle + \langle m\beta|H\frac{\partial|n\alpha\rangle}{\partial\lambda} = \langle m\beta|\sum_{\alpha'}\left[\frac{\partial|n\alpha'\rangle}{\partial\lambda}E^{(n)}_{\alpha',\alpha} + |n\alpha'\rangle\frac{\partial E^{(n)}_{\alpha',\alpha}}{\partial\lambda}\right]$$

$$\begin{aligned}\langle m\beta|\frac{\partial H}{\partial\lambda}|n\alpha\rangle &= \sum_{\alpha'}\frac{\partial E^{(n)}_{\alpha',\alpha}}{\partial\lambda}\langle m\beta|n\alpha'\rangle + \sum_{\alpha'}\langle m\beta|\frac{\partial|n\alpha'\rangle}{\partial\lambda}E^{(n)}_{\alpha',\alpha} - \sum_{\beta'}E^{(m)}_{\beta,\beta'}\langle m\beta'|\frac{\partial|n\alpha\rangle}{\partial\lambda} \\ &= \frac{\partial E^{(n)}_{\beta,\alpha}}{\partial\lambda}\delta_{mn} + (E^{(n)} - E^{(m)})\langle m\beta|\frac{\partial|n\alpha\rangle}{\partial\lambda}\end{aligned}$$

1. $m = n$. 1st: $\quad \dfrac{\partial E^{(n)}_{\alpha',\alpha}}{\partial\lambda} = \langle n\alpha'|\dfrac{\partial H}{\partial\lambda}|n\alpha\rangle = V_{n\alpha',n\alpha}$

2. $m \neq n$. 2nd: $\quad \langle m\beta|\dfrac{\partial|n\alpha\rangle}{\partial\lambda} = \dfrac{\langle m\beta|\frac{\partial H}{\partial\lambda}|n\alpha\rangle}{E^{(n)} - E^{(m)}} = \dfrac{V_{m\beta,n\alpha}}{E^{(n)} - E^{(m)}}$

   $\dfrac{\partial\langle m\beta|}{\partial\lambda}|n\alpha\rangle = \dfrac{\langle m\beta|\frac{\partial H}{\partial\lambda}}{E^{(m)} - E^{(n)}} = \dfrac{V_{m\beta,n\alpha}}{E^{(m)} - E^{(n)}}$

约定 $\langle n\beta|\partial_\lambda n\alpha\rangle = \langle\partial_\lambda n\beta|n\alpha\rangle = 0$.

0.1.1.3.3　有效哈密顿量

$$\begin{aligned}\frac{\partial}{\partial\lambda}E^{(n)}_{\alpha,\beta} &= V_{n\alpha,n\beta} \\ \frac{\partial^2}{\partial\lambda^2}E^{(n)}_{\alpha,\beta} &= 2\sum_{m\neq n}\sum_{\gamma}\frac{V_{n\alpha,m\gamma}V_{m\gamma,n\beta}}{E_n - E_m} \\ \frac{\partial}{\partial\lambda}|n\alpha\rangle &= \sum_{m\neq n}\sum_{\beta}|m\beta\rangle\frac{V_{m\beta,n\alpha}}{E_n - E_m}\end{aligned}$$

代入得到修正后的能量和波函数

$$\begin{aligned}E^{(n)}_{\alpha\beta}(\lambda) &= E_n\delta_{\alpha\beta} + V_{n\alpha,n\beta}\lambda + \sum_{m\neq n}\sum_{\gamma}\frac{V_{n\alpha,m\gamma}V_{m\gamma,n\beta}}{E_n - E_m}\lambda^2 + \cdots \\ |n\alpha(\lambda)\rangle &= |n\alpha\rangle + \sum_{m\neq n}\sum_{\beta}|m\beta\rangle\frac{V_{m\beta,n\alpha}}{E_n - E_m}\lambda + \cdots\end{aligned}$$

哈密顿量可写作各简并子空间哈密顿量的直和:

$$\begin{aligned}H^{\text{eff}}_n(\lambda) &= \sum_{\alpha,\beta}|n\alpha(\lambda)\rangle E^{(n)}_{\alpha,\beta}(\lambda)\langle n\beta(\lambda)| \\ H(\lambda) &= \bigoplus_n H^{\text{eff}}_n(\lambda)\end{aligned}$$

0.1.1.3.4　简并微扰论的例子

1. 两格点 Hubbard 模型.
   $H = -t\sum_{\langle i,j\rangle,\sigma}c^\dagger_{i\sigma}c_{j\sigma} + \text{h.c.} + U\sum_i n_{i\uparrow}n_{i\downarrow}$. 粒子数 $N = \sum_i n_i$ 守恒, 磁量子数 $S^z = \sum_i s^z_i = \sum_i \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$ 守恒. 考虑两格点 $N = 2$ 和 $S^z = 0$ 的子空间, 基矢选定为占据数表象 $|n_{1\uparrow}n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle$. 考虑 $S^z = 0$ 的限制, 可能存在的态为 $|1100\rangle$, $|0011\rangle$, $|1001\rangle$, $|0110\rangle$. 将排斥项 $U\sum_i n_{i\uparrow}n_{i\downarrow}$ 视为未微扰项 H_0, 跃迁项 $-t\sum_{\langle i,j\rangle,\sigma}c^\dagger_{i\sigma}c_{j\sigma} + \text{h.c.}$ 视为微扰项 V. 得到矩阵元

的方法是 $A_{mn} = \langle\psi_m|A|\psi_n\rangle$, 其中 $|\psi_m\rangle$ 为上述选定的基矢.

$$H_0 = Un_{1\uparrow}n_{1\downarrow} + Un_{2\uparrow}n_{2\downarrow} = \begin{pmatrix} U & & & \\ & U & & \\ & & 0 & \\ & & & 0 \end{pmatrix}$$

$$V = -tc^\dagger_{1\uparrow}c_{2\uparrow} - tc^\dagger_{2\uparrow}c_{1\uparrow} - tc^\dagger_{1\downarrow}c_{2\downarrow} - tc^\dagger_{2\downarrow}c_{1\downarrow} = \begin{pmatrix} & & -t & t \\ & & -t & t \\ -t & -t & & \\ t & t & & \end{pmatrix}$$

首先计算 H_0 的本征值和本征矢. 由矩阵可知其已经对角化, 对角线上元素为 U 和 0.

n	states	E_n
0	$\|1\uparrow 1\downarrow\rangle = \|1100\rangle = \|\overset{n}{0},\overset{\alpha}{1}\rangle = \|\psi_1\rangle,\quad \|2\uparrow 2\downarrow\rangle = \|0011\rangle = \|\overset{n}{0},\overset{\alpha}{2}\rangle = \|\psi_2\rangle$	U
1	$\|1\uparrow 2\downarrow\rangle = \|1001\rangle = \|\overset{n}{1},\overset{\alpha}{1}\rangle = \|\psi_3\rangle,\quad \|1\downarrow 2\uparrow\rangle = \|0110\rangle = \|\overset{n}{1},\overset{\alpha}{2}\rangle = \|\psi_4\rangle$	0

接下来按照简并微扰论的公式计算 $n=1$ 时波函数修正

$$\begin{aligned}
|\overset{n}{1},\overset{\alpha}{1}\rangle' &= |\overset{n}{1},\overset{\alpha}{1}\rangle + |\overset{m}{0},\overset{\beta}{1}\rangle\frac{V_{\substack{m\beta\ n\alpha\\01,11}}}{E_{\substack{n\\1}} - E_{\substack{m\\0}}} + |\overset{m}{0},\overset{\beta}{2}\rangle\frac{V_{\substack{m\beta\ n\alpha\\02,11}}}{E_{\substack{n\\1}} - E_{\substack{m\\0}}} + \cdots \\
&= |\overset{n}{1},\overset{\alpha}{1}\rangle + |\overset{m}{0},\overset{\beta}{1}\rangle\frac{t}{U} + |\overset{m}{0},\overset{\beta}{2}\rangle\frac{t}{U} + \cdots \\
|\overset{n}{1},\overset{\alpha}{2}\rangle' &= |\overset{n}{1},\overset{\alpha}{2}\rangle + |\overset{m}{0},\overset{\beta}{1}\rangle\frac{V_{\substack{m\beta\ n\alpha\\01,12}}}{E_{\substack{n\\1}} - E_{\substack{m\\0}}} + |\overset{m}{0},\overset{\beta}{2}\rangle\frac{V_{\substack{m\beta\ n\alpha\\02,12}}}{E_{\substack{n\\1}} - E_{\substack{m\\0}}} + \cdots \\
&= |\overset{n}{1},\overset{\alpha}{2}\rangle - |\overset{m}{0},\overset{\beta}{1}\rangle\frac{t}{U} - |\overset{m}{0},\overset{\beta}{2}\rangle\frac{t}{U} + \cdots
\end{aligned}$$

和有效哈密顿量(能量):

$$\begin{aligned}
E^{(\overset{n}{1})}_{\substack{\alpha\ \beta\\1,1}} &= E^{(\overset{n}{1})} + V_{\substack{n\alpha\ n\beta\\11,11}} + \frac{V_{\substack{n\alpha\ m\gamma\\11,01}}V_{\substack{m\gamma\ n\beta\\01,11}}}{E^{(\overset{n}{1})} - E^{(\overset{m}{0})}} + \frac{V_{\substack{n\alpha\ m\gamma\\11,02}}V_{\substack{m\gamma\ n\beta\\02,11}}}{E^{(\overset{n}{1})} - E^{(\overset{m}{0})}} = -\frac{2t^2}{U} \\
E^{\overset{(n)}{1}}_{\substack{\alpha\ \beta\\2,2}} &= E^{(\overset{n}{1})} + V_{\substack{n\alpha\ n\beta\\12,12}} + \frac{V_{\substack{n\alpha\ m\gamma\\12,01}}V_{\substack{m\gamma\ n\beta\\01,12}}}{E^{(\overset{n}{1})} - E^{(\overset{m}{0})}} + \frac{V_{\substack{n\alpha\ m\gamma\\12,02}}V_{\substack{m\gamma\ n\beta\\02,12}}}{E^{(\overset{n}{1})} - E^{(\overset{m}{0})}} = -\frac{2t^2}{U} \\
E^{(\overset{n}{1})}_{\substack{\alpha\ \beta\\1,2}} &= +V_{\substack{n\alpha\ n\beta\\11,12}} + \frac{V_{\substack{n\alpha\ m\gamma\\11,01}}V_{\substack{m\gamma\ n\beta\\01,12}}}{E^{(\overset{n}{1})} - E^{(\overset{m}{0})}} + \frac{V_{\substack{n\alpha\ m\gamma\\11,02}}V_{\substack{m\gamma\ n\beta\\02,12}}}{E^{(\overset{n}{1})} - E^{(\overset{m}{0})}} = \frac{2t^2}{U} \\
E^{(\overset{n}{1})}_{\substack{\alpha\ \beta\\2,1}} &= +V_{\substack{n\alpha\ n\beta\\12,11}} + \frac{V_{\substack{n\alpha\ m\gamma\\12,01}}V_{\substack{m\gamma\ n\beta\\01,11}}}{E^{(\overset{n}{1})} - E^{(\overset{m}{0})}} + \frac{V_{\substack{n\alpha\ m\gamma\\12,02}}V_{\substack{m\gamma\ n\beta\\02,11}}}{E^{(\overset{n}{1})} - E^{(\overset{m}{0})}} = \frac{2t^2}{U}
\end{aligned}$$

在 $n=1$ 的简并子空间中, 选定 $|\overset{n}{1},\overset{\alpha}{1}\rangle'$ 和 $|\overset{n}{1},\overset{\alpha}{2}\rangle'$ 为基矢, 有效哈密顿量为

$$H^{\mathrm{eff}}_{\substack{n\\1}} = \begin{pmatrix} E^{(\overset{n}{1})}_{\substack{\alpha\ \beta\\1,1}} & E^{(\overset{n}{1})}_{\substack{\alpha\ \beta\\1,2}} \\ E^{(\overset{n}{1})}_{\substack{\alpha\ \beta\\2,1}} & E^{(\overset{n}{1})}_{\substack{\alpha\ \beta\\2,2}} \end{pmatrix} = \begin{pmatrix} -\frac{2t^2}{U} & \frac{2t^2}{U} \\ \frac{2t^2}{U} & -\frac{2t^2}{U} \end{pmatrix}$$

此时对角元相同, 所以无法直接应用非简并微扰, 所以对该子空间进行严格对角化, 本征能量为 $\epsilon_1 = 0, \quad \epsilon_2 = -\dfrac{4t^2}{U}$, 对应的本征矢为

$$\begin{aligned}
|\epsilon_1\rangle &= \frac{1}{\sqrt{2}}\left(|\overset{n}{1},\overset{\alpha}{1}\rangle' + |\overset{n}{1},\overset{\alpha}{2}\rangle'\right) \\
|\epsilon_2\rangle &= \frac{1}{\sqrt{2}}\left(|\overset{n}{1},\overset{\alpha}{1}\rangle' - |\overset{n}{1},\overset{\alpha}{2}\rangle'\right)
\end{aligned}$$

2. 自旋-1 系统.

根据磁量子数选取基矢为 $|\overset{\alpha}{+1}\rangle, |\overset{\alpha}{0}\rangle, |\overset{\alpha}{-1}\rangle$. 考虑哈密顿量为 $H = H_0 + \lambda V = (S^z)^2 + \lambda(S^x + S_z)$.

$$S^x = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}, \quad S^z = \begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix} \Rightarrow H_0 = \begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 1\end{pmatrix}, \quad V = \lambda\begin{pmatrix}1 & 1/\sqrt{2} & 0\\ 1/\sqrt{2} & 0 & 1/\sqrt{2}\\ 0 & 1/\sqrt{2} & -1\end{pmatrix}$$

首先计算 H_0 的本征矢和本征值:

n	states	E_n
1	$\|\overset{n}{1},\overset{\alpha}{+1}\rangle = \|\psi_1\rangle$, $\|\overset{n}{1},\overset{\alpha}{-1}\rangle = \|\psi_3\rangle$	$E_1 = 1$
0	$\|\overset{n}{0},\overset{\alpha}{0}\rangle = \|\psi_2\rangle$	$E_0 = 0$

计算波函数的修正:

$$\begin{aligned}
|\overset{n}{1},\overset{\alpha}{\pm1}\rangle' &= |\overset{n}{1},\overset{\alpha}{\pm1}\rangle + |\overset{m}{0},\overset{\beta}{0}\rangle\frac{V_{\overset{m}{0}\overset{\beta}{0},\overset{n}{0}\overset{\alpha}{\pm1}}}{E^{(\overset{n}{1})} - E^{(\overset{m}{0})}}\lambda + \cdots\\
&= |\overset{n}{1},\overset{\alpha}{\pm1}\rangle + |\overset{m}{0},\overset{\beta}{0}\rangle\frac{1}{\sqrt{2}}\lambda + \cdots\\
|\overset{n}{0},\overset{\alpha}{0}\rangle' &= |\overset{n}{0},\overset{\alpha}{0}\rangle + |\overset{m}{1},\overset{\beta}{+1}\rangle\frac{V_{\overset{m}{1}\overset{\beta}{+1},\overset{n}{0}\overset{\alpha}{0}}}{E^{(\overset{n}{0})} - E^{(\overset{m}{1})}}\lambda + |\overset{m}{1},\overset{\beta}{-1}\rangle\frac{V_{\overset{m}{1}\overset{\beta}{-1},\overset{n}{0}\overset{\alpha}{0}}}{E^{(\overset{n}{0})} - E^{(\overset{m}{1})}}\lambda + \cdots\\
&= |\overset{n}{0},\overset{\alpha}{0}\rangle - (|\overset{m}{1},\overset{\beta}{+1}\rangle + |\overset{m}{1},\overset{\beta}{-1}\rangle)\frac{1}{\sqrt{2}}\lambda + \cdots
\end{aligned}$$

可见在 $n = 1$ 存在简并子空间. 选定 $|\overset{n}{1},\overset{\alpha}{+1}\rangle'$ 和 $|\overset{n}{1},\overset{\alpha}{-1}\rangle$ 作为基矢. 有效哈密顿量的矩阵元为

$$\begin{aligned}
E^{(\overset{n}{1})}_{\overset{\alpha}{+1},\overset{\beta}{+1}} &= E^{(\overset{n}{1})} + V_{\overset{n}{1}\overset{\alpha}{+1},\overset{n}{1}\overset{\beta}{+1}}\lambda + \frac{V_{\overset{n}{1}\overset{\alpha}{+1},\overset{m}{0}\overset{\gamma}{0}}V_{\overset{m}{0}\overset{\gamma}{0},\overset{n}{1}\overset{\beta}{+1}}}{E^{(\overset{n}{1})} - E^{(\overset{m}{0})}}\lambda^2 = 1 + \lambda + \frac{\lambda^2}{2}\\
E^{(\overset{n}{1})}_{\overset{\alpha}{-1},\overset{\beta}{-1}} &= E^{(\overset{n}{1})} + V_{\overset{n}{1}\overset{\alpha}{-1},\overset{n}{1}\overset{\beta}{-1}}\lambda + \frac{V_{\overset{n}{1}\overset{\alpha}{-1},\overset{m}{0}\overset{\gamma}{0}}V_{\overset{m}{0}\overset{\gamma}{0},\overset{n}{1}\overset{\beta}{-1}}}{E^{(\overset{n}{1})} - E^{(\overset{m}{0})}}\lambda^2 = 1 - \lambda + \frac{\lambda^2}{2}\\
E^{(\overset{n}{1})}_{\overset{\alpha}{+1},\overset{\beta}{-1}} &= V_{\overset{n}{1}\overset{\alpha}{+1},\overset{n}{1}\overset{\beta}{-1}}\lambda + \frac{V_{\overset{n}{1}\overset{\alpha}{+1},\overset{m}{0}\overset{\gamma}{0}}V_{\overset{m}{0}\overset{\gamma}{0},\overset{n}{1}\overset{\beta}{-1}}}{E^{(\overset{n}{1})} - E^{(\overset{m}{0})}}\lambda^2 = \frac{\lambda^2}{2}\\
E^{(\overset{n}{1})}_{\overset{\alpha}{-1},\overset{\beta}{+1}} &= V_{\overset{n}{1}\overset{\alpha}{-1},\overset{n}{1}\overset{\beta}{+1}}\lambda + \frac{V_{\overset{n}{1}\overset{\alpha}{-1},\overset{m}{0}\overset{\gamma}{0}}V_{\overset{m}{0}\overset{\gamma}{0},\overset{n}{1}\overset{\beta}{+1}}}{E^{(\overset{n}{1})} - E^{(\overset{m}{0})}}\lambda^2 = \frac{\lambda^2}{2}
\end{aligned}$$

有效哈密顿量为 $H^{\text{eff}}_{\overset{n}{1}} = \begin{pmatrix}1 + \lambda + \frac{\lambda^2}{2} & \frac{\lambda^2}{2}\\ \frac{\lambda^2}{2} & 1 - \lambda + \frac{\lambda^2}{2}\end{pmatrix}$, 此时对角元已经不等, 说明简并已经解除. 那么在这个更小的子空间中, 进一步使用微扰, 即一阶修正后的能量和波函数视为原始哈密顿量和波函数:

$$H^{\text{eff}}_{\overset{n}{1}} = \begin{pmatrix}1 + \lambda + \frac{\lambda^2}{2} & \frac{\lambda^2}{2}\\ \frac{\lambda^2}{2} & 1 - \lambda + \frac{\lambda^2}{2}\end{pmatrix} = \underbrace{\begin{pmatrix}1 + \lambda + \frac{\lambda^2}{2} & 0\\ 0 & 1 - \lambda + \frac{\lambda^2}{2}\end{pmatrix}}_{H_0'} + \underbrace{\begin{pmatrix}0 & \frac{\lambda^2}{2}\\ \frac{\lambda^2}{2} & 0\end{pmatrix}}_{V'}$$

$$\begin{aligned}
|\overset{n}{1},\overset{\alpha}{+1}\rangle'' &= |\overset{n}{1},\overset{\alpha}{+1}\rangle' + |\overset{n}{1},\overset{\beta}{-1}\rangle'\frac{V'_{\overset{\beta}{-1},\overset{\alpha}{+1}}}{E'_{\overset{\alpha}{+1}} - E'_{\overset{\beta}{-1}}} + \cdots = |\overset{n}{1},\overset{\alpha}{+1}\rangle' + |\overset{n}{1},\overset{\beta}{-1}\rangle'\frac{\lambda}{4} + \cdots\\
|\overset{n}{1},\overset{\alpha}{-1}\rangle'' &= |\overset{n}{1},\overset{\alpha}{-1}\rangle' + |\overset{n}{1},\overset{\beta}{+1}\rangle'\frac{V'_{\overset{\beta}{+1},\overset{\alpha}{-1}}}{E'_{\overset{\alpha}{-1}} - E'_{\overset{\beta}{+1}}} + \cdots = |\overset{n}{1},\overset{\alpha}{-1}\rangle' - |\overset{n}{1},\overset{\beta}{+1}\rangle'\frac{\lambda}{4} + \cdots
\end{aligned}$$

代入 $|\overset{n}{1},\overset{\alpha}{\pm1}\rangle'$ 即可得到进一步考虑了简并微扰的波函数, 注意要忽略 λ^2 阶:

$$\begin{aligned}
|\overset{n}{1},\overset{\alpha}{+1}\rangle'' &= |\overset{n}{1},\overset{\alpha}{+1}\rangle + |\overset{n}{1},\overset{\beta}{0}\rangle\frac{\lambda}{\sqrt{2}} + |\overset{n}{1},\overset{\beta}{-1}\rangle\frac{\lambda}{4}\\
|\overset{n}{1},\overset{\alpha}{-1}\rangle'' &= |\overset{n}{1},\overset{\alpha}{-1}\rangle + |\overset{n}{1},\overset{\beta}{0}\rangle\frac{\lambda}{\sqrt{2}} - |\overset{n}{1},\overset{\beta}{+1}\rangle\frac{\lambda}{4}
\end{aligned}$$

能量修正:

$$
\begin{aligned}
E''_{\overset{n}{1},\overset{\alpha}{+1}} &= E'_{\overset{n}{1},\overset{\alpha}{+1}} + V'_{\overset{n}{1},\overset{\alpha}{+1}\overset{\alpha}{+1}} + \frac{V'_{\overset{n}{1},\overset{\alpha}{+1}\overset{\beta}{-1}} V'_{\overset{n}{1},\overset{\beta}{-1}\overset{\alpha}{+1}}}{E'_{\overset{n}{1},\overset{\alpha}{+1}} - E'_{\overset{n}{1},\overset{\beta}{-1}}} = 1 + \lambda + \frac{\lambda^2}{2} + \mathcal{O}(\lambda^3) \\
E''_{\overset{n}{1},\overset{\alpha}{-1}} &= E'_{\overset{n}{1},\overset{\alpha}{-1}} + V'_{\overset{n}{1},\overset{\alpha}{-1}\overset{\alpha}{-1}} + \frac{V'_{\overset{n}{1},\overset{\alpha}{-1}\overset{\beta}{+1}} V'_{\overset{n}{1},\overset{\beta}{+1}\overset{\alpha}{-1}}}{E'_{\overset{n}{1},\overset{\alpha}{-1}} - E'_{\overset{n}{1},\overset{\beta}{+1}}} = 1 - \lambda + \frac{\lambda^2}{2} + \mathcal{O}(\lambda^3)
\end{aligned}
$$

0.1.2　含时微扰

0.1.2.1　含时微扰论

含时微扰论考虑的是时间演化算符 U 的修正. 设 $\dfrac{\partial H_0}{\partial t} = 0$, 则

$$
\begin{aligned}
H(t) &= H_0 + V(t), \quad H_0|n\rangle = E_n|n\rangle \\
\Rightarrow V(t) &= \sum_{m,n} |m\rangle\langle m|V(t)|n\rangle\langle n| = \sum_{m,n} |m\rangle V_{mn}(t)\langle n| \\
|\psi(t)\rangle &= U(t)|\psi(0)\rangle
\end{aligned}
$$

将时间演化算符拆分为 H_0 和 $V(t)$ 带来的时间演化

$$
\begin{aligned}
U(t) &= U_0(t)U_I(t) \\
|\psi_I(t)\rangle &= U_I(t)|\psi_I(0)\rangle \\
V_I(t) &= U_0^{-1}(t)V(t)U_0(t) = \sum_{mn} |m\rangle V_{mn}(t) e^{i(E_m - E_n)t}\langle n| \\
i\hbar\frac{\mathrm{d}}{\mathrm{d}t}U_I(t) &= V_I(t)U_I(t), \quad U_I(0) = \mathbb{I} \\
\Rightarrow |\psi_I(t)\rangle &= U_I(t)|\psi_I(0)\rangle, \quad U(t) = U_0(t)U_I(t)
\end{aligned}
$$

0.1.2.1.1　Dyson 级数

0.1.2.1.2　格林函数

0.1.2.1.3　费曼图

0.1.2.2　能级跃迁

0.1.2.2.1　跃迁概率　系统在 t_0 处于初态 $|i\rangle$, 在时刻 t 演化为 $G(t, t_0)|i\rangle$, 那么在 t 发现系统末态为 $|f\rangle$ 的概率为

$$
P_{i\to f} = |\langle f|G(t, t_0)|i\rangle|^2
$$

这种现象即为跃迁.

$$
\begin{aligned}
G(t, t_0) &\approx G_0(t, t_0) - i\int_{t_0}^{t} \mathrm{d}t_1 G_0(t, t_1)V(t_1)G_0(t_1, t_0) \\
G_0(t, t') &= \sum_n |n\rangle e^{-iE_n(t-t')}\langle n|
\end{aligned}
$$

$$
\begin{aligned}
\langle f|G(t, t_0)|i\rangle &\approx \langle f|G_0(t, t_0)|i\rangle - i\int_{t_0}^{t} \mathrm{d}t_1 \langle f|G_0(t, t_1)V(t_1)G_0(t_1, t_0)|i\rangle \\
&= e^{i(E_f t - E_i t_0)}\left(\delta_{fi} - i\int_{t_0}^{t_1} \langle f|V(t_1)|i\rangle e^{i(E_f - E_i)t_1}\right) \\
\Rightarrow P(i\to f) &= \frac{1}{\hbar^2}\left|\int_{t_0}^{t} \mathrm{d}t_1 \langle f|V(t_1)|i\rangle e^{i\omega_{fi}t_1}\right|^2, \quad \hbar\omega_{fi} = E_f - E_i
\end{aligned}
$$

0.1.2.2.2 Fermi 黄金规则 考虑系统初态 $|i\rangle$, 微扰为 $V(t) = \begin{cases} Ve^{-i\omega t}, & t > 0 \\ 0, & t < 0 \end{cases}$. 那么跃迁概率为

$$P_{i\to f}(t) = \frac{1}{\hbar^2}\left|\int_0^t \mathrm{d}t_1 \langle f|V|i\rangle e^{i(\omega_{fi}-\omega)t_1}\right|^2 = \frac{1}{\hbar^2}|\langle f|V|i\rangle|^2 \left(\frac{\sin\left[(\omega_{fi}-\omega)t/2\right]}{(\omega_{fi}-\omega)t/2}\right)^2$$
$$W_{i\to f} = \lim_{t\to\infty}\frac{P_{i\to f}(t)}{t} = \frac{2\pi}{\hbar}|\langle f|V|i\rangle|^2\delta(\omega_{fi}-\omega)$$

即长时极限下, 跃迁倾向于发生在与 ω 共振的能级, 即 $E_f - E_i = \hbar\omega$

0.1.2.2.3 绝热过程 微扰缓慢施加, 具有形式 $V(t) = \begin{cases} Ve^{t/\tau}, t < 0 \\ 0, t \geq 0 \end{cases}$. 设 $t_0 \to -\infty$ 的初态为 $|i\rangle$, 那么系统在 $t = 0$ 时末态为 $|f\rangle$ 的概率为

$$P_{i\to f} = \frac{1}{\hbar^2}\left|\int_{-\infty}^0 \mathrm{d}t_1 \langle f|V|i\rangle e^{t_1/\tau} e^{i\omega_{fi}t_1}\right|^2 = \frac{|\langle f|V|i\rangle|^2}{(E_f - E_i)^2 + \hbar^2/\tau^2}$$
$$\lim_{\tau\to\infty} P_{i\to f} = |\langle f|i(V)\rangle|^2 = \frac{|V_{fi}|^2}{(E_i - E_f)^2}$$

0.1.3 绝热近似

0.1.4 Berry 相位

0.1.4.1 Berry 相位的基本性质

0.1.4.2 单个自旋的 Berry 相位

0.1.4.3 Bloch 能带的 Berry 相位