

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 $U(t) = \tau \exp \left[-i \int_0^t dt' H(t') \right]$, 其中 $H(t) = H_0 + \lambda V(t)$.

0.1.1.2 非简并微扰论

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

0.1.1.2.1 HF 定理

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

0.1.1.2.2 能量的微扰修正

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

0.1.1.2.3 态的微扰修正

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

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:

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

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

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

$$\begin{aligned}1. \ m = n. \text{ 1st: } \frac{\partial E_{\alpha',\alpha}^{(n)}}{\partial \lambda} &= \langle n\alpha' | \frac{\partial H}{\partial \lambda} | n\alpha \rangle = V_{n\alpha',n\alpha} \\ \text{2nd: } \langle m\beta | \frac{\partial | n\alpha \rangle}{\partial \lambda} &= \frac{\langle m\beta | \frac{\partial H}{\partial \lambda} | n\alpha \rangle}{E^{(n)} - E^{(m)}} = \frac{V_{m\beta,n\alpha}}{E^{(n)} - E^{(m)}} \\ 2. \ m \neq n. \quad \frac{\partial \langle m\beta |}{\partial \lambda} | n\alpha \rangle &= \frac{\langle m\beta | \frac{\partial H}{\partial \lambda} | n\alpha \rangle}{E^{(m)} - E^{(n)}} = \frac{V_{m\beta,n\alpha}}{E^{(m)} - E^{(n)}}\end{aligned}$$

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

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

代入得到修正后的能量和波函数

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

哈密顿量可写作各简并子空间哈密顿量的直和:

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

0.1.1.3.4 简并微扰论的例子

1. 两格点 Hubbard 模型.

$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} + U \sum_i n_{i\uparrow} n_{i\downarrow}$. 粒子数 $N = \sum_i n_i$ 守恒, 磁量子数 $S^z = \sum_i s_i^z = \sum_i \frac{1}{2} (n_{i\uparrow} - n_{i\downarrow})$ 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 $-t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}$ 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.

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

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

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

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

和有效哈密顿量(能量):

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

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

$$H_1^{\text{eff}} = \begin{pmatrix} E_{\alpha\beta}^{(1)} & E_{\alpha\beta}^{(1)} \\ E_{\alpha\beta}^{(1)} & E_{\alpha\beta}^{(1)} \end{pmatrix} = \begin{pmatrix} -\frac{2t^2}{U} & \frac{2t^2}{U} \\ \frac{2t^2}{U} & -\frac{2t^2}{U} \end{pmatrix}$$

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 $\epsilon_1 = 0, \quad \epsilon_2 = -\frac{4t^2}{U}$, 对应的本征矢为

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

2. 自旋-1 系统.

根据磁量子数选取基矢为 $|+1\rangle, |0\rangle, |-1\rangle$. 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	$ 1, +1\rangle = \psi_1\rangle, \quad 1, -1\rangle = \psi_3\rangle$	$E_1 = 1$
0	$ 0, 0\rangle = \psi_2\rangle$	$E_0 = 0$

计算波函数的修正:

$$\begin{aligned} |1, \pm 1\rangle' &= |1, \pm 1\rangle + |0, 0\rangle \frac{V_{00,0\pm 1}^{m\beta, n\alpha}}{E^{(1)} - E^{(0)}} \lambda + \dots \\ &= |1, \pm 1\rangle + |0, 0\rangle \frac{1}{\sqrt{2}} \lambda + \dots \\ |0, 0\rangle' &= |0, 0\rangle + |1, +1\rangle \frac{V_{1+1,00}^{m\beta, n\alpha}}{E^{(0)} - E^{(1)}} \lambda + |1, -1\rangle \frac{V_{1-1,00}^{m\beta, n\alpha}}{E^{(0)} - E^{(1)}} \lambda + \dots \\ &= |0, 0\rangle - (|1, +1\rangle + |1, -1\rangle) \frac{1}{\sqrt{2}} \lambda + \dots \end{aligned}$$

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

$$\begin{aligned} E_{+1, +1}^{(1)} &= E^{(1)} + V_{1+1, 1+1}^{\alpha, n} \lambda + \frac{V_{1+1, 00}^{\alpha, m\gamma} V_{00, 1+1}^{m\gamma, n\beta}}{E^{(1)} - E^{(0)}} \lambda^2 = 1 + \lambda + \frac{\lambda^2}{2} \\ E_{-1, -1}^{(1)} &= E^{(1)} + V_{1-1, 1-1}^{\alpha, n} \lambda + \frac{V_{1-1, 00}^{\alpha, m\gamma} V_{00, 1-1}^{m\gamma, n\beta}}{E^{(1)} - E^{(0)}} \lambda^2 = 1 - \lambda + \frac{\lambda^2}{2} \\ E_{+1, -1}^{(1)} &= V_{1+1, 1-1}^{\alpha, n} \lambda + \frac{V_{1+1, 00}^{\alpha, m\gamma} V_{00, 1-1}^{m\gamma, n\beta}}{E^{(1)} - E^{(0)}} \lambda^2 = \frac{\lambda^2}{2} \\ E_{-1, +1}^{(1)} &= V_{1-1, 1+1}^{\alpha, n} \lambda + \frac{V_{1-1, 00}^{\alpha, m\gamma} V_{00, 1+1}^{m\gamma, n\beta}}{E^{(1)} - E^{(0)}} \lambda^2 = \frac{\lambda^2}{2} \end{aligned}$$

有效哈密顿量为 $H_1^{\text{eff}} = \begin{pmatrix} 1 + \lambda + \frac{\lambda^2}{2} & \frac{\lambda^2}{2} \\ \frac{\lambda^2}{2} & 1 - \lambda + \frac{\lambda^2}{2} \end{pmatrix}$, 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:

$$\begin{aligned} H_1^{\text{eff}} &= \begin{pmatrix} 1 + \lambda + \frac{\lambda^2}{2} & \frac{\lambda^2}{2} \\ \frac{\lambda^2}{2} & 1 - \lambda + \frac{\lambda^2}{2} \end{pmatrix} = \underbrace{\begin{pmatrix} 1 + \lambda + \frac{\lambda^2}{2} & 0 \\ 0 & 1 - \lambda + \frac{\lambda^2}{2} \end{pmatrix}}_{H'_0} + \underbrace{\begin{pmatrix} 0 & \frac{\lambda^2}{2} \\ \frac{\lambda^2}{2} & 0 \end{pmatrix}}_{V'} \\ |1, +1\rangle'' &= |1, +1\rangle' + |1, -1\rangle' \frac{V'_{-1, +1}}{E'_{+1} - E'_{-1}} + \dots = |1, +1\rangle' + |1, -1\rangle' \frac{\lambda}{4} + \dots \\ |1, -1\rangle'' &= |1, -1\rangle' + |1, +1\rangle' \frac{V'_{+1, -1}}{E'_{-1} - E'_{+1}} + \dots = |1, -1\rangle' - |1, +1\rangle' \frac{\lambda}{4} + \dots \end{aligned}$$

代入 $|1, \pm 1\rangle'$ 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:

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

能量修正:

$$E''_{1,+1} = E'_{1,+1} + V'_{1,+1} + \frac{V'_{1,+1} V'_{1,-1}}{E'_{1,+1} - E'_{1,-1}} = 1 + \lambda + \frac{\lambda^2}{2} + \mathcal{O}(\lambda^3)$$

$$E''_{1,-1} = E'_{1,-1} + V'_{1,-1} + \frac{V'_{1,-1} V'_{1,+1}}{E'_{1,-1} - E'_{1,+1}} = 1 - \lambda + \frac{\lambda^2}{2} + \mathcal{O}(\lambda^3)$$

0.1.2 含时微扰

0.1.2.1 含时微扰论

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

0.1.2.2.2 Fermi 黄金规则

0.1.2.2.3 绝热过程

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