Weyl semimetal in a magnetic field

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外尔半金属哈密顿量

$$H=\begin{pmatrix} M_z+\frac{1}{2}\boldsymbol{k}^2 & \alpha(k_x-ik_y) \\ \alpha(k_x+ik_y) & -M_z-\frac{1}{2}\boldsymbol{k}^2 \end{pmatrix}, \tag{1}$$

这里面内波矢 $\boldsymbol{k}=(k_x,k_y,0)$, $M_z=m+t\cos k_z$。M_z 看作外部参数。

考虑下面沿圆柱体 z 轴加外部磁场的外尔半金属, 选取对称规范, 即 $\boldsymbol{A}=\frac{B}{2}(-y,x,0)$。通过作以下变换

$$\boldsymbol{k}\to\boldsymbol{k}-\tilde{\boldsymbol{A}},\quad \tilde{\boldsymbol{A}}=\frac{\tilde{B}}{2}(-y,x,0),\quad \tilde{B}=eB/\hbar, \tag{2}$$

我们有

$$H=\begin{pmatrix} M_z+\frac{1}{2}[\boldsymbol{k}^2+\tilde{\boldsymbol{A}}^2-(\boldsymbol{k}\cdot\boldsymbol{A}+\boldsymbol{A}\cdot\boldsymbol{k})] & \alpha[k_x-A_x-i(k_y-A_y)] \\ \alpha[k_x-A_x+i(k_y-A_y)] & -M_z-\frac{1}{2}[\boldsymbol{k}^2+\tilde{\boldsymbol{A}}^2-(\boldsymbol{k}\cdot\tilde{\boldsymbol{A}}+\tilde{\boldsymbol{A}}\cdot\boldsymbol{k})] \end{pmatrix}. \tag{3}$$

由于 $\tilde{B}=eB/\hbar$, 磁长度 $l_B=\sqrt{\hbar/(eB)}$, 因此 $\tilde{B}=1/l_B^2$ (1 T 磁场的磁长度是 25.6 nm)。

将 k_x,k_y 变为 $-i\partial_x,-i\partial_y$, 具体如下

$$\frac{\boldsymbol{k}^2}{2}=-\frac{1}{2}\boldsymbol{\nabla}^2, \tag{4}$$

$$\frac{1}{2}(\boldsymbol{k}\cdot\tilde{\boldsymbol{A}}+\tilde{\boldsymbol{A}}\cdot\boldsymbol{k})=-\frac{i}{2}(\boldsymbol{\nabla}\cdot\tilde{\boldsymbol{A}}+\tilde{\boldsymbol{A}}\cdot\boldsymbol{\nabla}) \tag{5}$$

$$=-\frac{i}{2}((\boldsymbol{\nabla}\cdot\tilde{\boldsymbol{A}})+\tilde{\boldsymbol{A}}\cdot\boldsymbol{\nabla}+\tilde{\boldsymbol{A}}\cdot\boldsymbol{\nabla}) \tag{6}$$

$$=-i\tilde{\boldsymbol{A}}\cdot\boldsymbol{\nabla} \tag{7}$$

$$=i\frac{\tilde{B}}{2}(y\partial_x-x\partial_y) \tag{8}$$

$$=\frac{\tilde{B}}{2}L_z, \tag{9}$$

其中, $L_z=\boldsymbol{l}\times\boldsymbol{k}$, $\boldsymbol{l}=(x,y)$, $\boldsymbol{k}=-i\boldsymbol{\nabla}$。于是, 哈密顿量在实空间下变为

$$H=\begin{pmatrix} M_z-\frac{1}{2}(\boldsymbol{\nabla}^2-\tilde{\boldsymbol{A}}^2+\tilde{B}L_z) & \alpha[-i\partial_x-\partial_y+\frac{\tilde{B}}{2}(y+ix)] \\ \alpha[-i\partial_x+\partial_y+\frac{\tilde{B}}{2}(y-ix)] & -M_z+\frac{1}{2}(\boldsymbol{\nabla}^2-\tilde{\boldsymbol{A}}^2+\tilde{B}L_z) \end{pmatrix} \tag{10}$$

利用坐标变换, 即

$$x = r\cos\theta, \quad y = r\sin\theta, \quad r^2 = x^2 + y^2, \tag{11}$$

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}, \tag{12}$$

$$\frac{\partial}{\partial x} = \cos\theta\frac{\partial}{\partial r} - \frac{1}{r}\sin\theta\frac{\partial}{\partial \theta}, \tag{13}$$

$$\frac{\partial}{\partial y} = \sin\theta\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\frac{\partial}{\partial \theta}, \tag{14}$$

所以,

$$L_z = i(y\partial_x - x\partial_y) \tag{15}$$

$$= i[r\sin\theta(\cos\theta\frac{\partial}{\partial r} - \frac{1}{r}\sin\theta\frac{\partial}{\partial\theta}) - r\cos\theta(\sin\theta\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\frac{\partial}{\partial\theta}) \tag{16}$$

$$= -i\frac{\partial}{\partial\theta}, \tag{17}$$

$$k_x - A_x - i(k_y - A_y) = -i\partial_x - \partial_y + \frac{\tilde{B}}{2}(y + ix) \tag{18}$$

$$= -i(\cos\theta\frac{\partial}{\partial r} - \frac{1}{r}\sin\theta\frac{\partial}{\partial\theta}) - (\sin\theta\frac{\partial}{\partial r} + \frac{1}{r}\cos\theta\frac{\partial}{\partial\theta}) + \frac{\tilde{B}}{2}(r\sin\theta + ir\cos\theta) \tag{19}$$

$$= -ie^{-i\theta}\frac{\partial}{\partial r} - e^{-i\theta}\frac{\partial}{r\partial\theta} + i\frac{\tilde{B}r}{2}e^{-i\theta} \tag{20}$$

$$= e^{-i\theta}[(-i)(\frac{\partial}{\partial r} - i\frac{\partial}{r\partial\theta}) + i\frac{\tilde{B}r}{2}], \tag{21}$$

哈密顿量在极坐标空间下变为

$$H = \begin{pmatrix} M_z - \frac{1}{2}(\nabla^2 - \tilde{\boldsymbol{A}}^2 + \tilde{B}L_z) & \alpha\frac{\tilde{B}}{2}(-i\partial_x - \partial_y + y + ix) \\ \alpha\frac{\tilde{B}}{2}(-i\partial_x + \partial_y + y - ix) & -M_z + \frac{1}{2}(\nabla^2 - \tilde{\boldsymbol{A}}^2 + \tilde{B}L_z) \end{pmatrix} \tag{22}$$

$$= \begin{pmatrix} M_z - \frac{1}{2}(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} - \frac{\tilde{B}^2r^2}{4} - i\tilde{B}\frac{\partial}{\partial\theta}) & \alpha e^{-i\theta}[(-i)(\frac{\partial}{\partial r} - i\frac{\partial}{r\partial\theta}) + i\frac{\tilde{B}r}{2}] \\ \alpha e^{i\theta}[(-i)(\frac{\partial}{\partial r} + i\frac{\partial}{r\partial\theta}) - i\frac{\tilde{B}r}{2}] & -M_z + \frac{1}{2}(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} - \frac{\tilde{B}^2r^2}{4} - i\tilde{B}\frac{\partial}{\partial\theta}) \end{pmatrix}. \tag{23}$$

(24)

假设波函数具有一般形式

$$\psi = (\phi_n(r)e^{in\theta}, \varphi_n(r)e^{i(n+1)\theta})^T, \tag{25}$$

将其代入 $H\psi = E\psi$, 得到径向哈密顿量

$$\begin{pmatrix} M_z - \frac{1}{2}(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{n^2}{r^2} - \frac{\tilde{B}^2r^2}{4} + \tilde{B}n) & \alpha(-i\frac{\partial}{\partial r} - \frac{i(n+1)}{r} + i\frac{\tilde{B}r}{2}) \\ \alpha(-i\frac{\partial}{\partial r} + i\frac{n}{r} - i\frac{\tilde{B}r}{2}) & -M_z + \frac{1}{2}(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - \frac{(n+1)^2}{r^2} - \frac{\tilde{B}^2r^2}{4} + \tilde{B}(n+1)) \end{pmatrix}. \tag{26}$$

在区间 $[0,R]$ 的函数 $f(r)$ 可以用贝塞尔正交函数集 $J_\nu(\lambda_{\nu i}r)$ 来表示，

$$f(r)=\sum_{i=1}^{N}c_{\nu i}J_\nu(\lambda_{\nu i}r), \tag{27}$$

其中，$\lambda_{\nu i}=\mu_{\nu i}/R$, $\mu_{\nu i}$ 是 ν 阶贝塞尔函数（第一类）的第 i 个零点。

贝塞尔函数正交性

$$\int_0^R rJ_\nu(\lambda_{\nu i}r)J_\nu(\lambda_{\nu j}r)dr=\frac{R^2}{2}J_{\nu+1}^2(\mu_{\nu i})\delta_{ij}. \tag{28}$$

常用性质

$$\frac{d}{dr}\left[\frac{J_\nu(r)}{r^\nu}\right]=-\frac{J_{\nu+1}(r)}{r^\nu} \tag{29}$$

$$\frac{d}{dr}\left[x^\nu J_\nu(r)\right]=x^\nu J_{\nu-1}(r) \tag{30}$$

$$J_{\nu+1}(r)-\frac{2\nu J_\nu(r)}{r}+J_{\nu-1}(r)=0 \tag{31}$$

$$2J_\nu'(r)=J_{\nu-1}(r)-J_{\nu+1}(r) \tag{32}$$

$$J_{-\nu}=(-1)^\nu J_\nu \tag{33}$$

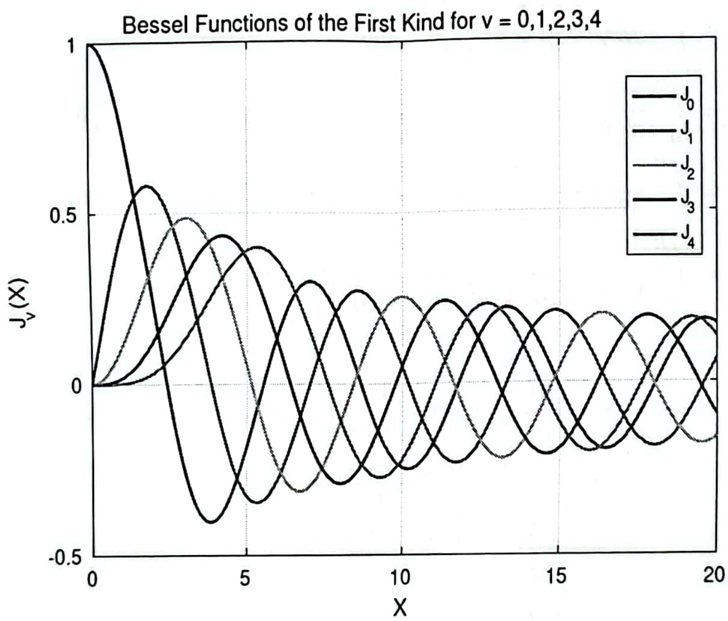

Figure 1: 第一类贝塞尔函数曲线图。

径向哈密顿量

$$\begin{pmatrix} M_z-\frac{1}{2}(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{n^2}{r^2}-\frac{\tilde{B}^2r^2}{4}+\tilde{B}n) & \alpha(-i\frac{\partial}{\partial r}-\frac{i(n+1)}{r}+i\frac{\tilde{B}r}{2}) \\ \alpha(-i\frac{\partial}{\partial r}+i\frac{n}{r}-i\frac{\tilde{B}r}{2}) & -M_z+\frac{1}{2}(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{(n+1)^2}{r^2}-\frac{\tilde{B}^2r^2}{4}+\tilde{B}(n+1)) \end{pmatrix}. \tag{34}$$

在贝塞尔函数基矢表示下，径向波函数为

$$\phi(r)=\sum_{i=1}^{N}c_{\nu i}\frac{\sqrt{2}}{RJ_{\nu+1}(\mu_{\nu i})}J_\nu(\lambda_{\nu i}r),\ \varphi(r)=\sum_{j=1}^{N}c_{\kappa j}\frac{\sqrt{2}}{RJ_{\kappa+1}(\mu_{\kappa i})}J_\kappa(\lambda_{\kappa i}r), \tag{35}$$

其中，$\frac{\sqrt{2}}{RJ_{\nu+1}(\mu_{\nu i})}$ 是归一化系数。

下面计算径向哈密顿量矩阵元。为了方便矩阵元积分计算，贝塞尔函数阶数选取 $\nu=n,\kappa=n+1$，与角动量量子数一致。

$$\begin{pmatrix} H^{(n,n)} & H^{(n,n+1)} \\ H^{(n+1,n)} & H^{(n+1,n+1)} \end{pmatrix}\Psi=E\Psi, \tag{36}$$

其中，$\Psi=(c_{n1},\cdots,c_{nN},c_{n+1,1},\cdots,c_{n+1,N})^T$，径向哈密顿量矩阵元分别为

$$H_{ij}^{(n,n)}=\int_0^R\frac{2}{R^2J_{n+1}(\mu_{ni})J_{n+1}(\mu_{nj})}rJ_n(\lambda_{ni}r)H_1J_n(\lambda_{nj}r)dr, \tag{37}$$

$$H_{ij}^{(n,n+1)}=\int_0^R\frac{2}{R^2J_{n+1}(\mu_{ni})J_{n+2}(\mu_{n+1,j})}rJ_n(\lambda_{ni}r)H_2J_{n+1}(\lambda_{n+1,j}r)dr, \tag{38}$$

$$H_{ij}^{(n+1,n)}=\int_0^R\frac{2}{R^2J_{n+2}(\mu_{n+1,i})J_{n+1}(\mu_{nj})}rJ_{n+1}(\lambda_{n+1,i}r)H_3J_n(\lambda_{nj}r)dr, \tag{39}$$

$$H_{ij}^{(n+1,n+1)}=\int_0^R\frac{2}{R^2J_{n+2}(\mu_{n+1,i})J_{n+2}(\mu_{n+1,j})}rJ_{n+1}(\lambda_{n+1,i}r)H_4J_{n+1}(\lambda_{n+1,j}r)dr. \tag{40}$$

$$(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{n^2}{r^2})J_n(\lambda_{ni}r)=\frac{\partial}{\partial r}[\frac{\partial}{\partial r}J_n(\lambda_{ni}r)]+\frac{1}{r}\frac{\partial}{\partial r}J_n(\lambda_{ni}r)-\frac{n}{r}[\frac{n}{r}J_n(\lambda_{ni}r)] \tag{41}$$

$$=\frac{\partial}{\partial r}(\lambda_{ni}\frac{J_{n-1}(\lambda_{ni}r)-J_{n+1}(\lambda_{ni}r)}{2})+\frac{\lambda_{ni}}{r}\frac{J_{n-1}(\lambda_{ni}r)-J_{n+1}(\lambda_{ni}r)}{2} -\frac{n\lambda_{ni}}{r}\frac{J_{n+1}(\lambda_{ni}r)+J_{n-1}(\lambda_{ni}r)}{2} \tag{42}$$

$$=\frac{\lambda_{ni}^2}{4}[J_{n-2}(\lambda_{ni}r)-J_n(\lambda_{ni}r)-J_n(\lambda_{ni}r)+J_{n+2}(\lambda_{ni}r)] -\frac{\lambda_{ni}(n-1)}{2r}J_{n-1}(\lambda_{ni}r)-\frac{\lambda_{ni}(n+1)}{2r}J_{n+1}(\lambda_{ni}r) \tag{43}$$

$$=\frac{\lambda_{ni}^2}{4}[J_{n-2}(\lambda_{ni}r)-J_n(\lambda_{ni}r)-J_n(\lambda_{ni}r)+J_{n+2}(\lambda_{ni}r)] -\frac{\lambda_{ni}^2}{4}[J_{n+2}(\lambda_{ni}r)+J_n(\lambda_{ni}r)+J_n(\lambda_{ni}r)+J_{n-2}(\lambda_{ni}r)] \tag{44}$$

$$=-\lambda_{ni}^2J_n(\lambda_{ni}r), \tag{45}$$

$$(\frac{\partial}{\partial r}+\frac{n+1}{r})J_{n+1}(\lambda_{n+1,i}r)=\lambda_{n+1,i}\frac{J_n(\lambda_{n+1,i}r)-J_{n+2}(\lambda_{n+1,i}r)}{2}+\lambda_{n+1,i}\frac{J_{n+2}(\lambda_{n+1,i}r)+J_n(\lambda_{n+1,i}r)}{2}$$

$$=\lambda_{n+1,i}J_n(\lambda_{n+1,i}r), \tag{46}$$

$$(\frac{\partial}{\partial r}-\frac{n}{r})J_n(\lambda_{ni}r)=\lambda_{ni}\frac{J_{n-1}(\lambda_{ni}r)-J_{n+1}(\lambda_{ni}r)}{2}-\lambda_{ni}\frac{J_{n-1}(\lambda_{ni}r)+J_{n+1}(\lambda_{ni}r)}{2}$$

$$=-\lambda_{ni}J_{n+1}(\lambda_{ni}r). \tag{47}$$

记 $A_{ij}^{(m,n)}=\dfrac{2}{R^2J_{m+1}(\mu_{mi})J_{n+1}(\mu_{nj})}$,

$$H_{ij}^{(n,n)}=\int_0^R A_{ij}^{(n,n)}rJ_n(\lambda_{ni}r)H_1J_n(\lambda_{nj}r)dr \tag{48}$$

$$=\int_0^R A_{ij}^{(n,n)}rJ_n(\lambda_{ni}r)\left[M_z-\frac{1}{2}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{n^2}{r^2}-\frac{\tilde{B}^2r^2}{4}+\tilde{B}n\right)\right]J_n(\lambda_{nj}r)dr \tag{49}$$

$$=(M_z-\frac{1}{2}\tilde{B}n+\frac{1}{2}\lambda_{ni}^2)\delta_{ij}+\frac{1}{8}\tilde{B}^2A_{ij}^{(n,n)}\int_0^R r^3J_n(\lambda_{ni}r)J_n(\lambda_{nj}r)dr, \tag{50}$$

$$H_{ij}^{(n+1,n+1)}=\int_0^R A_{ij}^{(n+1,n+1)}rJ_{n+1}(\lambda_{n+1,i}r)H_4J_{n+1}(\lambda_{n+1,j}r)dr \tag{51}$$

$$=\int_0^R A_{ij}^{(n+1,n+1)}rJ_{n+1}(\lambda_{n+1,i}r)\left[-M_z+\frac{1}{2}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{(n+1)^2}{r^2}-\frac{\tilde{B}^2r^2}{4}+B(n+1)\right)\right]$$
$$\times J_{n+1}(\lambda_{n+1,j}r)dr \tag{52}$$

$$=[-M_z+\frac{1}{2}\tilde{B}(n+1)-\frac{1}{2}\lambda_{n+1,i}^2]\delta_{ij}-\frac{1}{8}\tilde{B}^2A_{ij}^{(n+1,n+1)}\int_0^R r^3J_{n+1}(\lambda_{n+1,i}r)J_{n+1}(\lambda_{n+1,j}r)dr. \tag{53}$$

$$H_{ij}^{(n,n+1)}=\int_0^R A_{ij}^{(n,n+1)}rJ_n(\lambda_{ni}r)H_2J_{n+1}(\lambda_{n+1,j}r)dr \tag{54}$$

$$=\int_0^R A_{ij}^{(n,n+1)}rJ_n(\lambda_{ni}r)\left[-i\alpha\left(\frac{\partial}{\partial r}+\frac{n+1}{r}-\frac{\tilde{B}r}{2}\right)\right]J_{n+1}(\lambda_{n+1,j}r)dr \tag{55}$$

$$=-i\alpha A_{ij}^{(n,n+1)}\lambda_{n+1,j}\int_0^R rJ_n(\lambda_{ni}r)J_n(\lambda_{n+1,j}r)dr+i\alpha\frac{\tilde{B}}{2}\int_0^R A_{ij}^{(n,n+1)}r^2J_n(\lambda_{ni}r)J_{n+1}(\lambda_{n+1,j}r)dr \tag{56}$$

$$=-i\alpha A_{ij}^{(n,n+1)}\lambda_{n+1,j}\times\left[-\frac{R(\lambda_{ni}J_{n-1}(\lambda_{ni}R)J_n(\lambda_{n+1,j}R)-\lambda_{n+1,j}J_n(\lambda_{ni}R)J_{n-1}(\lambda_{n+1,j}R))}{\lambda_{ni}^2-\lambda_{n+1,j}^2}\right]$$
$$+i\alpha\frac{\tilde{B}}{2}\int_0^R A_{ij}^{(n,n+1)}r^2J_n(\lambda_{ni}r)J_{n+1}(\lambda_{n+1,j}r)dr \tag{57}$$

$$=i\alpha\frac{2\mu_{n+1,j}\mu_{ni}}{R(\mu_{ni}^2-\mu_{n+1,j}^2)}\times\frac{J_{n-1}(\mu_{ni})J_n(\mu_{n+1,j})}{J_{n+1}(\mu_{ni})J_{n+2}(\mu_{n+1,j})}+i\alpha\frac{\tilde{B}}{2}\int_0^R A_{ij}^{(n,n+1)}r^2J_n(\lambda_{ni}r)J_{n+1}(\lambda_{n+1,j}r)dr \tag{58}$$

$$=i\alpha\frac{2\mu_{n+1,j}\mu_{ni}}{R(\mu_{ni}^2-\mu_{n+1,j}^2)}+i\alpha\frac{\tilde{B}}{2}\int_0^R A_{ij}^{(n,n+1)}r^2J_n(\lambda_{ni}r)J_{n+1}(\lambda_{n+1,j}r)dr \tag{59}$$

$$H_{ij}^{(n+1,n)} = \int_0^R A_{ij}^{(n+1,n)} r J_{n+1}(\lambda_{n+1,i} r) H_3 J_n(\lambda_{nj} r) dr \tag{60}$$

$$= \int_0^R A_{ij}^{(n+1,n)} r J_{n+1}(\lambda_{n+1,i} r) \left[-i\alpha(\frac{\partial}{\partial r} - \frac{n}{r} + \frac{\tilde{B}r}{2}) \right] J_n(\lambda_{nj} r) dr \tag{61}$$

$$= -i\alpha A_{ij}^{(n+1,n)} \lambda_{nj} \int_0^R r J_{n+1}(\lambda_{n+1,i} r) J_{n+1}(\lambda_{nj} r) dr - i\alpha \frac{\tilde{B}}{2} \int_0^R r J_{n+1}(\lambda_{n+1,i} r) J_{n+1}(\lambda_{nj} r) dr \tag{62}$$

$$= -i\alpha A_{ij}^{(n+1,n)} \lambda_{nj} \times \left[-\frac{R(\lambda_{n+1,i} J_n(\lambda_{n+1,i} R) J_{n+1}(\lambda_{nj} R) - \lambda_{nj} J_{n+1}(\lambda_{n+1,i} R) J_n(\lambda_{nj} R))}{\lambda_{n+1,i}^2 - \lambda_{nj}^2} \right]$$

$$- i\alpha \frac{\tilde{B}}{2} A_{ij}^{(n+1,n)} \int_0^R r^2 J_{n+1}(\lambda_{n+1,i} r) J_n(\lambda_{nj} r) dr \tag{63}$$

$$= i\alpha \frac{2\lambda_{n+1,i}\lambda_{nj}}{R(\lambda_{n+1,i}^2 - \lambda_{nj}^2)} \times \frac{J_n(\lambda_{n+1,i} R) J_{n+1}(\lambda_{nj} R)}{J_{n+2}(\lambda_{n+1,i} R) J_{n+1}(\lambda_{nj} R)} - i\alpha \frac{\tilde{B}}{2} A_{ij}^{(n+1,n)} \int_0^R r^2 J_{n+1}(\lambda_{n+1,i} r) J_n(\lambda_{nj} r) dr \tag{64}$$

$$= i\alpha \frac{2\mu_{n+1,i}\mu_{nj}}{R(\mu_{n+1,i}^2 - \mu_{nj}^2)} - i\alpha \frac{\tilde{B}}{2} A_{ij}^{(n+1,n)} \int_0^R r^2 J_{n+1}(\lambda_{n+1,i} r) J_n(\lambda_{nj} r) dr \tag{65}$$

若 $n < 0$, 上面结果似乎不影响？