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相对论性氢原子径向算符矩阵元的通项计算公式

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给出了相对论性氢原子径向算符矩阵元 $\langle n'_1, K_1, j_1, m_{j1} | r^p | n'_2, K_2, j_2, m_{j2} \rangle$ 的通项计算公式.

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在利用量子力学研究氢原子的某些问题时, 经常要计算氢原子的径向算符矩阵元. 氢原子径向算符矩阵元的计算要涉及到复杂的积分, 计算起来非常困难. 文献[1—4]给出了某些特定条件下非相对论性氢原子径向算符矩阵元的计算结果. 本文推导出了一个普遍适用的计算相对论性氢原子径向算符矩阵元的通项计算公式.

相对论性氢原子的定态 Dirac 方程为

$$(c\,\alpha\cdot\boldsymbol{p} + mc^2\beta - e\phi(r))\,\psi = E\psi \tag{1}$$

$$\left(\boldsymbol{p} = -\,\mathrm{i}\hbar\,\nabla, \quad \phi(r) = \frac{Ze}{r}\right).$$

相对论性氢原子的守恒量完全集可以取为[5] $(H, \boldsymbol{K}, \boldsymbol{J}^2, \boldsymbol{J}_z)$, 能级公式为

$$E = E_{n'K} = mc^2\left[1 + \frac{\alpha^2 Z^2}{(n' + \sqrt{K^2 - \alpha^2 Z^2})^2}\right]^{-\frac{1}{2}}, \tag{2}$$

其中

$$n' = 0, 1, 2 \cdots,$$

$$|K| = j + \frac{1}{2} = 1, 2, 3 \cdots,$$

$$\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}.$$

相应的本征函数可表示如下[5]:

$$\psi_{n'Kjm_j} = \begin{pmatrix} f_{n'K}(r)\,\phi^A_{jm_j} \\ \mathrm{i}g_{n'K}(r)\,\phi^B_{jm_j} \end{pmatrix} \qquad \left(\text{当 } K = j + \frac{1}{2} \text{ 时}\right), \tag{3}$$

$$\psi_{n'Kjm_j} = \begin{pmatrix} f_{n'K}(r)\,\phi^B_{jm_j} \\ \mathrm{i}g_{n'K}(r)\,\phi^A_{jm_j} \end{pmatrix} \qquad \left(\text{当 } K = -\left(j + \frac{1}{2}\right) \text{ 时}\right), \tag{4}$$

其中

$$\phi^A_{jm_j} = \begin{pmatrix} \sqrt{\dfrac{j+m_j}{2j}}\, Y_{j-1/2,\, m_j-1/2} \\ \sqrt{\dfrac{j-m_j}{2j}}\, Y_{j-1/2,\, m_j+1/2} \end{pmatrix}, \tag{5}$$

$$\phi^B_{jm_j} = \begin{pmatrix} -\sqrt{\dfrac{j-m_j+1}{2j+2}}\, Y_{j+1/2,\, m_j-1/2} \\ \sqrt{\dfrac{j+m_j+1}{2j+2}}\, Y_{j+1/2,\, m_j+1/2} \end{pmatrix}. \tag{6}$$

我们可把相对论性氢原子波函数(3)式和(4)式统一地表示为

$$\phi_{n'Kjm_j} = \begin{pmatrix} f_{n'K}(r)[\mathrm{sgn}(|K|+K)\,\phi^A_{jm_j} + \mathrm{sgn}(|K|-K)\,\phi^B_{jm_j}] \\ \mathrm{i}g_{n'K}(r)[\mathrm{sgn}(|K|-K)\,\phi^A_{jm_j} + \mathrm{sgn}(|K|+K)\,\phi^B_{jm_j}] \end{pmatrix}, \tag{7}$$

这里

$$\mathrm{sgn}(x) = \begin{cases} 1, & x > 0, \\ 0, & x = 0, \\ -1, & x < 0 \end{cases} \tag{8}$$

为符号函数.

根据文献[6, 7]可得相对论性氢原子的归一化径向函数为

$$\begin{aligned} f_{n'K}(r) = {}& H_{n'K}\sqrt{1+\varepsilon_{n'K}}\left(\frac{2Z}{Na_0}\right)^{s+1/2} r^{s-1}\exp\left(-\frac{Zr}{Na_0}\right) \\ & \times\left[(N+K)\mathrm{F}\left(-n', 2s+1, \frac{2Zr}{Na_0}\right) - n'\mathrm{F}\left(-n'+1, 2s+1, \frac{2Zr}{Na_0}\right)\right], \end{aligned} \tag{9}$$

$$\begin{aligned} g_{n'K}(r) = {}& H_{n'K}\sqrt{1-\varepsilon_{n'K}}\left(\frac{2Z}{Na_0}\right)^{s+1/2} r^{s-1}\exp\left(-\frac{Zr}{Na_0}\right) \\ & \times\left[(N+K)\mathrm{F}\left(-n', 2s+1, \frac{2Zr}{Na_0}\right) + n'\mathrm{F}\left(-n'+1, 2s+1, \frac{2Zr}{Na_0}\right)\right], \end{aligned} \tag{10}$$

其中

$$H_{n'K} = \frac{1}{2\Gamma(2s+1)}\sqrt{\frac{\Gamma(n'+2s+1)}{N(N+K)}},$$

$$N = \left[\alpha^2 Z^2 + \left(n' + \sqrt{K^2-\alpha^2 Z^2}\right)^2\right]^{1/2},$$

$$\varepsilon_{n'K} = \frac{E_{n'K}}{mc^2} = \left[1 + \frac{\alpha^2 Z^2}{\left(n'+\sqrt{K^2-\alpha^2 Z^2}\right)^2}\right]^{-1/2},$$

$$s = \sqrt{K^2-\alpha^2 Z^2},$$

$$\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137},$$

$$a_0 = \frac{\hbar^2}{m e^2}\ (\text{玻尔半径}).$$

相对论性氢原子径向算符矩阵元为

$$\langle n'_1, K_1, j_1, m_{j1} | r^p | n'_2, K_2, j_2, m_{j2}\rangle$$

$$= \delta_{j_1,j_2}\delta_{m_{j1},m_{j2}}\int_0^\infty [f_{n'_1K_1}(r)f_{n'_2K_2}(r) + g_{n'_1K_1}(r)g_{n'_2K_2}(r)]r^{p+2}\mathrm{d}r$$

$$= \delta_{j_1,j_2}\delta_{m_{j1},m_{j2}}H_{n'_1K_1}H_{n'_2K_2}\sqrt{(1+\varepsilon_{n'_1K_1})(1+\varepsilon_{n'_2K_2})}\left(\frac{2Z}{N_1a_0}\right)^{s_1+\frac{1}{2}}\left(\frac{2Z}{N_2a_0}\right)^{s_2+\frac{1}{2}}$$

$$\times\int_0^\infty r^{s_1+s_2+p}\mathrm{e}^{-\left[\frac{Z(N_1+N_2)r}{N_1N_2a_0}\right]}\left[(N_1+K_1)\mathrm{F}\left(-n'_1, 2s_1+1, \frac{2Zr}{N_1a_0}\right)\right.$$

$$\left.-n'_1\mathrm{F}\left(-n'_1+1, 2s_1+1, \frac{2Zr}{N_1a_0}\right)\right]\left[(N_2+K_2)\mathrm{F}\left(-n'_2, 2s_2+1, \frac{2Zr}{N_2a_0}\right)\right.$$

$$\left.-n'_2\mathrm{F}\left(-n'_2+1, 2s_2+1, \frac{2Zr}{N_2a_0}\right)\right]\mathrm{d}r$$

$$+\delta_{j_1,j_2}\delta_{m_{j1},m_{j2}}H_{n'_1K_1}H_{n'_2K_2}\sqrt{(1-\varepsilon_{n'_1K_1})(1-\varepsilon_{n'_2K_2})}\left(\frac{2Z}{N_1a_0}\right)^{s_1+\frac{1}{2}}\left(\frac{2Z}{N_2a_0}\right)^{s_2+\frac{1}{2}}$$

$$\times\int_0^\infty r^{s_1+s_2+p}\mathrm{e}^{-\left[\frac{Z(N_1+N_2)r}{N_1N_2a_0}\right]}\left[(N_1+K_1)\mathrm{F}\left(-n'_1, 2s_1+1, \frac{2Zr}{N_1a_0}\right)\right.$$

$$\left.+n'_1\mathrm{F}\left(-n'_1+1, 2s_1+1, \frac{2Zr}{N_1a_0}\right)\right]\left[(N_2+K_2)\mathrm{F}\left(-n'_2, 2s_2+1, \frac{2Zr}{N_2a_0}\right)\right.$$

$$\left.+n'_2\mathrm{F}\left(-n'_2+1, 2s_2+1, \frac{2Zr}{N_2a_0}\right)\right]\mathrm{d}r. \qquad (11)$$

为求得(11)式, 我们先来计算形如下式的积分:

$$\int_0^\infty z^w\mathrm{e}^{-\lambda z}\mathrm{F}(-n_1, \mu_1+1, k_1z)\mathrm{F}(-n_2, \mu_2+1, k_2z)\mathrm{d}z. \qquad (12)$$

合流超几何函数与广义拉盖尔函数有如下关系[8]:

$$\mathrm{F}(-n, \mu+1, z) = \frac{n!\Gamma(\mu+1)}{\Gamma(n+\mu+1)}\mathrm{L}_n^\mu(z). \qquad (13)$$

把(13)式代入(12)式有

$$\int_0^\infty z^w\mathrm{e}^{-\lambda z}\mathrm{F}(-n_1, \mu_1+1, k_1z)\mathrm{F}(-n_2, \mu_2+1, k_2z)\mathrm{d}z$$

$$= \frac{n_1!\Gamma(\mu_1+1)n_2!\Gamma(\mu_2+1)}{\Gamma(n_1+\mu_1+1)\Gamma(n_2+\mu_2+1)}\int_0^\infty z^w\mathrm{e}^{-\lambda z}\mathrm{L}_{n_1}^{\mu_1}(k_1z)\mathrm{L}_{n_2}^{\mu_2}(k_2z)\mathrm{d}z. \qquad (14)$$

把广义拉盖尔函数的级数形式

$$\mathrm{L}_n^u(z) = \sum_{q=0}^n(-1)^q\begin{pmatrix}n+\mu\\ n-q\end{pmatrix}\frac{z^q}{q!} \qquad (15)$$

代入(14)式, 有

$$\int_0^\infty z^w\mathrm{e}^{-\lambda z}\mathrm{F}(-n_1, \mu_1+1, k_1z)\mathrm{F}(-n_2, \mu_2+1, k_2z)\mathrm{d}z$$

$$= \frac{n_1!\Gamma(\mu_1+1)n_2!\Gamma(\mu_2+1)}{\Gamma(n_1+\mu_1+1)\Gamma(n_2+\mu_2+1)}$$

$$\times \sum_{q=0}^{n_1}\left[(-1)^q \frac{k_1^q}{q!}\begin{pmatrix} n_1+\mu_1 \\ n_1-q\end{pmatrix}\int_0^\infty z^{w+q}e^{-\lambda z}L_{n_2}^{\mu_2}(k_2 z)dz\right]$$

$$= \frac{n_1!\Gamma(\mu_1+1)n_2!\Gamma(\mu_2+1)}{\Gamma(n_1+\mu_1+1)\Gamma(n_2+\mu_2+1)}$$

$$\times \sum_{q=0}^{n_1}\left[(-1)^q \frac{k_1^q}{q!}\begin{pmatrix} n_1+\mu_1 \\ n_1-q\end{pmatrix}\left(\frac{1}{k_2}\right)^{w+q}\int_0^\infty (k_2 z)^{w+q}\exp\left[-\frac{\lambda}{k_2}(k_2 z)\right]L_{n_2}^{\mu_2}(k_2 z)d(k_2 z)\right]. \tag{16}$$

再把积分公式[9]

$$\int_0^\infty t^\beta e^{-vt}L_n^c(t)dt = \frac{\Gamma(\beta+1)\Gamma(c+n+1)}{n!\Gamma(c+1)}\nu^{-\beta-1}F\left(-n,\beta+1,c+1,\frac{1}{\nu}\right) \tag{17}$$

代入(16)式, 得

$$\int_0^\infty z^w e^{-\lambda z}F(-n_1,\mu_1+1,k_1 z)F(-n_2,\mu_2+1,k_2 z)dz$$

$$= \frac{n_1!\Gamma(\mu_1+1)}{\Gamma(n_1+\mu_1+1)}\sum_{q=0}^{n_1}\left[(-1)^q \frac{k_1^q}{q!}\begin{pmatrix} n_1+\mu_1 \\ n_1-q\end{pmatrix}\Gamma(w+q+1)\lambda^{-w-q-1}\right.$$

$$\left.\times F\left(-n_2,w+q+1,\mu_2+1,\frac{k_2}{\lambda}\right)\right]. \tag{18}$$

把(18)式代入(11)式, 得

$$\langle n_1', K_1, j_1, m_{j1} | r^p | n_2', K_2, j_2, m_{j2}\rangle$$

$$= \delta_{j_1,j_2}\delta_{m_{j1},m_{j2}}H_{n_1'K_1}H_{n_2'K_2}\left(\frac{2}{N_1}\right)^{s_1+1/2}\left(\frac{2}{N_2}\right)^{s_2+1/2}\left(\frac{a}{Z}\right)^p$$

$$\times\left\{\left[\sqrt{(1-\varepsilon_{n_1'K_1})(1-\varepsilon_{n_2'K_2})}+\sqrt{(1+\varepsilon_{n_1'K_1})(1+\varepsilon_{n_2'K_2})}\right]Q_1\right.$$

$$+\left[\sqrt{(1-\varepsilon_{n_1'K_1})(1-\varepsilon_{n_2'K_2})}-\sqrt{(1+\varepsilon_{n_1'K_1})(1+\varepsilon_{n_2'K_2})}\right]Q_2$$

$$+\left[\sqrt{(1-\varepsilon_{n_1'K_1})(1-\varepsilon_{n_2'K_2})}-\sqrt{(1+\varepsilon_{n_1'K_1})(1+\varepsilon_{n_2'K_2})}\right]Q_3$$

$$\left.+\left[\sqrt{(1-\varepsilon_{n_1'K_1})(1-\varepsilon_{n_2'K_2})}+\sqrt{(1+\varepsilon_{n_1'K_1})(1+\varepsilon_{n_2'K_2})}\right]Q_4\right\}, \tag{19}$$

其中

$$Q_1 = (N_1+K_1)(N_2+K_2)\frac{n_1'!\Gamma(2s_1+1)}{\Gamma(n_1'+2s_1+1)}\sum_{q=0}^{n_1'}\left[\frac{(-1)^q}{q!}\left(\frac{2}{N_1}\right)^q\begin{pmatrix} n_1'+2s_1 \\ n_1'-q\end{pmatrix}\right.$$

$$\times\left(\frac{N_1N_2}{N_1+N_2}\right)^{s_1+s_2+p+q+1}\Gamma(s_1+s_2+p+q+1)$$

$$\left.\times F\left(-n_2', s_1+s_2+p+q+1, 2s_2+1, \frac{2N_1}{N_1+N_2}\right)\right], \tag{20}$$

$$O_2 = n_2'(N_1+K_1)\frac{n_1'!\Gamma(2s_1+1)}{\Gamma(n_1'+2s_1+1)}\sum_{q=0}^{n_1'}\left[\frac{(-1)^q}{q!}\left(\frac{2}{N_1}\right)^q\begin{pmatrix} n_1'+2s_1 \\ n_1'-q\end{pmatrix}\right.$$

$$\times\left(\frac{N_1N_2}{N_1+N_2}\right)^{s_1+s_2+p+q+1}\Gamma(s_1+s_2+p+q+1)$$

$$\times F\left[-n_2'+1, s_1+s_2+p+q+1, 2s_2+1, \frac{2N_1}{N_1+N_2}\right]\Bigg], \tag{21}$$

$$Q_3 = n_1'(N_2+K_2)\frac{(n_1'-1)!\Gamma(2s_1+1)}{\Gamma(n_1'+2s_1)}\sum_{q=0}^{n_1'-1}\left[\frac{(-1)^q}{q!}\left(\frac{2}{N_1}\right)^q\right.$$
$$\times\binom{n_1'+2s_1-1}{n_1'-q-1}\left(\frac{N_1N_2}{N_1+N_2}\right)^{s_1+s_2+p+q+1}\Gamma(s_1+s_2+p+q+1)$$
$$\left.\times F\left[-n_2', s_1+s_2+p+q+1, 2s_2+1, \frac{2N_1}{N_1+N_2}\right]\right], \tag{22}$$

$$Q_4 = n_1'n_2'\frac{(n_1'-1)!\Gamma(2s_1+1)}{\Gamma(n_1'+2s_1)}\sum_{q=0}^{n_1'-1}\left[\frac{(-1)^q}{q!}\left(\frac{2}{N_1}\right)^q\binom{n_1'+2s_1-1}{n_1'-q-1}\right.$$
$$\times\left(\frac{N_1N_2}{N_1+N_2}\right)^{s_1+s_2+p+q+1}\Gamma(s_1+s_2+p+q+1)$$
$$\left.\times F\left[-n_2'+1, s_1+s_2+p+q+1, 2s_2+1, \frac{2N_1}{N_1+N_2}\right]\right]. \tag{23}$$

(19)式即为相对论性氢原子径向算符矩阵元的通项计算公式. 积分公式(17)式要求 $\mathrm{Re}\,\beta>-1$ 和 $\mathrm{Re}\,\nu>0$. 即要求(16)式中 $\mathrm{Re}(w+q)>-1$, $\mathrm{Re}\,\lambda>0$. 由于 $q\geqslant 0$, 所以对任给 $\mathrm{Re}\,w>-1$, $\mathrm{Re}\,\lambda>0$, (18)式均成立, 进而由(11)式可知, (19)式适用于任何 $\mathrm{Re}\,p>-(1+s_1+s_2)$ 的情况.

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UNIVERSAL FORMULA FOR CALCULATING THE MATRIX ELEMENT OF RADIAL OPERATOR OF RELATIVISTIC HYDROGEN ATOM

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ABSTRACT

The universal formula for calculating the matrix element of radial operator of relativistic hydrogen atom is established.

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