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三维各向同性谐振子径向矩阵元的递推关系*

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推导出三维各向同性谐振子径向矩阵元$\langle nl|r^p|n'l'\rangle$所满足的递推关系.

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各向同性谐振子势是量子力学中可精确求解的问题之一[1,2]. 它在原子核的壳层结构模型[3]中得到了广泛的应用,在原子核结构研究中占有重要的地位. 在处理实际问题时经常需要计算径向矩阵元$\langle nl|r^p|n'l'\rangle$的值. 最近侯春风等[4]给出了这个矩阵元的通项表达式,然而表达式中含有阶乘运算和伽马函数,所以对于高幂次来说,不仅计算过程极为繁琐,而且计算精度也不高. 为了克服这些不足,本文给出不同幂次矩阵元之间所满足的递推关系. 利用本文所给的递推关系,只需知道几个低幂次矩阵元的值,就可以非常方便地算出任意幂次的矩阵元的值因而具有极大的适用性. 下面我们就推导出这一递推关系.

取$\Psi(r,\theta,\varphi)=\frac{u(r)}{r}Y(\theta,\varphi)$,则三维各向同性谐振子的径向方程为

$$\frac{\mathrm{d}^2u_{nl}(r)}{\mathrm{d}r^2}+\left[2E-r^2-\frac{l(l+1)}{r^2}\right]u_{nl}(r)=0, \tag{1}$$

其能量本征值为

$$E=2n+l+3/2. \tag{2}$$

对于状态nl和状态$n'l'$,(1)式分别化为

$$\frac{\mathrm{d}^2u_{nl}(r)}{\mathrm{d}r^2}+\left[(4n+2l+3)-r^2-\frac{l(l+1)}{r^2}\right]u_{nl}(r)=0, \tag{3}$$

$$\frac{\mathrm{d}^2u_{n'l'}(r)}{\mathrm{d}r^2}+\left[(4n'+2l'+3)-r^2-\frac{l'(l'+1)}{r^2}\right]u_{n'l'}(r)=0, \tag{4}$$

而矩阵元为

$$\langle nl|r^p|n'l'\rangle=\int_0^\infty r^pu_{nl}(r)u_{n'l'}(r)\mathrm{d}r. \tag{5}$$

以$r^pu_{n'l'}(r)$乘(3)式各项并积分$\int_0^\infty\cdots\mathrm{d}r$,等号左边方括号内的三项显然给出$r^p$,$r^{p+2}$和$r^{p-2}$的矩阵元,而第一项进行二次分部积分,则得如下结果:

$$\begin{aligned}&-\int_0^\infty r^p\frac{\mathrm{d}u_{nl}}{\mathrm{d}r}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r+\int_0^\infty pr^{p-1}u_{nl}\frac{\mathrm{d}u_{u'l'}}{\mathrm{d}r}\mathrm{d}r\\&=[l(l+1)-p(p-1)]\langle nl|r^{p-2}|n'l'\rangle\\&\quad-(4n+2l+3)\langle nl|r^p|n'l'\rangle\\&\quad+\langle nl|r^{p+2}|n'l'\rangle.\end{aligned} \tag{6}$$

再以$r^pu_{nl}(r)$乘(4)式各项并积分$\int_0^\infty\cdots\mathrm{d}r$,等号左边方括号内的三项依然给出$r^p$,$r^{p+2}$和$r^{p-2}$的矩阵元,而第一项分部积分一次,得到

$$\begin{aligned}&-\int_0^\infty r^p\frac{\mathrm{d}u_{nl}}{\mathrm{d}r}\frac{\mathrm{d}u_{u'l'}}{\mathrm{d}r}\mathrm{d}r-\int_0^\infty pr^{p-1}u_{nl}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r\\&=l'(l'+1)\langle nl|r^{p-2}|n'l'\rangle\\&\quad-(4n'+2l'+3)\langle nl|r^p|n'l'\rangle\\&\quad+\langle nl|r^{p+2}|n'l'\rangle.\end{aligned} \tag{7}$$

联合(6)和(7)式得到

$$\begin{aligned}&-\int_0^\infty r^p\frac{\mathrm{d}u_{nl}}{\mathrm{d}r}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r\\&=\frac{1}{2}[l(l+1)+l'(l'+1)\\&-p(p-1)]\langle nl|r^{p-2}|n'l'\rangle-(2n+2n'+l\\&+l'+3)\langle nl|r^p|n'l'\rangle+\langle nl|r^{p+2}|n'l'\rangle,\end{aligned} \tag{8}$$

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$$\int_0^\infty p r^{p-1} u_{nl} \frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r = \frac{1}{2}[l(l+1) - l'(l'+1) - p(p-1)]\langle nl|r^{p-2}|n'l'\rangle - (2n-2n'+l-l')\langle nl|r^p|n'l'\rangle. \tag{9}$$

下面再用 $r^{p+1}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}$ 乘(3)式各项并积分 $\int_0^\infty\cdots\mathrm{d}r$，其中对等号左边第一项进行一次分部积分得到

$$-\int_0^\infty (p+1) r^p \frac{\mathrm{d}u_{nl}}{\mathrm{d}r}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r - \int_0^\infty r^{p+1}\frac{\mathrm{d}u_{nl}}{\mathrm{d}r}\frac{\mathrm{d}^2u_{n'l'}}{\mathrm{d}r^2}\mathrm{d}r = l(l+1)\int_0^\infty r^{p-1}u_{nl}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r - (4n+2l+3)\cdot\int_0^\infty r^{p+1}u_{nl}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r + \int_0^\infty r^{p+3}u_{nl}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r. \tag{10}$$

再用 $r^{p+1}\frac{\mathrm{d}u_{nl}}{\mathrm{d}r}$ 乘(4)式各项并积分 $\int_0^\infty\cdots\mathrm{d}r$，其中对等号左边方括号内的三项各进行一次分部积分得到

$$\int_0^\infty r^{p+1}\frac{\mathrm{d}u_{nl}}{\mathrm{d}r}\frac{\mathrm{d}^2u_{n'l'}}{\mathrm{d}r^2}\mathrm{d}r = -l'(l'+1)(p-1)\langle nl|r^{p-2}|n'l'\rangle - l'(l'+1)\int_0^\infty r^{p-1}u_{nl}\frac{\mathrm{d}u_{u'l'}}{\mathrm{d}r}\mathrm{d}r + (4n'+2l'+3)(p+1)\langle nl|r^p|n'l'\rangle + (4n'+2l'+3)\int_0^\infty r^{p+1}u_{nl}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r - (p+3)\langle nl|r^{p+2}|n'l'\rangle - \int_0^\infty r^{p+3}u_{nl}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r. \tag{11}$$

把(11)式代入(10)式并化简合并同幂次项的积分得到

$$-\int_0^\infty (p+1) r^p \frac{\mathrm{d}u_{nl}}{\mathrm{d}r}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r = -l'(l'+1)(p-1)\langle nl|r^{p-2}|n'l'\rangle + [l(l+1) - l'(l'+1)]\int_0^\infty r^{p-1}u_{nl}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r + (4n'+2l'+3)(p+1)\langle nl|r^p|n'l'\rangle - 2(2n-2n'+l-l')\int_0^\infty r^{p+1}u_{nl}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r - (p+3)\langle nl|r^{p+2}|n'l'\rangle. \tag{12}$$

上式等号右边第二项的积分可直接利用(9)式来代换，第四项的积分则需在(9)式中用 $p\to p+2$，然后代换这一项的积分，二项的积分代换后，再对(12)式进行化简最后可得到

$$-\int_0^\infty r^p \frac{\mathrm{d}u_{nl}}{\mathrm{d}r}\frac{\mathrm{d}u_{n'l'}}{\mathrm{d}r}\mathrm{d}r = \left\{\frac{[l(l+1)-l'(l'+1)]^2}{2p(p+1)} - \frac{[l(l+1)+l'(l'+1)](p-1)}{2(p+1)}\right\}\cdot\langle nl|r^{p-2}|n'l'\rangle + \left\{(2n+2n'+l+l'+3) - \frac{2[l(l+1)-l'(l'+1)](2n-2n'+l-l')}{p(p+2)}\right\}\cdot\langle nl|r^p|n'l'\rangle + \left\{\frac{2(2n-2n'+l-l')^2}{(p+1)(p+2)} - \frac{p+3}{p+1}\right\}\langle nl|r^{p+2}|n'l'\rangle. \tag{13}$$

对比(8)与(13)式，即得矩阵元的递推关系

$$\left\{\frac{(2n-2n'+l-l')^2}{(p+1)(p+2)} - \frac{p+2}{p+1}\right\}\langle nl|r^{p+2}|n'l'\rangle = \left\{\frac{[l(l+1)-l'(l'+1)](2n-2n'+l-l')}{p(p+2)} - (2n+2n'+l+l'+3)\right\}\langle nl|r^p|n'l'\rangle + \left\{\frac{p[l(l+1)+l'(l'+1)]}{2(p+1)} - \frac{p(p-1)}{4} - \frac{[l(l+1)-l'(l'+1)]^2}{4p(p+1)}\right\}\langle nl|r^{p-2}|n'l'\rangle. \tag{14}$$

由上式可知，只要知道了矩阵元 $\langle nl|r|n'r'\rangle$，$\langle nl|r^2|n'l'\rangle$ 和 $\langle nl|r^3|n'l'\rangle$ 的值，就可利用(14)式算出所需要的任意幂次的矩阵元.

在(14)式中，令 $n'=n$，$l'=l$，即得平均值的递推公式

$$(p+2)\langle nl|r^{p+2}|nl\rangle - (p+1)(4n+2l+3)\cdot\langle nl|r^p|nl\rangle + \frac{p[(2l+1)^2-p^2]}{4}\cdot\langle nl|r^{p-2}|nl\rangle = 0. \tag{15}$$

这与文献[5]给出的平均值的递推公式完全一致。由此可见，本文给出的矩阵元的递推公式更具有一般性.

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RECURRENCE FORMULA FOR RADIAL MATRIX ELEMENTS OF THREE-DIMENSIONAL ISOTROPIC HARMONIC OSCILLATOR*

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ABSTRACT

The recurrence formula for radial matrix elements $\langle nl \mid r^p \mid n'l' \rangle$ of three-dimensional isotropic harmonic oscillator are derived.

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