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Analytical formulae and recurrence relations of bound-continuous transition matrix element for Coulomb wavefunctions*

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In this paper, the analytical formulae of bound-continuous transition matrix elements for Coulomb wavefunctions are obtained, and the recurrence relations of different power order transition matrix elements are also derived. The results may be useful in a great diversity of scattering problems for atoms or molecules.

Keywords: Coulomb wavefunctions, bound-continuous transition matrix elements, analytical formulae, recurrence relations

PACC: 0365, 0365N, 3115

1. Introduction

The theoretical prediction of many properties of atoms or molecules requires the knowledge of the matrix elements of r^s operators. There has been a long history of attempts to calculate the matrix elements of r^s operators for Coulomb wavefunctions in bound states.[1−8] The explicit expressions and the general formula for matrix elements of r^s operators for relativistic-Coulomb wavefunctions have been given.[9−14] However, the study of characteristics of the scattering states for atoms or molecules such as (e, 2e) collisions[15−17] and photoionization[18−21] requires bound-continuous transition matrix elements. In previous papers,[22,23] bound-continuous transition matrix elements between some bound states and scattering states have been given. The purpose of the present paper is to derive the analytical formulae and the recurrence relations of bound-continuous transition matrix elements for Coulomb wavefunctions. In Section 2, we will give the general analytical formulae of bound-continuous transition matrix elements for Coulomb wavefunctions. In order to simplify the calculation of radial matrix elements in the case of high powers of r operator, we will derive the recurrence relation of different powers of the bound-continuous transition matrix elements in Section 3. The approach we use in this section is related to the one developed recently for the case of bound states of n-dimensional isotropic harmonic oscillator and the Hartmann potential.[24−27]

2. Analytical formulae of bound-continuous transition matrix elements

Letting

$$\Psi(r,\theta,\phi)=\frac{u(r)}{r}Y(\theta,\varphi) \tag{1}$$

and then separating the variables of the Schrödinger equation with the Coulomb potential $V(r)=-Ze^2/r$, we can obtain the radial equation ($\hbar=m=e=1$)

$$\frac{\mathrm{d}^2u(r)}{\mathrm{d}r^2}+\left(2E+\frac{2Z}{r}-\frac{l(l+1)}{r^2}\right)u(r)=0. \tag{2}$$

For the bound states, $E<0$, solving the above equation gives the normalized radial wavefunctions and the exact energy equation[28,29]

$$u_{nl}(r)=N_{nl}\left(\frac{2Zr}{n}\right)^{l+1}\mathrm{e}^{-\frac{Zr}{n}}L_{n+l}^{2l+1}\left(\frac{2Zr}{n}\right), \tag{3}$$

$$E_n=-\frac{Z^2}{2n^2}\,,\quad n=n_r+l+1=1,2,3\cdots, \tag{4}$$

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where n is the principal quantum number, and l is the angular quantum number, and N_{nl} is the normalization constant of the radial wavefunctions of bound states

$$N_{nl} = -\left[\frac{Z(n-l-1)!}{n^2[(n+l)!]^3}\right]^{1/2}, \tag{5}$$

and the associated Laguerre polynomial is

$$L_{n+l}^{2l+1}(x) = \sum_{t=0}^{n-l-1}(-1)^{t+2l+1} \times \frac{[(n+l)!]^2 x^t}{(n-l-1-t)!(2l+1+t)!t!}. \tag{6}$$

For the scattering states, $E > 0$, solving the above equation gives, on the "$k/2\pi$ scale", the normalized radial wavefunctions[28,29]

$$u_{kl}(r) = C_{kl}(2kr)^{l+1}\mathrm{e}^{-\mathrm{i}kr}F(l+1+\mathrm{i}Z/k, 2l+2, 2\mathrm{i}kr), \tag{7}$$

where $k = \sqrt{2E}$ and C_{kl} is the normalization constant of the radial wavefunctions of scattering states

$$C_{kl} = \frac{|\Gamma(l+1-\mathrm{i}Z/k)|\,\mathrm{e}^{\pi Z/2k}}{(2l+1)!}. \tag{8}$$

The bound-continuous transition matrix elements for Coulomb wavefunctions are

$$\langle nl|\, r^s\, |kl'\rangle = \int_0^\infty u_{nl}^*(r)u_{kl'}(r)r^s\mathrm{d}r. \tag{9}$$

Substituting Eqs.(3) and (7) into Eq.(9), we have

$$\begin{aligned}&\langle nl|\, r^s\, |n\,l'\rangle \\ =&N_{nl}C_{kl'}\left(\frac{2Z}{n}\right)^{l+1}(2k)^{l'+1} \\ &\times\int_0^\infty r^{l+l'+2+s}\mathrm{e}^{-(Z/n+\mathrm{i}k)r}L_{n+l}^{2l+1}(2Zr/n) \\ &\times F(l'+1+\mathrm{i}Z/k, 2l'+2, 2\mathrm{i}kr)\,\mathrm{d}r.\end{aligned} \tag{10}$$

Substituting Eq.(6) into Eq.(10), the above expression can be written as

$$\begin{aligned}&\langle nl|\, r^s\, |kl'\rangle \\ =&N_{nl}C_{kl'}(2k)^{l'+1}\sum_{t=0}^{n-l-1}(-1)^{t+2l+1} \\ &\times\frac{[(n+l)!]^2}{(n-l-1-t)!(2l+1+t)!t!}\left(\frac{2Z}{n}\right)^{t+l+1} \\ &\times\int_0^\infty r^{l+l'+t+2+s}\mathrm{e}^{-(Z/n+\mathrm{i}k)r} \\ &\times F(l'+1+\mathrm{i}Z/k, 2l'+2, 2\mathrm{i}kr)\,\mathrm{d}r.\end{aligned} \tag{11}$$

By using the integral formulae containing confluent hypergeometric function[29]

$$\begin{aligned}&\int_0^\infty z^v\mathrm{e}^{-\lambda z}F(\alpha,\gamma,kz)\mathrm{d}z \\ =&\Gamma(v+1)\lambda^{-v-1}F(\alpha, v+1, \gamma, k/\lambda),\end{aligned} \tag{12}$$

and substituting Eqs.(5) and (8) into Eq.(11), after simplifying, we have

$$\begin{aligned}&\langle nl|\, r^s\, |kl'\rangle \\ =&\left[\frac{Z(n-l-1)!}{n^2(n+l)!}\right]^{1/2} \\ &\times\frac{|\Gamma(l'+1-\mathrm{i}Z/k)|\,\mathrm{e}^{\pi Z/2k}}{(2l'+1)!}(2k)^{l'+1}\sum_{t=0}^{n_r}(-1)^t \\ &\times\frac{(n+l)!}{(n-l-1-t)!\;(2l+1+t)!\;t!}\left(\frac{2Z}{n}\right)^{t+l+1} \\ &\times\Gamma(l+l'+s+t+3)(Z/n+\mathrm{i}k)^{-(l+l'+s+t+3)} \\ &\times F\Bigg(l'+1+\mathrm{i}Z/k, l+l'+s+t+3, \\ &2l'+2, \frac{2\mathrm{i}k}{Z/n+\mathrm{i}k}\Bigg).\end{aligned} \tag{13}$$

The above expression is a general expression of the bound-continuous transition matrix elements for Coulomb wavefunctions. The radial wavefunctions of bound states $u_{nl}(r)$ is a real function, and the radial wavefunctions of scattering states $u_{kl'}(r)$ is a complex function, so we have $\langle kl'|\, r^s\, |nl\rangle = \langle nl|\, r^s\, |kl'\rangle^*$.

3. Recurrence relations of bound-continuous transition matrix elements

We have obtained the general formulae of the bound-continuous transition matrix elements for Coulomb wavefunctions in Section 2. In order to simplify the calculation of the bound-continuous transition matrix elements in the case of high powers of r operator, the recurrence relations for them are derived in this section.

In analogy to the practice of the recurrence relation of radial matrix elements for the bound states of the n-dimensional isotropic harmonic oscillator and the Hartmann potential,[24−27] for the bound state nl and the scattering state kl', we can re-write Eq.(2) as

$$\frac{\mathrm{d}^2u_{nl}(r)}{\mathrm{d}r^2} + \left[-\frac{Z^2}{n^2} + \frac{2Z}{r} - \frac{l(l+1)}{r^2}\right]u_{nl}(r) = 0, \tag{14}$$

$$\frac{\mathrm{d}^2u_{kl'}(r)}{\mathrm{d}r^2} + \left[k^2 + \frac{2Z}{r} - \frac{l'(l'+1)}{r^2}\right]u_{kl'}(r) = 0. \tag{15}$$

It can be shown from Eqs.(3) and (7) that

$$r \to 0\ , \quad u_{nl}(r) \to r^{l+1}, \quad u_{kl}(r) \to r^{l+1};$$
$$r \to \infty, \quad u_{nl}(r) \to r^n \mathrm{e}^{-Zr/n},$$
$$u_{kl}(r) \to 2\sin(kr - l\pi/2 + (Z\ln 2kr)/k + \delta_l). \quad (16)$$

If $s > -(l + l' + 1)$, we have

$$r^s u_{kl'} \frac{\mathrm{d}u_{nl}}{\mathrm{d}r}\bigg|_0^\infty = 0, \quad r^{s-1} u_{nl} u_{kl'}\bigg|_0^\infty = 0,$$
$$r^s \frac{\mathrm{d}u_{kl'}}{\mathrm{d}r} u_{nl}\bigg|_0^\infty = 0, \quad r^{s+1} \frac{\mathrm{d}u_{nl}}{\mathrm{d}r}\frac{\mathrm{d}u_{kl'}}{\mathrm{d}r}\bigg|_0^\infty = 0. \quad (17)$$

Firstly, we multiply each term of Eq.(14) by $r^s u_{kl'}(r)$ and integrate $\int_0^\infty \cdots \mathrm{d}r$. Obviously, the three terms in the square brackets are bound-continuous transition matrix elements of r^s and r^{s-1} and r^{s-2}. Integrating the first term twice by parts and using Eq.(17), we obtain the result

$$-\int_0^\infty r^s \frac{\mathrm{d}u_{nl}(r)}{\mathrm{d}r}\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r$$
$$+\int_0^\infty s r^{s-1} u_{nl}(r)\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r$$
$$= [l(l+1) - s(s-1)] \langle nl|\, r^{s-2}\, |kl'\rangle$$
$$- 2Z \langle nl|\, r^{s-1}\, |kl'\rangle + (Z^2/n^2) \langle nl|\, r^s\, |kl'\rangle\ . \quad (18)$$

Secondly, we multiply each term of Eq.(15) by $r^s u_{nl}(r)$ and integrate $\int_0^\infty \cdots \mathrm{d}r$. Obviously, the three terms in the square brackets are bound-continuous transition matrix elements of r^s and r^{s-1} and r^{s-2}. Integrating the first term once by parts and using Eq.(17), we have

$$-\int_0^\infty r^s \frac{\mathrm{d}u_{nl}(r)}{\mathrm{d}r}\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r$$
$$-\int_0^\infty s r^{s-1} u_{nl}(r)\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r$$
$$= l'(l'+1) \langle nl|\, r^{s-2}\, |kl'\rangle$$
$$- 2Z \langle nl|\, r^{s-1}\, |kl'\rangle - k^2 \langle nl|\, r^s\, |kl'\rangle\ . \quad (19)$$

Comparing Eq.(18) with Eq.(19), we have

$$-\int_0^\infty r^s \frac{\mathrm{d}u_{nl}(r)}{\mathrm{d}r}\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r$$
$$= \frac{1}{2}[l(l+1) + l'(l'+1) - s(s-1)] \langle nl|\, r^{s-2}\, |kl'\rangle$$
$$- 2Z \langle nl|\, r^{s-1}\, |kl'\rangle$$
$$+ \frac{1}{2}(Z^2/n^2 - k^2) \langle nl|\, r^s\, |kl'\rangle\ , \quad (20)$$

$$\int_0^\infty s r^{s-1} u_{nl}(r)\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r$$
$$= \frac{1}{2}[l(l+1) - l'(l'+1) - s(s-1)] \langle nl|\, r^{s-2}\, |kl'\rangle$$
$$+ \frac{1}{2}(Z^2/n^2 + k^2) \langle nl|\, r^s\, |kl'\rangle\ . \quad (21)$$

Thirdly, we multiply each term of Eq.(14) by $r^{s+1}\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}$ and integrate $\int_0^\infty \cdots \mathrm{d}r$. Integrating the first term once by parts and using Eq.(17), the result is

$$-\int_0^\infty (s+1) r^s \frac{\mathrm{d}u_{nl}(r)}{\mathrm{d}r}\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r$$
$$-\int_0^\infty r^{s+1} \frac{\mathrm{d}u_{nl}(r)}{\mathrm{d}r}\frac{d^2 u_{kl'}(r)}{\mathrm{d}r^2}\mathrm{d}r$$
$$= l(l+1)\int_0^\infty r^{s-1} u_{nl}(r)\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r$$
$$- 2Z\int_0^\infty r^s u_{nl}(r)\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r$$
$$+ (Z^2/n^2)\int_0^\infty r^{s+1} u_{nl}(r)\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r\ . \quad (22)$$

Finally, we multiply each term of Eq.(15) by $r^{s+1}\frac{\mathrm{d}u_{nl}(r)}{\mathrm{d}r}$ and integrate $\int_0^\infty \cdots \mathrm{d}r$. Integrating each term in the square bracket once by parts and using Eq.(17), we have

$$\int_0^\infty r^{s+1}\frac{\mathrm{d}u_{nl}(r)}{\mathrm{d}r}\frac{d^2u_{kl'}(r)}{\mathrm{d}r^2}\mathrm{d}r$$

$$= -l'(l'+1)(s-1)\langle nl|\, r^{s-2}\,|kl'\rangle - l'(l'+1)\int_0^\infty r^{s-1}u_{nl}(r)\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r + (s+1)k^2\langle nl|\, r^s\,|kl'\rangle$$

$$+ k^2\int_0^\infty r^{s+1}u_{nl}(r)\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r + 2sZ\langle nl|\, r^{s-1}\,|kl'\rangle + 2Z\int_0^\infty r^s u_{nl}(r)\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r\ . \tag{23}$$

Substituting Eq.(23) into (22), after simplifying, we have

$$-\int_0^\infty (s+1)r^s\frac{\mathrm{d}u_{nl}(r)}{\mathrm{d}r}\frac{\mathrm{d}u_{kl}(r)}{\mathrm{d}r}\mathrm{d}r$$

$$= -l'(l'+1)(s-1)\langle nl|\, r^{s-2}\,|kl'\rangle + (l-l')(l+l'+1)\int_0^\infty r^{s-1}u_{nl}(r)\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r + (s+1)k^2\langle nl|\, r^s\,|kl'\rangle$$

$$+ [Z^2/n^2+k^2]\int_0^\infty r^{s+1}u_{nl}(r)\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r + 2sZ\langle nl|\, r^{s-1}\,|kl'\rangle\ . \tag{24}$$

The two terms containing integrals on the right-hand side of the above expression may be replaced by the recurrence formula (21), and after simplifying, we have

$$-\int_0^\infty r^s\frac{\mathrm{d}u_{nl}(r)}{\mathrm{d}r}\frac{\mathrm{d}u_{kl'}(r)}{\mathrm{d}r}\mathrm{d}r$$

$$=\frac{(Z^2/n^2+k^2)^2}{2(s+1)(s+2)}\langle nl|\, r^{s+2}\,|kl'\rangle + \left[\frac{(l-l')(l+l'+1)(Z^2/n^2+k^2)}{s(s+2)} - \frac{Z^2/n^2-k^2}{2}\right]\langle nl|\, r^s\,|kl'\rangle$$

$$+ \frac{2sZ}{s+1}\langle nl|\, r^{s-1}\,|kl'\rangle + \left\{-\frac{[l(l+1)+l'(l'+1)](s-1)}{2(s+1)} + \frac{[(l-l')(l+l'+1))]^2}{2s(s+1)}\right\}\langle nl|\, r^{s-2}\,|kl'\rangle\ . \tag{25}$$

Comparing Eq.(20) with Eq.(25), we have the recurrence relation of the bound-continuous transition matrix elements for Coulomb wavefunctions, i.e.

$$s(Z^2/n^2+k^2)^2\langle nl|\, r^{s+2}\,|kl'\rangle$$

$$=2(s+1)\left[s(s+2)(Z^2/n^2-k^2) - (l-l')(l+l'+1)(Z^2/n^2+k^2)\right]\langle nl|\, r^s\,|kl'\rangle$$

$$- 4Zs(s+2)(2s+1)\langle nl|\, r^{s-1}\,|kl'\rangle + (s+2)[(l-l')^2-s^2][s^2-(l+l'+1)^2]\langle nl|\, r^{s-2}\,|kl'\rangle\,. \tag{26}$$

The above expression is the recurrence relation of different powers of bound-continuous transition matrix elements for Coulomb wavefunctions. It is valid only if $s > -(l+l'+1)$. The formula (26) shows that if the values of $\langle nl|\, r\,|kl'\rangle$, $\langle nl|\, r^2\,|kl'\rangle$ and $\langle nl|\, r^3\,|kl'\rangle$ are given, the bound-continuous transition matrix elements of any power of the radial r for Coulomb wavefunctions may be calculated.

4. Conclusion

In this paper, we have obtained the analytical formulae and the recurrence relation of bound-continuous transition matrix elements for Coulomb wavefunctions. The problem of how to calculate the bound-continuous transition matrix elements for Coulomb wavefunctions has been solved. Using those formulae, we can calculate values of different powers of bound-continuous transition matrix elements for Coulomb wavefunctions.

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