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Polarization, correlation, and distortion effects in excitation processes

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Analytical expressions are derived for the asymptotic correlated three-body state of a Coulomb compound consisting of a continuum particle and an electron bound to a residual ion. The extension of these expressions to finite distances is also given. The distortion of the continuum particle's motion by the Coulomb nuclear field and the field of the bound electron is investigated as well as the amount of polarization of the bound system due to coupling of the bound electron to the continuum particle. [S1050-2947(98)50609-9]

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In recent years, considerable progress has been made in the analytical description of highly excited few-particle Coulomb complexes. Such excited systems are usually generated upon the impact of photons and charged particles. E.g., for photon- and electron-impact fragmentation processes that lead to three interacting continuum particles, a number of analytical approaches have been put forward [1–6]. One strategy to derive approximate expressions for the three-body wave functions is to start from the asymptotic eigenstates of the three-particle Hamiltonian and to search for reasonable extensions of these states to finite distances [2,5,7]. One well-known approximation obtained this way [1,2,5] regards the three-body Coulomb system as the sum of three, in configuration space, noninteracting two-body subsystems (on the two-body energy shell). The mathematical reflection of this point of view is that the three-body continuum state Ψ_{3C} is a product of three two-body Coulomb waves (on the two-body energy shell), each simulating the interaction within a specific two-body subsystem, i.e. (atomic units are used throughout; outgoing wave boundary conditions are considered),

$$\begin{aligned}\Psi_{3C}(\mathbf{r}_a,\mathbf{r}_b) = (2\pi)^{-3}\ & \exp(i\mathbf{k}_a\cdot\mathbf{r}_a + i\mathbf{k}_b\cdot\mathbf{r}_b)\\ & \times N_a\, {}_1F_1[i\alpha_a,1,-ik_a(r_a+\hat{\mathbf{k}}_a\cdot\mathbf{r}_a)]\\ & \times N_b\, {}_1F_1[i\alpha_b,1,-ik_b(r_b+\hat{\mathbf{k}}_b\cdot\mathbf{r}_b)]\\ & \times N_{ab}\, {}_1F_1[i\alpha_{ab},1,-ik_{ab}(r_{ab}+\hat{\mathbf{k}}_{ab}\cdot\mathbf{r}_{ab})],\end{aligned} \tag{1}$$

where $\mathbf{r}_{a/b}$ are the coordinates of the continuum particles escaping with momenta $\mathbf{k}_{a/b}$ (with respect to a residual ion), $N_j=\Gamma(1-i\alpha_j)\exp(-\pi\alpha_j/2)$, $j\in\{a,b,ab\}$ are normalization constants, ${}_1F_1[a,b,x]$ is the confluent hypergeometric function, and $\mathbf{r}_{ab}=\mathbf{r}_a-\mathbf{r}_b$ is the interparticle relative coordinate with $\mathbf{k}_{ab}$ being its conjugate momentum. In Eq. (1) the Sommerfeld parameters are $\alpha_j=-Z/k_j$, $j=a,b$, and $\alpha_{ab}=1/(2k_{ab})$, where Z is the charge of the residual ion.

This resulting $3C$ wave function, so called since it consists of three Coulomb waves, has, in some cases, considerable success in predicting the relative angular distributions of correlated electron pairs emitted upon photon and particle impact [2,8,9]. In addition to the, meanwhile well-known shortcomings of this model [5,9,10], its mathematical structure suggests that it is only designed for total breakup reactions without regard to any virtual intermediate excitations.

The basic mathematical concept of starting from asymptotic states and then propagating to finite distances has, however, been recently employed to consider intermediate and direct excitations [11,12]. In Ref. [11] a scheme has been proposed to include the (off-shell) virtual excitations to discrete and continuum levels in the three-body scattering states. In actual calculations of ionization probabilities, however, only virtual continuum states have been included.

In a second approach by Dewangan [12] a version of the $3C$ wave function has been suggested to deal with direct electron-impact excitation of hydrogen. He applied the theory to the $1s\rightarrow 2p$ transitions and evaluated the angular correlation parameters λ and R ($\lambda=\langle f_0 f_0^*\rangle/\sigma$, $R=\mathrm{Re}\langle f_1 f_0^*\rangle/\sigma$, where f_{m_ℓ} is the excitation amplitude of the magnetic sublevel m_ℓ, σ is the differential cross section, and $\langle\cdots\rangle$ denotes the average over spin). Remarkable agreement with experimental data was found in the backward direction for the R parameter, yet some serious discrepancies remained unexplained at a certain angular region.

Dewangan suggested that a wave function for the projectile electron and the excited atom can be obtained from Eq. (1) upon a straightforward replacement of the ejected-electron Coulomb wave,

$$(2\pi)^{-3/2}N_b\,\exp(i\mathbf{k}_b\cdot\mathbf{r}_b)\,{}_1F_1[i\alpha_b,1,-ik_b(r_b+\hat{\mathbf{k}}_b\cdot\mathbf{r}_b)],$$

by a bound atomic eigenfunction $\Phi_f(\mathbf{r}_b)$ for the excited target state in the exit channel. Subsequently the wave vector k_b is set to zero. This *ad hoc* replacement reduces Eq. (1) to the two-center wave function (TCW)

$$\begin{aligned}\Psi^-_{\mathrm{TCW}}(\mathbf{r}_a,\mathbf{r}_b) & = (2\pi)^{-3/2}|\Gamma(1+i\alpha_a)|^2\,\exp(i\mathbf{k}_a\cdot\mathbf{r}_a)\\ & \times {}_1F_1[i\alpha_a,1,-ik_a(r_a+\hat{\mathbf{k}}_a\cdot\mathbf{r}_a)]\\ & \times {}_1F_1\{-i\alpha_a,1,-\tfrac{1}{2}[ik_a(r_{ab}+\hat{\mathbf{k}}_a\cdot\mathbf{r}_{ab})]\}.\end{aligned} \tag{2}$$

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To maintain proper asymptotic behavior $\mathbf{r}_{ab}$ is to be replaced by $2\mathbf{r}_{ab}$.

The procedure leading to Ψ^{-}_{TCW} is motivated by physical and practical considerations, yet it leaves in the dark the actual mathematical justification and foundations for the expression (2). Nonetheless, as shown in Ref. [12], the comparison with the experimental findings shows that some of the physics of the excitation process is captured by Ψ^{-}_{TCW}. Therefore, it seems worthwhile to derive Eq. (2) from first principles, which might open the way for more elaborate methods beyond that of Eq. (2). The relation of the approximation (2) to conventional perturbative approaches has been discussed in Ref. [12].

In this work a mathematical method is sought to derive (asymptotic) eigenstates of highly excited three-body systems with one particle moving in the continuum of a two-body compound. For clarity a system consisting of two electrons and a heavy ion with charge Z is considered; the general case can be treated along the same lines (mass-polarization terms then have to be neglected).

The time-independent Schrödinger equation for this system reads

$$\left[\Delta_a+\Delta_b+\frac{2Z}{r_a}+\frac{2Z}{r_b}-\frac{2}{r_{ab}}+2E\right]\psi(\mathbf{r}_a,\mathbf{r}_b)=0. \tag{3}$$

The total energy E is the sum of the energy of the continuum electron $k_a^2/2$ and that of the bound electron in a state specified by the principle, orbital, and magnetic quantum numbers n,ℓ,m, respectively, i.e.,

$$E=-\frac{Z^2}{2n^2}+\frac{k_a^2}{2}. \tag{4}$$

The unperturbed state of the bound electron b has the form [13]

$$\zeta^b_{n,\ell,m}(\mathbf{r}_b)=\frac{1}{r_b^{n-1}}\chi_{n,\ell}(r_b)\exp\left(-\frac{Zr_b}{n}\right)\mathrm{Y}_{\ell,m}(\hat{\mathbf{r}}_b), \tag{5}$$

where $\chi_{n,\ell}(r_b)$ and $\mathrm{Y}_{\ell,m}(\hat{\mathbf{r}}_b)$ are, respectively, the radial wave functions and the spherical harmonics in the notation of Ref. [13]. The asymptotic uniform motion of the projectile electron is generally $(Z\neq 1)$ modified by a Coulomb phase. Therefore, for the solution of Eq. (3) we make the ansatz

$$\Psi(\mathbf{r}_a,\mathbf{r}_b)=\overline{\psi}(\mathbf{r}_a,\mathbf{r}_b)\,\frac{\exp\left(-\frac{Zr_b}{n}\right)}{r_b}\sum_{k=0}^{\infty}\xi_k, \tag{6}$$

with the definition $\overline{\psi}(\mathbf{r}_a,\mathbf{r}_b)=\exp(i\mathbf{k}_a\cdot\mathbf{r}_a+i\phi)$. In Eq. (6) ϕ is a (complex) function yet to be determined and

$$\xi_k=\frac{1}{r_b^k}\chi_{n,\ell}(r_b)\mathrm{Y}_{\ell,m}(\hat{\mathbf{r}}_b). \tag{7}$$

Substitution of Eq. (6) into Eq. (3) yields

$$\left[-\left(\frac{2Z}{n}+\frac{2}{r_b}\right)\frac{\partial}{\partial r_b}+\Delta_b+2i\mathbf{k}_a\cdot\boldsymbol{\nabla}_a+\Delta_a+\frac{2Z}{r_b}+\frac{2Z}{r_a}-\frac{2}{r_{ab}}\right]e^{i\phi}\sum\xi_k=0. \tag{8}$$

Furthermore we deduce the differential equation

$$\left[\Delta_a+\Delta_b+i(\Delta_a+\Delta_b)\phi-(\boldsymbol{\nabla}_a\phi)^2-(\boldsymbol{\nabla}_b\phi)^2+2i(\boldsymbol{\nabla}_b\phi\cdot\boldsymbol{\nabla}_b+\boldsymbol{\nabla}_a\phi\cdot\boldsymbol{\nabla}_a)-2i\left(\frac{Z}{n}+\frac{1}{r_b}\right)\left(\frac{\partial\phi}{\partial r_b}-i\frac{\partial}{\partial r_b}\right)-2\mathbf{k}_a\cdot\boldsymbol{\nabla}_a\phi+2i\mathbf{k}_a\cdot\boldsymbol{\nabla}_a+\frac{2Z}{r_b}+\frac{2Z}{r_a}-\frac{2}{r_{ab}}\right]\sum\xi_k=0. \tag{9}$$

Asymptotically, terms that fall off faster than the Coulomb potential can be neglected. Therefore, we end up with an asymptotic differential equation from which the function ϕ can be determined:

$$\frac{iZ}{n}\frac{\partial\phi}{\partial r_b}+\mathbf{k}_a\cdot\boldsymbol{\nabla}_a\phi-\frac{Z}{r_a}-\frac{Z}{r_b}+\frac{1}{r_{ab}}=0. \tag{10}$$

For the solution of Eq. (10) an ansatz is appropriate that possesses the form

$$\phi^{\pm}=-in\,\ln(r_b)+\Phi^{\pm}, \tag{11}$$

$$\Phi^{\pm}=\mp\frac{Z}{k_a}\ln(k_ar_a\mp\mathbf{k}_a\cdot\mathbf{r}_a)+\tilde{\phi}^{\pm}, \tag{12}$$

where $\tilde{\phi}^{\pm}$ is a complex function yet to be specified. Incoming- or outgoing-wave boundary conditions can be accounted for by choosing the $+$ or $-$ sign in Eq. (12), respectively. The first term in Eq. (11) leads in Eq. (6) to a real exponential factor that describes the behavior of the state of the electron bound to the residual ion. For the following this term is basically irrelevant and can be included in the functions ξ_k, as defined in Eq. (7). The first term in Eq. (12) signifies the dephasing of the unbound electron a by virtue of the nuclear field and can thus be considered as a measure of the distortion of this electron's motion due to coupling to the residual ion.

The phase $\tilde{\phi}^{\pm}$ in Eq. (12) is due to the electronic correlation. Substitution of Eq. (11) into Eq. (10) leads, in case of incoming-wave boundary conditions, to

$$\frac{iZ}{n}\frac{\partial\tilde{\phi}^{+}}{\partial r_b}+\mathbf{k}_a\cdot\boldsymbol{\nabla}_a\tilde{\phi}^{+}+\frac{1}{r_{ab}}=0. \tag{13}$$

Equation (13) can be solved by the ansatz

$$\tilde{\phi}^{+}=\frac{1}{\lambda}\ln(\lambda r_{ab}+\mathbf{c}\cdot\mathbf{r}_{ab}). \tag{14}$$

Here the independent *complex* quantities λ and $\mathbf{c}$ are still to be determined. Upon substituting Eq. (14) into Eq. (13) and after some lengthy algebraic manipulations we obtain

$$\mathbf{c}=-\mathbf{k}_a+i\frac{Z}{n}\hat{\mathbf{r}}_b,$$

$$\lambda^2=\left(\mathbf{k}_a-i\frac{Z}{n}\hat{\mathbf{r}}_b\right)^2. \tag{15}$$

In a similar manner we obtain for outgoing-wave boundary conditions

$$\tilde{\phi}^-=-\frac{1}{\lambda}\ln(\lambda r_{ab}-\mathbf{c}\cdot\mathbf{r}_{ab}). \tag{16}$$

From Eqs. (15) it follows that if $r_a\gg r_b$, $k_a\gg Z/n$, then Eq. (12) simplifies to $\Phi^{\pm}=\mp(Z-1)/k_a\ln(k_a r_a\mp\mathbf{k}_a\cdot\mathbf{r}_a)$. Thus, for a two-body compound consisting of a neutral bound system $(Z-1=0)$ and a continuum electron, there is no distortion of the asymptotic uniform motion of the continuum particle and no polarization of the bound system due to the presence of the free electron in the asymptotic region.

In the general case, to get an insight into the amount of polarization of the bound state and the phase distortion of the in- or outgoing electrons due to interelectronic correlation, it is instructive to inspect the real and imaginary parts of the complex function $\exp(i\tilde{\phi}^-)$.

To this end we rewrite λ as

$$\lambda=x+iy, \tag{17}$$

where x,y are real quantities. Thus, $\tilde{\phi}^-$ attain the form

$$\tilde{\phi}^-=\frac{\lambda^*}{|\lambda|^2}\ln[v^2+u^2]^{1/2}+i\ \arctan\left(\frac{u}{v}\right). \tag{18}$$

The real functions v,u are given by

$$v=xr_{ab}-\mathbf{k}_a\cdot\mathbf{r}_{ab},$$

$$u=yr_{ab}+\frac{Z}{n}\hat{\mathbf{r}}_b\cdot\mathbf{r}_{ab}. \tag{19}$$

On the other hand, we can characterize the complex function $\exp(i\tilde{\phi}^-)$ in the Gauss plane by the real phase φ and the amplitude A, i.e.,

$$\exp(i\tilde{\phi}^-)=A\ \exp(i\varphi). \tag{20}$$

The amplitude A describes the polarization of the initial state due to the electronic correlation, whereas φ is a measure for the distortion of the continuum particle's motion. For A we obtain

$$A=\exp(-\mathrm{Im}\ \tilde{\phi}^-)=[v^2+u^2]^{y/2|\lambda|^2}\ \exp\left[-\frac{x}{|\lambda|^2}\arctan\frac{u}{v}\right]. \tag{21}$$

In an analogous way the phase φ is represented by

$$\varphi=\mathrm{Re}\ \tilde{\phi}^-=\ln[v^2+u^2]^{x/2|\lambda|^2}+\left[\frac{y}{|\lambda|^2}\arctan\frac{u}{v}\right]. \tag{22}$$

Expressions for x and y are then derived by substituting Eq. (18) into Eq. (13), which yields two coupled differential equations. After algebraic manipulations the final expressions for x and y are deduced as

$$x=\left\{\left[\frac{1}{4}\left(k_a^2-\frac{Z^2}{n^2}\right)^2+\frac{Z^2}{n^2}(\hat{\mathbf{r}}_b\cdot\mathbf{k}_a)^2\right]^{1/2}+\frac{1}{2}\left(k_a^2-\frac{Z^2}{n^2}\right)\right\}^{1/2}, \tag{23}$$

$$y=-\frac{Z(\hat{\mathbf{r}}_b\cdot\mathbf{k}_a)}{xn}. \tag{24}$$

In the limit of fast projectile electrons $k_a\gg Z/n$ the quantities x and y reduce to $x\approx k_a$ and $y=-Z\hat{\mathbf{r}}_b\cdot\hat{\mathbf{k}}_a/n$, respectively, and the amplitude A simplifies to unity, which means that the polarization of the bound state diminishes in this asymptotic case.

The above asymptotic analysis can be extended to finite distances (the mathematical details are somewhat more involved). The term $\bar{\psi}$ in Eq. (6) then reads [cross terms of the kinetic-energy operators that appear in Eq. (9) had to be neglected]

$$\bar{\psi}^{\mp}=\mathcal{N}\exp(i\mathbf{k}_a\cdot\mathbf{r}_a)\ {}_1F_1[\pm i\alpha_a,1,\mp ik_a(r_a\pm\hat{\mathbf{k}}_a\cdot\mathbf{r}_a)]\times{}_1F_1[\pm i\alpha_\lambda,1,\mp i(\lambda r_{ab}\mp\mathbf{c}\cdot\mathbf{r}_{ab})], \tag{25}$$

where the complex vector $\mathbf{c}$ and λ are given by Eqs. (15) and $\alpha_\lambda=1/\lambda$. The normalization constant $\mathcal{N}=(2\pi)^{-3/2}|\Gamma(1+i\alpha_a)|^2$ is derived from the requirement that the asymptotic flux generated by Eq. (6) should be equivalent to that of the plane wave [7].

It is straightforward to show that the wave function Ψ^-_{TCW}, as given by Eq. (2), derives from Eqs. (25) and (6) in the high-energy limit, i.e., $k_a\gg Z/n$ [cf. Eq. (15)], provided that in Eq. (2) we replace $\mathbf{r}_{ab}$ by $2\mathbf{r}_{ab}$. That the wave function [Eqs. (25) and (6)] satisfies the proper asymptote without any further modification is to be expected since this property was imposed in the course of the derivation of Eqs. (25) and (6).

Summarizing, in this work we envisaged correlated three-body wave functions for Coulomb compounds consisting of a bound two-body subsystem and a continuum particle. The asymptotic properties have been explored and the extension to finite distances has been pointed out. In addition, we studied the relation of the derived expressions to the polarization of the bound system and the distortion of the continuum particle's motion. In the high-energy limit $(k_a\gg Z/n)$, the present wave function has already been employed for the calculations of the angular correlation parameters of the $1s\rightarrow 2p$ transitions in hydrogen with encouraging results as compared to experiment [12].

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