Three-Body Coulomb Continuum Problem

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A symmetric representation of the three-body Coulomb continuum wave function as a product of three two-body Coulomb wave functions is modified to allow for three-body effects whereby the Sommerfeld parameter describing the strength of interaction of any two particles is affected by the presence of the third particle. This approach gives excellent agreement with near-threshold *absolute* $(e,2e)$ ionization cross sections. In particular a recently observed deep minimum in noncoplanar geometry is reproduced for the first time.

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The problem of the motion of three Coulomb interacting particles at energies above the complete dissociation threshold is one of the basic unsolved problems of atomic physics. Such a three-body Coulomb continuum state is the final state achieved in the processes of electron impact ionization and double photoionization. Recent angular correlation data on both of these fundamental processes have provided the most detailed and rigorous tests of current theories. In the case of electron impact ionization of neutral atoms, in the final state two electrons move in the field of a singly positively charged ion. In the case of double photoionization of neutral atoms two electrons move in the field of a doubly charged ion. Hence, in general, all three two-body Coulomb interactions are of comparable strength and there is no reason to neglect one interaction in comparison to others. Nevertheless, as is traditional in atomic physics, usually prominence is given to the electron-nucleus interactions and the electron-electron interaction is included in some approximate way. In other words the six-dimensional wave function of the three-body continuum is expressed in the coordinates $\mathbf{r}_a, \mathbf{r}_b$ of two electrons a, b with respect to the nucleus. No explicit dependence on the electron coordinate $\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b$ is included. In the most popular form of such general distorted-wave theories the final three-body state is represented simply by a product of two electron-nucleus Coulomb wave functions but with effective charges dependent upon the momenta $\mathbf{k}_a, \mathbf{k}_b$ of both electrons relative to the fixed nucleus [1–4]. Thereby the electron-electron interaction is represented merely by a dynamic screening, due to the presence of a second electron, of the nuclear charge seen by one electron. A criterion by which the effective nuclear charges may be chosen was put forward by Peterkop [5] and Rudge and Seaton [6] (see also [7]), based on a consideration of the classical motion of three Coulomb particles in the total three-body Coulomb potential at asymptotically large distances. Recently [8], the electron-electron interaction has been explicitly included in the form of an asymptotic phase factor.

In a completely quantum-mechanical treatment of the impact-ionization and photoionization processes, the full symmetry of the three two-body Coulomb interactions has been taken into account [9]. In this case the three-body wave function is represented as a product of three two-body Coulomb wave functions, one for each pair of interacting particles. Each pair is considered to interact separately with a relative energy on the two-body energy shell and with electric charges unscreened by the presence of the third particle. Although this approximation has been very successful in describing angular distributions of ionized electrons, for both electron impact and photoionization [9,10], it suffers from several deficiencies. The most serious of these concerns the absolute value of cross sections obtained for low total energy of the continuum electrons. In this case it appears that the absolute values are much too low. The reason can be traced to the appearance of two-body normalization factors in the three Coulomb (3C) product wave function. The normalization factor corresponding to the repulsive electron-electron interaction goes exponentially to zero as the total energy above threshold $E = E_a + E_b = (k_a^2 + k_b^2)/2$ of the two electrons goes to zero. This exponential decrease causes the magnitude of the cross section also to decrease exponentially, a behavior which is at variance with the Wannier threshold law and with experiment.

The main result of this paper is to formulate a strategy to correct this deficiency of the 3C wave function while still maintaining the philosophy that all three Coulomb interactions should be included on an equal footing. This will be done by the introduction of effective Sommerfeld parameters in the two-body factors in the 3C wave function. The Sommerfeld parameter $\alpha = Z_1 Z_2 \mu_{12}/k_{12}$ is a measure of the strength of the Coulomb interaction between particles of charges Z_1 and Z_2, reduced mass μ_{12}, and momentum $k_{12} = \mu_{12}|\mathbf{k}_1 - \mathbf{k}_2|$ conjugate to $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. Here new Sommerfeld parameters which are functions of *all three* relative momenta will be introduced. This corresponds to the modification of a particular two-body Coulomb interaction by the presence of the third particle, the degree of modification being dependent upon the momenta of the two particles relative to the third in question. Such a modification represents a dynamic screening (DS) of the three two-body

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Coulomb interactions and hence the new wave function will be designated DS3C. The functional form of the wave function and the T-matrix element are exactly as used before [9,11,12]; only the Sommerfeld parameters in the two-body wave functions are changed. The momentum-dependent Sommerfeld parameters β_i are introduced simply by a linear transformation from the original set α_i, i.e.,

$$\beta_i = \sum_{j=1}^{3} A_{ij}\alpha_j, \tag{1}$$

where the nine coefficients $A_{ij} \in R$ and $i = a, b$ or ab designate the two-body interaction of the two electrons with the nucleus and the electron-electron interaction, respectively. In the particular case of two electrons in the field of a nucleus the original two-body Sommerfeld parameters are

$$\alpha_a = -\frac{Z}{k_a}, \quad \alpha_b = -\frac{Z}{k_b}, \quad \alpha_{ab} = \frac{1}{2k_{ab}} \tag{2}$$

for nuclear charge Z (atomic units are used throughout).

The coefficients A_{ij} must be determined on the basis of physical considerations. One condition, a generalization of that given by Peterkop [5] for a product of two Coulomb functions, is that

$$\beta_a + \beta_b + \beta_{ab} = \alpha_a + \alpha_b + \alpha_{ab} \; . \tag{3}$$

In the classical interpretation of the asymptotic motion given by Peterkop, i.e., the relative coordinates $\mathbf{r}_i = (\mathbf{k}_i/\mu_i)t$, where t is the time, the right hand side of (3) is proportional to the total Coulomb potential. Hence the transformation (1) preserves the value of the asymptotic Coulomb potential. This also guarantees the fulfilment of the boundary conditions [13]. Here the further necessary conditions will be imposed by the requirement that in the limit $k_i \to 0$ ($i = a, b, ab$) the two particles concerned interact undisturbed by the third, i.e., $\beta_i = \alpha_i$.

In this work attention will be concentrated on the symmetric case $k_a = k_b = k$ where recent data are available. Then only the limit $k_{ab} \to 0$, i.e., two electrons have zero relative momentum, arises. In addition, in the collinear configuration the electrons see an effective nuclear charge of $Z - 1/4$ as demanded by an expansion about the potential saddle in this configuration [14]. It is readily established that these conditions are satisfied by

$$\beta_a = \beta_b = -\frac{4Z - \sin\Theta}{4k} \tag{4}$$

and

$$\beta_{ab} = \frac{1 - \sin^2\Theta}{2k\sin\Theta}, \tag{5}$$

where $\Theta = (\cos^{-1}\hat{\mathbf{k}}_a \cdot \hat{\mathbf{k}}_b)/2$ varies from $\pi/2$ (collinear configuration) to zero (electrons emerging parallel with the same energy). Note that when $\Theta = \pi/2$, $\beta_{ab} = 0$. Hence when the nucleus is between the two electrons the electron-electron interaction is subsumed completely in an effective electron-nuclear interaction. As Θ decreases from $\pi/2$ to zero the nucleus moves off the interelectronic line and the electron-electron interaction is slowly switched on, reaching its unscreened value for $\Theta = 0$.

It will now be shown that calculations on $(e, 2e)$ collisions using the DS3C wave function with the Sommerfeld parameters (4) and (5) give excellent agreement with *absolute* experimental data. In addition, a recently observed new feature, a deep minimum in $(e, 2e)$ cross sections, which is not predicted by distorted-wave calculations, is reproduced for the first time using the DS3C wave function.

Since the only absolute data available are on helium, it is necessary to introduce one free parameter, an effective charge Z_{eff} for the motion of the electrons in the He^+ core. We stress that this is the only parameter in the theory. The T-matrix element is the same as used in Refs. [11,12], where the perturbation potential in the incident channel is the Coulomb interaction with the nucleus and both helium electrons; one is ionized and the other remains in its ground state.

In Fig. 1 is shown the collinear equal-energy-sharing triply differential cross section (TDCS) at 2 eV above threshold as a function of the angle of the interelectronic axis with respect to the beam direction. The data are absolute and the theory is in excellent agreement in both magnitude and shape. The singlet and triplet cross sections are shown also, the latter being zero at $\theta = \pi/2$, from symmetry requirements. In the inset is shown the cross section calculated with the original 3C wave function [11,12]. Not only is the cross section more than 3 orders of magnitude too small, but also the subsidiary maximum centered around $\pi/2$ is absent.

In Fig. 2 the cross section for equal-energy sharing 2 eV above threshold is shown for the arrangement where θ_a is fixed at 330° and θ_b varied. The cross section is vanishingly small for parallel emission and again there is excellent agreement with absolute data. In particular a small shoulder around $\theta_b = \pi/2$ is reproduced.

Murray and Read [15,16] have recently measured equal-energy, equal-angle cross sections for varying angles ψ of the incident beam to the plane spanned by $\hat{\mathbf{k}}_a$ and $\hat{\mathbf{k}}_b$. The angle ψ was varied between zero (coplanar geometry) and $\pi/2$ (equatorial geometry). In particular they observed, for $\psi = 67.5°$, a remarkably deep minimum near $\theta = 70°$, where 2θ is the relative angle of the two emerging electrons. The origin of this dip has remained unexplained and in particular does not appear in distorted-wave theories. However, in Fig. 3 it is shown that the minimum for incident energy 64.6 eV, final electron energy 20 eV, and $\psi = 67.5°$ is reproduced by the DS3C wave function. The calculations show that the dip is a true zero, itself remarkable since the T-matrix element is a sum of different interactions between the four particles involved in the collision. The theoretical and experimental minima are not quite coincident but in

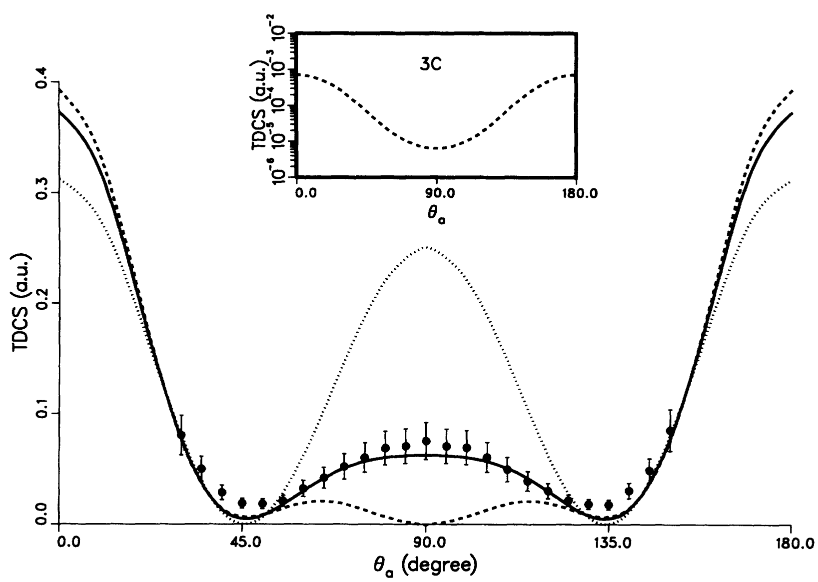

FIG. 1. The TDCS for collinear configuration with $E_a = E_b = 1$ eV, as a function of the angle of the interelectronic axis with respect to the beam direction. Continuous line: calculations using the DS3C wave function; singlet (dotted line) and triplet (dashed line) cross sections are also shown. The inset shows the results with the 3C wave function. The experimental data are taken from Ref. [2].

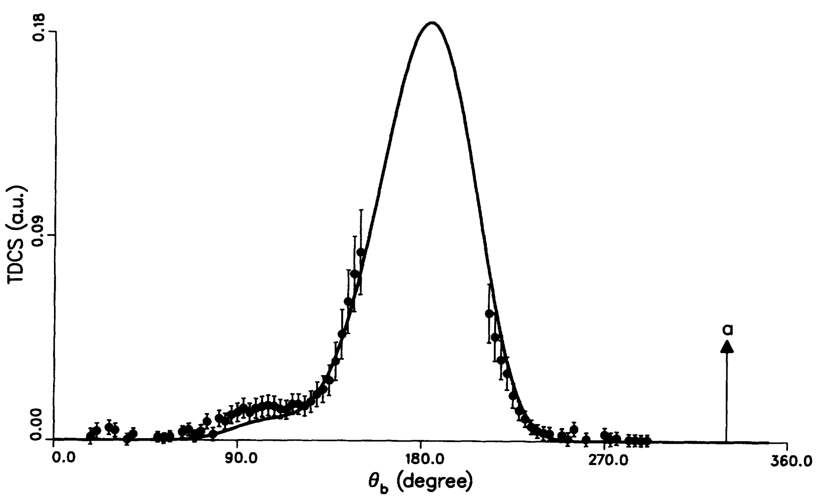

FIG. 2. As Fig. 1 but with $\theta_a = 330°$ fixed (which is designated by the arrow) and θ_b variable.

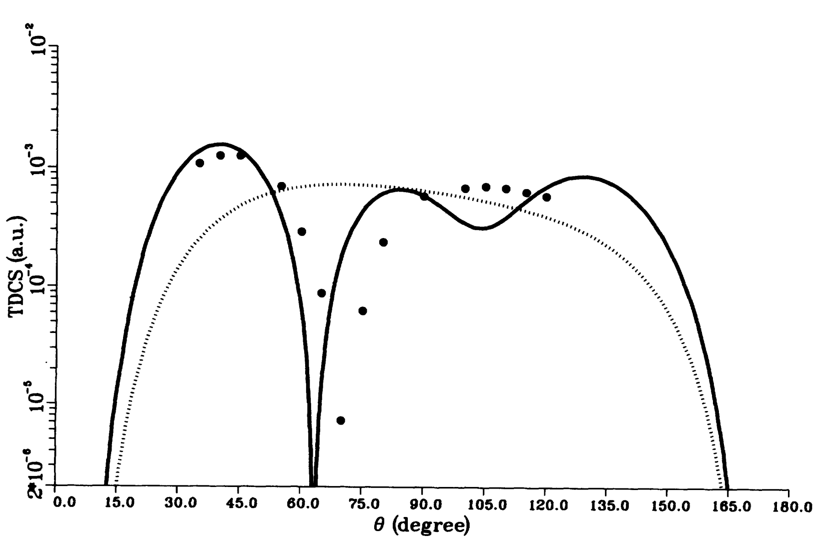

FIG. 3. The experimental results for $He(e,2e)He^+$ with $E_a = E_b = 20$ eV from Ref. [16] compared with calculated TDCS using the DS3C (continuous line) and 3C (dotted line) wave functions. The data have been normalized to theory at $\theta = 90°$.

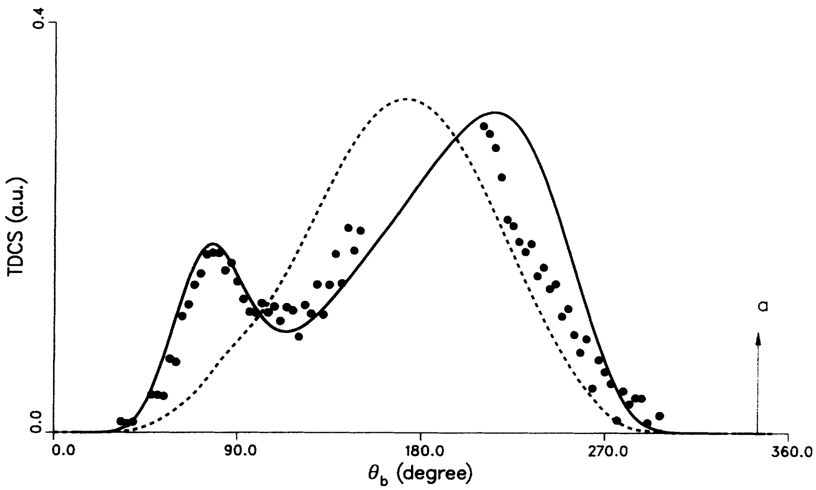

FIG. 4. TDCS for ionization of hydrogen with $E_a = E_b = 6.8$ eV, $\theta_a = 345°$, and θ_b variable. Continuous line: results using DS3C wave function. Dashed line: results using 3C wave function. Data are from Ref. [17].

view of the sensitivity of the dip position (e.g., to the initial-state wave function used) in the theory and the fact that the experimental resolution is $\approx 6°$, the agreement should be considered satisfactory. Also shown in Fig. 3 are the results using the 3C wave function where the deep minimum is completely absent.

In the case of an atomic hydrogen target the data are not absolute and theory and experiment must be normalized to each other. Previous calculations [17] using the 3C wave function showed qualitative agreement with the data but certain details were not reproduced. For example, as shown in Fig. 4 for the case of $E_a = E_b = 6.8$ eV with $\theta_a = 345°$ (designated by the arrow in Fig. 4), only a single peak arises in the 3C calculations, in disagreement with experiment. The new calculation, however, reproduces also the subsidiary peak near $\theta_b = 80°$. This peak arises from the electron-electron scattering contribution to the T-matrix element.

In summary, it has been shown that a new approach to the three-body Coulomb continuum, in which the two-body Coulomb interactions involve Sommerfeld parameters dependent upon all three relative momenta, gives absolute $(e, 2e)$ cross sections in excellent agreement with experiment. This modification of the symmetric 3C wave function has removed its major deficiency (namely, the inability to predict absolute cross sections near threshold) and significantly improved the agreement with the detailed shape of angular distributions. We have performed more extensive calculations than are shown here for different geometries and in all cases have achieved agreement with experiment. Further, it has been shown here that a recently observed deep minimum in equal-energy, equal-angle $(e, 2e)$ cross sections is reproduced. Its origin appears to be not kinematic but to arise from a quantum interference between the various two-body Coulomb interactions contributing to the ionization amplitude.

It should be remarked that in a recent paper Alt and Mukhamedzhanov [13] showed that a correct description of the asymptotic region where two particles are close together but far away from the third leads to the introduction of position-dependent relative momenta. Our approach is very similar in philosophy to theirs and indeed it can be shown that in the Peterkop interpretation of the asymptotic motion our limits are compatible with theirs.

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