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$v/2$ electron emission in ion-atom collisions with short-range potentials

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Exact differential ionization probabilities have been calculated for inelastic ion-atom collisions in one dimension with interaction potentials of zero range. The ionization spectrum confirms the existence of the so-called $v/2$ electrons; i.e., a hump in the spectrum at a velocity close to half of the velocity of the projectile at intermediate collision energies while the customary electron-capture-to-continuum (ECC) and electron-loss-to-continuum (ELC) peaks are missing. The enhancement near $v/2$ disappears at high energies with the binary-encounter peak being the predominant feature, while shoulder structures develop near the target and projectile velocities which resemble but do not coincide with ECC and ELC peaks.

In recent years a newly discovered ionization phenomenon has gained considerable attention: the $v/2$ electrons, i.e., electrons ejected with velocities of about half the velocity of the projectile v. The traditional picture of the velocity distribution of ionized electrons was characterized by a two-center structure of electrons centered in velocity space either about the target, "direct ionization" or "electron-loss to continuum" (ELC),[1,2] or about the projectile, "electron-capture to continuum" (ECC).[3,4] These structures are closely associated with corresponding two-body final-state interactions for the ejected electrons with the target and the projectile. The binary encounter peak resulting from a head-on collision of the projectile with the electrons plays a somewhat special role in that the final state is a free electron of velocity $2v$ well separated in velocity space from either the target or the projectile and not subject to significant final-state interactions. Recent theoretical and experimental results have amended this global picture of the electron distribution by a new feature: electrons "stranded" in between the two Coulomb centers giving rise to a hump near $v/2$. "In between" refers here to both the coordinate space and the velocity space. Such a feature is clearly a true three-body effect caused by simultaneous interactions of comparable strengths of the electrons with both the target and the projectile.

First direct theoretical evidence for $v/2$ electrons was found by Olson[5] using classical-trajectory Monte Carlo (CTMC) method. He noted a considerable fraction of ejected electrons with velocities approximately equal to half the projectile velocity stranded between the projectile and target ions. In a quantum-mechanical formulation $v/2$ electrons were indirectly observed by Winter and Lin[6] in a three-center expansion coupled-state calculation. They noted that a considerable fraction of ionization probability is localized in the united-atom orbitals centered halfway in between the target and the projectile. More recently, and more clearly, CTMC calculations by Olson[7] have revealed that the ionization probability peaks at intermediate collision velocities ($v \simeq 1$ a.u.) near $v_e = v/2$ and shifts toward the target ($v_e = 0$) at higher collision velocities. Experimental evidence for $v/2$ electrons has been found, but, as of yet, is somewhat ambiguous, in part because of inherent difficulties in low-energy electron spectroscopy. Meckbach *et al.*[8] observed a narrowly focused ridge in forward direction stretching from the ECC peak down to velocities close to $v/2$ in $H^+ + He$ collisions. The height of this ridge, however, is likely to be overestimated because of experimental finite target size distortions of the spectra.[9] Olson *et al.*[10] reported on a hump near $v/2$ at angles near 20° for the same system and a shift[11] of this hump to lower velocities for He^{2+} projectiles, i.e., larger projectile charge.

Invoking their unique location in phase space a qualitative interpretation of the $v/2$ electron distribution relies on the evolution of the electrons near the saddle point between the two Coulomb centers in the exit channel. Postcollisional evolution of a wave packet centered about

the midpoint in phase space under the influence of a two-center[8] or single-center[12] Coulomb distortion has been shown to lead to a formation of a ridge in the emission spectra.

In the present communication we report on a theoretical investigation of $v/2$ electron emission in one-dimensional (1D) ion-atom collisions with zero-ranged (δ-function) potentials. While being a drastic simplification, this 1D δ-function problem has surprisingly many features in common with the 3D Coulomb problem, for example the well-known Stückelberg oscillations for quasiresonant charge transfer.[13] The major interest in the model in the present context stems from the fact that it is one of the few exactly solvable nontrivial three-body problems in quantum mechanics. This model is therefore well suited to study the $v/2$ emission which is thought to be an intrinsic three-body effect. Low-order Fadeev expansions of the three-body scattering amplitude in terms of two-body amplitudes, commonly used in 3D calculations of ionization in ion-atom collisions, on the other hand, are expected to converge only slowly (if at all) for these three-body final states. The δ potential is also of interest from a different point of view: It enables one to explore the ionization spectrum in the absence of any long-range forces, and hence, proper saddle points (in this model the saddle point is degenerated to a flat "plane"). As we will discuss below $v/2$ electron emission is present in absence of a saddle point and of long-range forces pointing to a more general mechanism being responsible for its occurrence.

Using a classical constant-velocity trajectory for the internuclear motion, $R(t)=vt$, the time-dependent "electronic" Hamiltonian for the 1D δ problem is given by (in a.u.)

$$H=-\frac{1}{2}\frac{\partial^2}{\partial x^2}-Z_P\delta\left(x-\frac{v}{2}t\right)-Z_T\delta\left(x+\frac{v}{2}t\right). \tag{1}$$

In Eq. (1) we have adopted the "center-of-velocity" (c.v.) frame. It should be noted that the solutions of the time-dependent Hamiltonian Eq. (1) are Galilean invariant if translation factors for projectile (target) centered orbitals are included.[14] Accordingly the resulting transition probabilities are independent of the chosen frame. The projectile and the target with "nuclear charges" $Z_{P,T}$ propagate with speed $v'_{P,T}=\pm v/2$ in the c.v. frame, and the hump of $v/2$ electrons is localized around the origin with momentum $k'\simeq 0$. As usual, the internuclear potential has been neglected since it gives rise only to an irrelevant phase factor in the wave function within a constant-velocity approximation. The asymptotic initial and final states are defined with reference to the "atomic" Hamiltonian

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2}-Z_{T,P}\delta(x)\right)\phi_{T,P}=\epsilon_{T,P}\phi_{T,P}. \tag{2}$$

Equation (2) possesses only the bound state with

$$\epsilon_{T,P}=-\tfrac{1}{2}Z_{T,P}^2, \tag{3}$$

and

$$\phi_{T,P}=\sqrt{Z_{T,P}}\,e^{-Z_{T,P}|x|}, \tag{4}$$

which closely resembles a hydrogenic $1s$ state, and an infinite number of continuum states. The lack of an excited bound-state spectrum points to the absence of ELC or ECC peaks because of vanishing density of states near threshold.

The time-dependent Schrödinger equation

$$H\psi(x,t)=i\frac{\partial\psi(x,t)}{\partial t} \tag{5}$$

has been solved exactly for the Hamiltonian operator [Eq. (1)][13,15] to determine the elastic and the charge-transfer probabilities. Upon slight modifications the same methods can be used to determine the differential ionization amplitude $a(k)$,

$$a(k)=\langle k(\infty)\,|\,\hat{P}(\infty)U(\infty,-\infty)\,|\,\phi_T(-\infty)\rangle, \tag{6}$$

where $U(t_1,t_0)$ is the time-evolution operator belonging to the Hamiltonian in Eq. (1). In Eq. (6) we have used the initial condition that the electron is in an atomic eigenstate at $t=-\infty$. The free-particle wave function is given by

$$\langle x\,|\,k(t)\rangle=\frac{1}{\sqrt{2\pi}}e^{ikx-k^2t/2}, \tag{7}$$

and the projection onto the continuum portion of the Hilbert space is given by

$$\hat{P}(t)=1-|\,\phi_T(t)\rangle\langle\phi_T(t)\,|-|\,\phi_P(t)\rangle\langle\phi_P(t)\,|\,. \tag{8}$$

Using standard identities for the S matrix the ionization amplitude can be rewritten as

$$a(k)=\langle\psi_k^-(0)\,|\,\psi_T^+(0)\rangle-\langle k\,|\,\phi_T\rangle\langle\psi_T^-(0)\,|\,\psi_T^+(0)\rangle -\langle k\,|\,\phi_P\rangle\langle\psi_P^-(0)\,|\,\psi_T^+(0)\rangle, \tag{9}$$

where

$$|\,\psi_T^+(0)\rangle=U(0,-\infty)\,|\,\phi_T(-\infty)\rangle, \tag{10a}$$

$$|\,\psi_{T,P}^-(0)\rangle=U(0,\infty)\,|\,\phi_{T,P}(\infty)\rangle, \tag{10b}$$

$$|\,\psi_k^-(0)\rangle=U(0,\infty)\,|\,k(\infty)\rangle, \tag{10c}$$

and $\langle k\,|\,\phi_{T,T}\rangle$ are the bound-state wave functions [Eq. (4)] in momentum space. Explicit expressions for Eq. (10a) and (10b) have been given in Ref. 13. In a similar way we find for scattering of a plane-wave subject to the boundary conditions [Eq. (10c)] as $t\to\infty$,

$$\psi_k^-(x,t)=\frac{1}{\sqrt{2\pi}}e^{ikx-ik^2t/2}+e^{ivx/2-iv^2t/8}\sum_s a_s e^{-k_s|x-vt/2|+ik_s^2t/2}+e^{-ivx/2-iv^2t/8}\sum_s b_s e^{-q_s|x+vt/2|+iq_s^2t/2}, \tag{11}$$

where the coefficients are defined through the recursion relations

$$k_{s+1}=q_s+iv,\quad q_{s+1}=k_s+iv\,, \tag{12a}$$

$$a_{s+1}=\frac{Z_P b_s}{k_{s+1}-Z_P},\quad b_{s+1}=\frac{Z_T a_s}{q_{s+1}-Z_T}\,, \tag{12b}$$

with

$$k_0=i\,|k-v/2|,\quad q_0=i\,|k+v/2|\,, \tag{12c}$$

$$a_0=\frac{1}{\sqrt{2\pi}}\frac{Z_P}{k_0-Z_P},\quad b_0=\frac{1}{\sqrt{2\pi}}\frac{Z_T}{q_0-Z_T}\,, \tag{12d}$$

The differential ionization probability of an electron with momentum k is given by

$$p(k)=|a(k)|^2. \tag{13}$$

The numerical accuracy of $p(k)$ which requires a numerical integration has been checked by calculating the total ionization probability

$$P_I=\int_{-\infty}^{\infty}p(k)\,dk\,, \tag{14}$$

which, by unitarity considerations, must equal $1-P_{\text{elastic}}-P_{\text{capture}}$.

Due to scaling properties[13] the only independent parameters in the δ model are Z_P/v and Z_T/v. Figure 1 shows the ionization spectrum for the symmetric collision system $Z_P/v=Z_T/v=1$. A broad peak near $k'\simeq 0$ ($k/v=\frac{1}{2}$) is indeed clearly visible. ECC and ELC peaks are missing as expected. This is a combined effect of the short-ranged potential and the confinement of the motion to one dimension. The position of the $v/2$ hump is slightly shifted toward the projectile by $\Delta k\simeq 0.1v$. Figure 2 shows the variation of the peak position as a function of the asymmetry ratio of the system $\gamma=Z_P/Z_T$ at a collision velocity of $v=1$. While the dependence on γ is not monotonic there appears to be an overall trend in shifting the peak position towards lower velocities (from 0.7 to 0.48) as Z_P increases. This is in somewhat surprising agreement with the shift of the classical saddle point in the 3D Coulomb problem.[11] The reason for this is not yet known. The contribution of this ionization mechanism to total ionization probability P_I as determined by integration

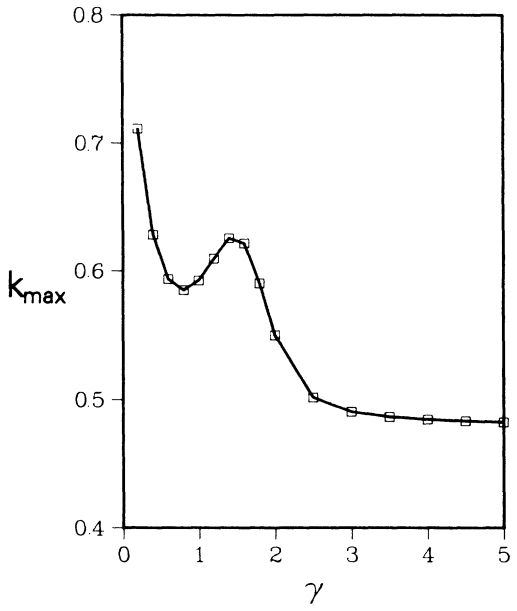

FIG. 2. $v/2$ electron peak position $k_{\max}$ (in units of v) vs the ratio of projectile and target charges $\gamma(=Z_P/Z_T)$.

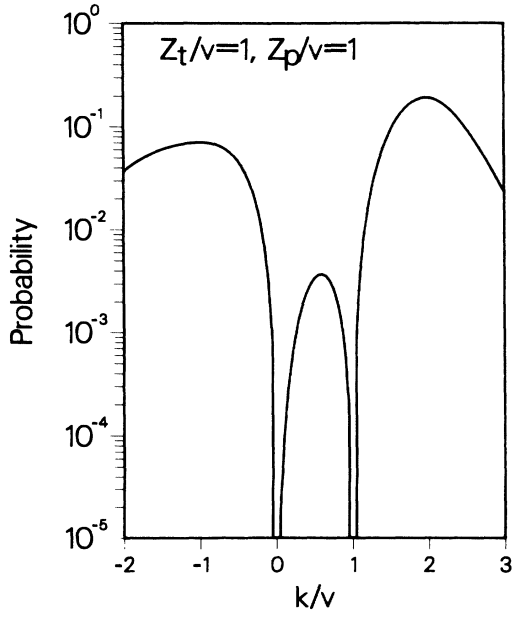

FIG. 1. Differential ionization probability vs electron momentum k (in units of the projectile velocity v). $Z_{P,T}$: projectile (target) charge. The $v/2$ electron hump is located at $k/v\simeq\frac{1}{2}$ while both ELC ($k/v=0$) and ECC ($k/v=1$) vanish.

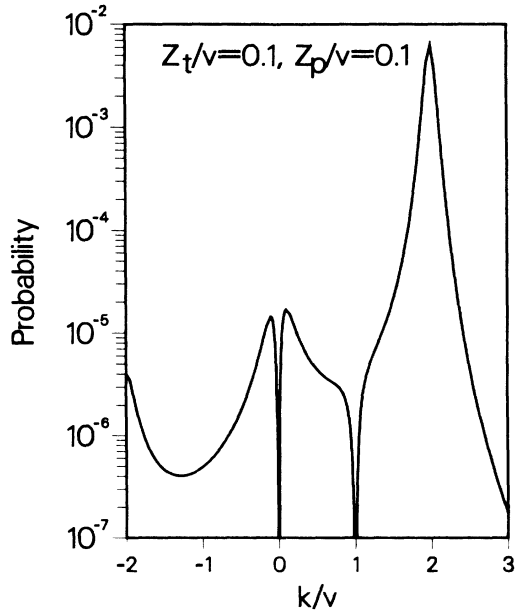

FIG. 3. Same notation as Fig. 1 except for smaller ratios of Z_T/v and Z_P/v.

over the broad peak ($-v/2 \leq k' \leq v/2$) does not exceed a few percent, indicating that the additional $v/2$ feature in the spectrum does not substantially influence the total ionization cross section for this system. In the limit of high collision velocities ($Z_P/v = Z_T/v = 0.1$) the $v/2$ electron peak disappears (Fig. 3). The binary encounter peak in the forward direction becomes the predominant feature at higher collision velocities while the emission cross section is still zero at threshold for the binary systems (electron target, electron projectile), i.e., at $k = 0$ and $k = v$. The spectrum displays now an enhancement near the projectile and target velocities which is similar but not identical to ELC and ECC peaks. In addition, structures at higher velocities in both forward and backward direction become visible, which can be analyzed in terms of a perturbative multiple scattering series.[16] We have also observed more complicated structures in the ionization spectrum at small velocities ($Z_{P,T}/v > 2$).

The occurrence of a $v/2$ emission feature independent of the range of the potential involved can be understood in terms of a quasimolecular potential-energy diagram [i.e., the static limit of the Schrödinger Eq. (1)]. The δ molecule has one binding and one antibinding state which is directly promoted to the continuum at small distances $R_c \simeq 1$ a.u. in a nonadiabatic collision. While in detail quite different, the quasimolecular orbital promotion mechanism for ionization is present both in the 1D δ problem and the 3D Coulomb problem. This mechanism is effective at small distances irrespective of the long-range nature of the potential. The low-energy portion of the quasimolecular ionization spectrum (in the c.v. frame) leads to the enhancement near $v/2$ in the laboratory frame. This ionization process at small distances can be considered to be the likely candidate for the primary mechanism generating the wave packet which is then subject to postcollisional distortion[8,12] in the 3D Coulomb problem.

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