Threshold law for the triplet state for electron-impact ionization in the Temkin-Poet model

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We derive the analytical threshold behavior for the triplet cross section for electron-impact ionization in the Temkin-Poet model. The analytical results indicate that the most recent numerical calculations may fail to reproduce the correct threshold behavior in an energy regime below about $E=0.1$ a.u. We also present an analytical expression for the energy distribution of the two electrons near threshold. [S1050-2947(97)04704-5]

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The Temkin-Poet model [1–3] for the three-body Coulomb system consisting of a nucleus with charge Z and two electrons has received considerable attention during recent years. It is also known as the s-wave model because the interaction between the electrons is replaced by its monopole part $1/r_>$ (where $r_>$ denotes the larger of the distances of each electron from the nucleus) and the single-particle angular momenta are confined to zero. It is perhaps the simplest model for a three-body Coulomb system that still retains the crucial feature of mutual long-range interactions. It has become the ideal testing ground for numerical methods that hope to describe the full three-body problem [3–7].

Early attempts to formulate a threshold law for the s-wave model concentrated on the fact that the equations of motion are separable for $r_1>r_2$ and vice versa. The basic solutions in the case of hydrogen $(Z=1)$ are products of free particle solutions for one of the electrons and Coulomb waves for the second electron. The singlet or triplet symmetry of the wave function is ensured by superimposing an infinite set of such basic solutions at a fixed total energy and enforcing the appropriate boundary condition. Based on this ansatz Temkin derived a power law proportional to $E^{1.5}$ for the singlet cross sections where E is the total energy of the two free electrons [2].

Recent time-dependent calculations for the Temkin-Poet model [9,10], however, suggest a quite different scenario for electron-impact ionization. The major part of the wave function that contributes to ionization remains confined near the "ridge" $r_1=r_2$ as it propagates outwards towards large interparticle separation. It thus shows surprising similarity with earlier time-dependent calculations for a collinear configuration of the three particles [11].

This similarity supports the idea that the Wannier picture of ridge propagation also holds for the Temkin-Poet model where the potential in the hyperangle $\alpha=\arctan(r_2/r_1)$ has the form of a cusp $\sim|\pi/4-\alpha|$ around $\alpha=\pi/4$ rather than an inverted harmonic oscillator as in the collinear configuration. It is important to emphasize that this picture of ridge propagation must be distinguished from the original Wannier analysis based on classical trajectories [12], which is not possible for the Temkin-Poet model because of the lack of ionizing trajectories in a certain energy range even above zero energy [13].

An analytical theory for the threshold behavior of ionization cross sections is not only inherently important but it is also of relevance to numerical methods with regard to the question of their convergence in the threshold region. We derive here an analytical threshold law for the ionization cross section and the single differential cross section in triplet symmetry for the Temkin-Poet model. The single differential triplet cross section is of special interest because different types of large-scale basis set calculations show good agreement in the triplet case while there are disagreements for the singlet [8]. The energy distribution for ionization in triplet symmetry at fixed total energy is thus a most suitable candidate for comparison between the analytical theory and numerical results if the latter ones are performed close enough to threshold.

A theory that incorporates the picture of ridge propagation in a purely quantum-mechanical fashion has been formulated recently [15]. Since it has already been described in detail for the special case of the singlet cross section of the Temkin-Poet model [16] we only give a brief outline for our purposes.

With the approximation of a fixed nucleus the Schrödinger equation for the Temkin-Poet model reads in hyperspherical coordinates $\alpha=\arctan(r_2/r_1)$ and $R=(r_1^2+r_2^2)^{1/2}$,

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial R^2}-\frac{1}{2R^2}\left(\frac{\partial^2}{\partial\alpha^2}+\frac{1}{4}-2RC(\alpha)\right)-E\right]\Psi(R,\alpha)=0. \tag{1}$$

The potential function $C(\alpha)$ is given by

$$C(\alpha)=\begin{cases}-Z/\cos\alpha-Z/\sin\alpha+1/\cos\alpha & 0\leqslant\alpha\leqslant\pi/4\\ -Z/\cos\alpha-Z/\sin\alpha+1/\sin\alpha & \pi/4\leqslant\alpha\leqslant\pi/2.\end{cases} \tag{2}$$

Single differential cross sections are related to the construction of adiabatic wave functions $\varphi_\mu(R;\alpha)$ at fixed hyperradius whose Schrödinger equation is given by

$$\left[\frac{\partial^2}{\partial\alpha^2}+\frac{1}{4}-2RC(\alpha)+2R^2\varepsilon_\mu(R)\right]\varphi_\mu(R;\alpha)=0. \tag{3}$$

The adiabatic energies $\varepsilon_\mu(R)$ show avoided crossings at real values of the hyperradius R. Asymptotically they converge towards the threshold energies of the scattering channels. For a sufficiently large imaginary part of the hyper-radius they connect smoothly to a single-valued function $\varepsilon(R)$ [14]. Double escape is characterized by following the system along a path in that part of the complex hyper-radius plane where $\varepsilon(R)$ is single valued. The transition probability between an initial adiabatic state to a final state in which both particles are ionized is then given by the hidden crossing theory [15] as

$$P_{\mathrm{asy}}(E)=\exp\left[-2\,\mathrm{Im}\int_{R_0}^{\infty}\sqrt{2[E-\varepsilon(R)]}dR\right]. \tag{4}$$

The path of integration starts at a small radius R_0 at the boundary of the reaction zone, which is of the order of a few bohr radii. We chose $R_0=4$ a.u. in our calculations.

Absolute values of the differential cross section $d\sigma/d\epsilon_2$ as a function of the energy ϵ_2 of one of the electrons involve an additional factor $P_{\mathrm{inner}}(E)$, which derives from contributions to the transition probability from the reaction zone at $R<R_0$. To determine $P_{\mathrm{inner}}(E)$ the adiabatic energy surface $\varepsilon(R)$ must be calculated fully quantum mechanically at small interparticle distance. However, since at small interparticle separation the Coulomb interaction dominates the total energy E, near threshold this factor is only weakly dependent on the energy and is not needed to determine the form of the threshold law. The differential ionization cross section is given by

$$\frac{d\sigma}{d\epsilon_2}(E)=\frac{d\sigma_{\mathrm{asy}}}{d\epsilon_2}(E)P_{\mathrm{inner}}(E), \tag{5}$$

where

$$\frac{d\sigma_{\mathrm{asy}}}{d\epsilon_2}(E)=\frac{\pi}{2E+1}P_{\mathrm{asy}}(E)\frac{1}{E\sin(2\alpha)}|\varphi_{\mathrm{asy}}(R_E,\alpha)|^2. \tag{6}$$

The energy distribution is determined by the absolute square of the asymptotic form of the wave function in the lowest ionization channel. The radius R_E at which $\varphi_{\mathrm{asy}}(R_E,\alpha)$ has to be evaluated is inversely proportional to the total energy and relates to the transition from the Coulomb zone where the potential energy $C(\alpha)/R$ dominates the three-particle motion to the asymptotically free zone where the escaping particles are virtually free.

Instead of taking a path in the complex hyper-radius plane the asymptotic part $P_{\mathrm{asy}}(E)$ of the transition probability can be calculated by replacing the exact $\varepsilon(R)$ by its asymptotic expansion $\varepsilon_{\mathrm{asy}}(R)$ and integrating Eq. (4) along the real axis. Formally the ionization channels emerge when the adiabatic Schrödinger equation (3) is solved for negative values of the hyper-radius. To avoid confusion with the actual physical hyper-radius R we rename it ρ.

After expanding the potential function (2) around the unstable equilibrium $x=\pi/4-\alpha=0$ and introducing a new variable

$$z=\sqrt{2}(-\rho)^{1/3}\left(\frac{\pi}{4}-\alpha\right) \tag{7}$$

the Schrödinger equation (3) for the asymptotic adiabatic wave function becomes

$$\left[\frac{d^2}{dz^2}-z-\frac{3}{2\sqrt{2}(-\rho)^{1/3}}z^2+2\Delta(\rho)\right]\varphi_{\mathrm{asy}}(z)=0,\quad z\geqslant 0. \tag{8}$$

$\Delta(\rho)$ has been introduced in connection with the asymptotic adiabatic energy

$$\varepsilon_{\mathrm{asy}}(\rho)=\frac{\sqrt{2}}{(-\rho)}+\frac{2\Delta(\rho)}{(-\rho)^{4/3}}-\frac{1}{4\rho^2}. \tag{9}$$

If the quadratic term in z is neglected, Eq. (8) becomes an equation for the Airy function, which is subject to the boundary condition

$$\varphi_{\mathrm{asy}}(\alpha=\pi/4)=0 \tag{10}$$

since the wave function for the triplet state must vanish when the electrons are at equal distances from the nucleus. A solution is the Airy function $\mathrm{Ai}(z-2\Delta)$ with $2\Delta=2.338$ independent of ρ. The value of 2Δ is chosen so that the Airy function has only one node in the hyperangle (at $\alpha=\pi/4$) that corresponds to the first excited adiabatic state $\varphi_1(R_E,\alpha)$. The corresponding wave function of Ref. [16] in the singlet case was the nodeless ground state with the boundary condition of vanishing derivative at $\alpha=\pi/4$. The change in the boundary conditions accounts for a different value of 2Δ, but otherwise the solution is unchanged. The adiabatic wave function in the hyperangle must be normalized to unity for negative values of ρ, which gives the normalization constant

$$\mathcal{N}^2(\rho)=A(-\rho)^{1/3}, \tag{11}$$

where $A=0.4912$. The contribution of the quadratic term in Eq. (8) is calculated in first-order perturbation theory, which gives the expectation value

$$\langle x^2\rangle=\frac{1.434\mathcal{N}^2}{(-\rho)\sqrt{2}}. \tag{12}$$

Inserting this result into Eq. (9), the asymptotic dependence of the adiabatic energy on ρ is

$$\varepsilon_{\mathrm{asy}}(\rho)=\frac{C_0}{(-\rho)}+\frac{C_1}{(-\rho)^{4/3}}+\frac{C_2}{(-\rho)^{5/3}} \tag{13}$$

with the numerical values $C_0=\sqrt{2}$, $C_1=2.338$, $C_2=1.057$. The dependence of the asymptotic adiabatic energy on ρ is the same as for the singlet case derived in Ref. [16] but the numerical values of A, C_1, and C_2 differ due to the different boundary condition imposed.

The adiabatic wave function at a large value of the hyperradius $R_E=4C_0/E$ is given by

$$\varphi_{\mathrm{asy}}(R_E,\alpha)=\mathcal{N}(R_E)\ \mathrm{Ai}(z_E-2\Delta) \tag{14}$$

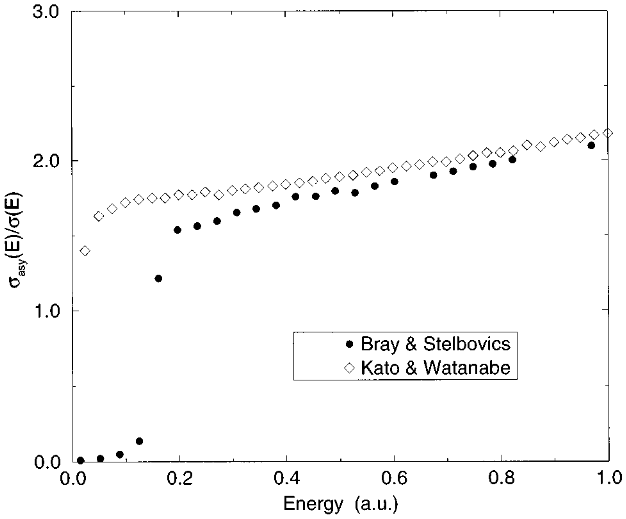

FIG. 1. Ratio $\sigma_{asy}(E)/\sigma(E)$ for the triplet cross sections in the Temkin-Poet model. The filled circles are the CCC data points from Ref. [5]. The diamonds correspond to the HSCC data from Ref. [6].

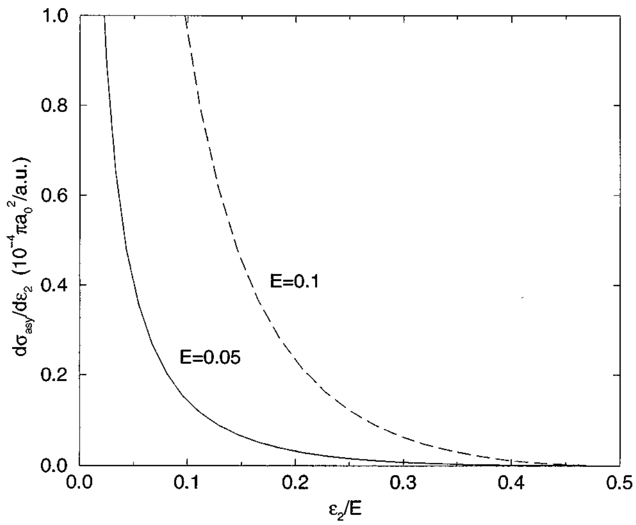

FIG. 2. Energy distribution $d\sigma_{asy}/d\epsilon_2$ as a function of the energy ϵ_2 of one of the electrons for the triplet cross section in the Temkin-Poet model. Energies: $E=0.05$ and 0.1 a.u.

with

$$z_E=\sqrt{2}\exp\left[-\frac{i\pi}{3}\right]R_E^{1/3}\left(\frac{\pi}{4}-\alpha\right). \tag{15}$$

The integral Eq. (4) is evaluated by expanding the integrand up to order $R^{-7/6}$ (in the limit $E\rightarrow 0$) inclusively using the expression (13) for the asymptotic adiabatic energy. The result is

$$P_{asy}(E)=\exp\{-\sqrt{3}[C_1 f(1/3;C_0,E)+C_2 f(2/3,C_0,E) -\tfrac{1}{2}C_1^2 g(5/3,C_0,E)]\} \tag{16}$$

with

$$f(\tau;C_0,E)=\frac{\rho_0^{-\tau}}{\tau\sqrt{2E}}\;{}_2F_1[1/2,\tau;\tau+1;-C_0/(ER_0)] \tag{17}$$

and

$$g(\tau;C_0,E)=\frac{\rho_0^{-\tau}}{2\tau\sqrt{2E^3}}\;{}_2F_1[3/2,\tau;\tau+1;-C_0/(ER_0)]. \tag{18}$$

Integrating the energy distribution over ϵ_2 or equivalently over the hyperangle gives the integrated cross section

$$\sigma_{asy}(E)=\frac{1}{2E+1}\,\frac{A}{2\sqrt{6\Delta}}\exp[2^{2/3}\sqrt{3\pi}\Delta E^{-1/6}]P_{asy}(E). \tag{19}$$

Using the limiting form of f and g as E goes to zero in Eq. (19) the threshold behavior takes the form

$$\sigma_{asy}(E)\sim\frac{1}{2E+1}\exp[-aE^{-1/6}+bE^{1/6}]. \tag{20}$$

The numerical values of the coefficients are $a=15.766$ and $b=-1.162$ for the triplet cross section. For the singlet cross section the corresponding values are $a=6.870$ and $b=2.770$ [16]. The triplet cross section is much smaller than the singlet cross section since a is more than twice as big in the triplet case. This reduction in the cross section is a consequence of the requirement that the wave function must have a node on the ''ridge'' ($\alpha=\pi/4$) in the triplet case. Note that the correction term containing b reduces the triplet cross section even further in contrast to the singlet cross section where b is positive.

The exponential threshold law in the Temkin-Poet model in contrast to the Wannier power law, which arises both in the fully three-dimensional problem [15] and in a restricted collinear configuration of the three particles [17], may be connected to the fact that in the classical version of the Temkin-Poet model ionization is forbidden in a limited energy range even above total energy zero [13], as it is well known that classically forbidden motion often leads to a quantum-mechanical law with exponential behavior in the energy.

One way to extract the contribution of the factor $P_{inner}(E)$ to the cross section is to build the ratio between the asymptotic contribution to the integrated cross section Eq. (19) and integrated cross sections taken from *ab initio* calculations. This ratio has been plotted in Fig. 1 using the data of the convergent close coupling (CCC) method of Bray and Stelbovics [5] and the hyperspherical close coupling (HSCC) method of Kato and Watanabe [6]. Figure 1 shows that at energies above $E=0.4$ a.u. both methods give quite similar results and the ratio σ_{asy}/σ depends only weakly on the energy and can be very well fitted by a linear function of the energy with small positive slope. The striking feature is a sudden drop of the ratio at $E=0.2$ a.u. for the CCC data and at $E=0.1$ a.u. for the HSCC data. In contrast, theory predicts a smooth behavior of P_{inner} near the ionization threshold [15]. We argue from this fact that the drop of the ratio near threshold may indicate the region of energy below which the *ab initio* calculations fail to converge. It is reasonable that the region of convergence extends to lower energy for the HSCC calculations compared to the CCC calculations be-

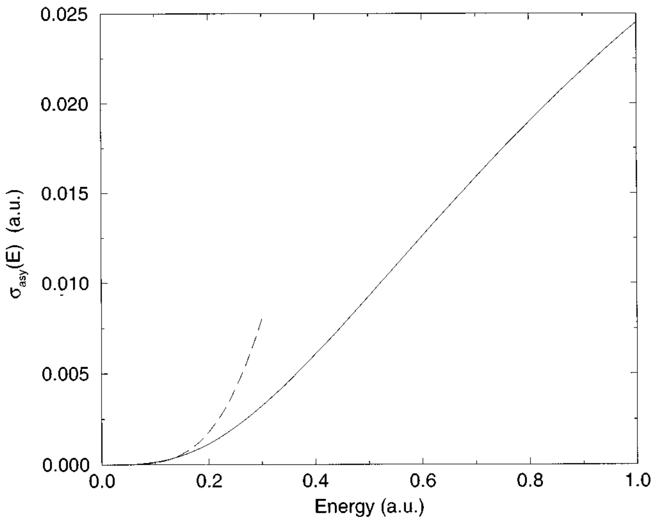

FIG. 3. Solid line: Asymptotic cross sections $\sigma_{\rm asy}(E)$ for the Temkin-Poet model in triplet symmetry according to Eq. (19). The dashed line indicates the threshold behavior given by Eq. (20).

cause the hyperspherical channel functions are better adapted to the problem in the threshold region than the independent particle basis used in the latter.

In Fig. 2 we present the asymptotic contribution Eq. (5) to the single differential cross section at two different total energies $E=0.05$ and 0.1 a.u. Note that $P_{\rm inner}(E)$ contributes with an energy-dependent part only but is independent of the hyperangle, so it does not change the shape of the energy distribution. The lowest energy for which a single differential cross section has been calculated to date for the Temkin-Poet model by *ab initio* methods is $E=1.5$ a.u. [8]. This is clearly beyond the range where the asymptotic theory presented here is valid and we therefore make no attempt to compare our results with these data. Our main result is that the asymptotic theory predicts an energy distribution that is governed by the square of an Airy function in the hyperangle.

Expression (19) for the asymptotic contribution to the integrated cross section is plotted together with the limiting behavior Eq. (20) in Fig. 3. It is seen that the threshold law only holds in a very limited energy range of approximately 0.1 a.u. One advantage of the theory presented here is that the general expression (19) for the asymptotic contribution to the cross section holds over a much wider energy range than the threshold law itself.

For future research *ab initio* calculations of energy distributions for the Temkin-Poet model and comparison with the energy distributions predicted by the asymptotic theory presented here would be most valuable.

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