Angular asymmetry of low-energy electron emission in ion-atom collisions

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We show that two factors contribute to the forward-backward angular asymmetry in low-energy electron emission by ion impact: the deviation of the target potential from a pure Coulomb potential and the two-center effect. We perform calculations with various theories that include these two effects: the continuum-distorted-wave–eikonal-initial-state (CDW-EIS) and the CDW approximations based on distorted-wave perturbation theory and a close-coupling calculation using a discrete representation of the continuum. The various theories give consistent results on the asymmetry but discrepancies remain between theory and experiment.

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The electron emission spectrum in ion-atom collisions presents characteristic features. At low electron energies, the doubly differential cross section as a function of electron energy and angle decreases slowly with increasing electron energy. It has a finite value for zero electron energy. At forward angles and when the electron velocity is equal to that of the projectile, the spectrum shows a characteristic cusp due to the ejected electron-projectile interaction. Finally, there appears, for larger electron energies and for emission angles smaller than 90°, the binary encounter peak which arises from a binary collision between the projectile and the target electron. Up to now, much effort has been devoted to the study of these structures while the low-energy part of the spectrum has been partially overlooked (see, e.g., [1], and references therein). This is due in part to the difficulties involved in accurate measurements of low-energy electrons. Still, the data of Rudd *et al.* [2] already included results for electron energies as low as 1 eV. The main interest of the low-energy electrons lies in their dominant contribution to the total ionization cross section. Theoretically it is well known that, when the residual target is an ion, any cross section differential in electron energy is finite at threshold and that low-energy electrons are mainly produced in dipolar transitions which, at high impact energies, are well represented in the first Born approximation. As the projectile energy decreases, the *two-center effect* [3], due to the influence of the projectile field on the final state of the ejected electron, becomes important even for low-energy electrons. It produces an increase of the electron yield in the forward direction and a (larger) decrease in the backward direction. This is the most significant deviation with respect to the first Born predictions. Alternatively, the latter effect has been studied at high impact energies by increasing the projectile charge [3–5].

In a recent series of papers, Suárez and co-workers have produced a set of results for the collision of 106 keV H^+ with a Ne target [6–8]. They have found a significant forward-backward asymmetry with respect to 90° electron emission, which they have assigned to two-center effects. In the present contribution we wish to discuss the origin of the forward-backward asymmetry in the angular distribution of low-energy electrons and perform quantitative calculations for confrontation with experiment.

We consider throughout a one-electron description of the target in which the target electrons move independently in a central potential (e.g., the Hartree-Fock potential of the ground state of the target atom). We analyze the angular behavior of the doubly differential cross section for ejection of an electron with final energy $E_k=k^2/2$ into the solid angle $d\Omega_k$ in terms of the expansion

$$S(\theta)=\frac{d\sigma}{dE_k d\Omega_k}=\sum_L \beta_L(k)P_L(\cos\theta), \tag{1}$$

where θ is the ejection angle with respect to the projectile velocity and P_L is a Legendre polynomial. We have verified that values of L up to $L=2$ are the most important for the present study. Higher orders are at least one order of magnitude smaller. We introduce the asymmetry parameter

$$\alpha(k)=\frac{[S(0)-S(\pi)]}{[S(0)+S(\pi)]}=\frac{\Sigma_j\beta_{2j+1}(k)}{\Sigma_j\beta_{2j}(k)}\simeq\frac{\beta_1(k)}{[\beta_0(k)+\beta_2(k)]}. \tag{2}$$

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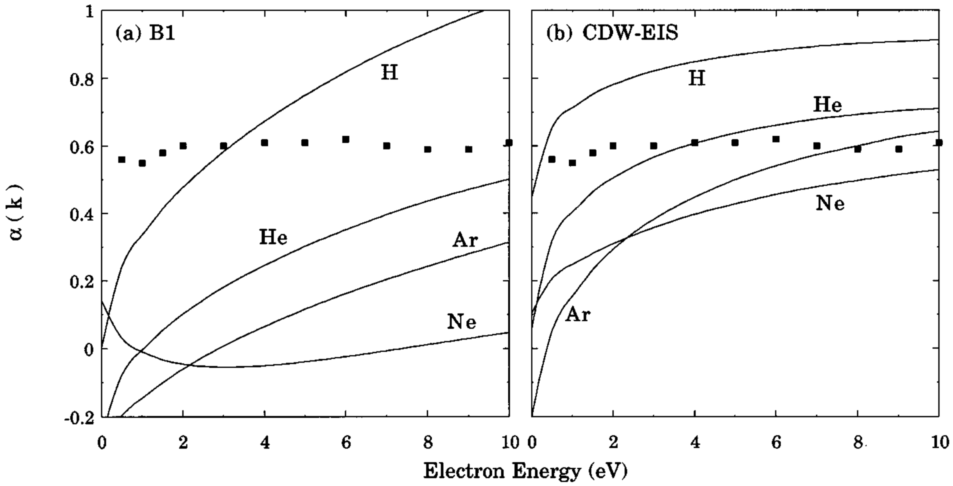

FIG. 1. Asymmetry parameter (α) as a function of electron energy for 100 keV proton impact on different targets calculated with (a) first Born and (b) CDW-EIS approximation. Full squares: experimental results for Ne from [7].

This parameter of asymmetry is more useful than, for example, (β_1/β_0), because it gives the relative importance of the asymmetric (odd) contributions in Eq. (2) with respect to *all* the significant symmetric (even) terms.

Consider first the case of the first Born approximation. The coefficients $\beta_L(k)$ may be calculated explicitly as [9]

$$\beta_L(k)=\sum_{\ell\ell'}\cos[\delta_\ell(k)-\delta_{\ell'}(k)]\begin{pmatrix}\ell & \ell' & L\\ 0 & 0 & 0\end{pmatrix}A^L_{\ell\ell'}(k). \quad (3)$$

The phase shifts $\delta_\ell(k)$ are the ones associated with the scattering of an electron with momentum k and angular momentum ℓ by the target potential. When the target potential is a pure Coulomb potential, the phase shifts $\delta_\ell(k)$ are the pure Coulomb phase shifts $\delta^c_\ell(k)$ and one gets

$$\lim_{k\to 0}[\delta^c_\ell(k)-\delta^c_{\ell'}(k)]=(\ell-\ell')\pi/2. \quad (4)$$

Therefore, due to the properties of Wigner's $3j$ symbol which is zero unless $\ell+\ell'+L$ is even, $\beta_L(k)$ is zero in this limit for odd values of L and the distribution of ejected electrons is symmetric around 90°. It has been shown by Burgdörfer [10] that this is due to the particular symmetry of the Coulomb problem. For nonzero ejection energies, the pure Coulomb phase shift $\delta^c_\ell=\Gamma(1+\ell-\mathrm{i}/k)$ varies rapidly with k. Then, odd terms in the expansion (1) are no longer zero and a forward-backward asymmetry develops. Any approximate treatment of the target which makes use of a pure Coulomb potential for the definition of the final continuum state (even with an effective charge) yields the same result, independently of the approximation for the initial bound state of the target electron.

However, if the ejected electron does not move in a pure Coulomb field, as is the case for any multielectron target, $\delta_\ell(k)=\delta^c_\ell(k)+\sigma_\ell(k)$ where $\sigma_\ell(k)$ is the additional phase shift caused by the deviation of the target potential from a pure Coulomb one. As a consequence, $\beta_L(0)$ is usually different from zero *even for odd values of L* and the Born approximation gives a forward-backward asymmetry in the angular distribution when $k\to 0$, in contradiction with what has been assumed in previous discussions of the problem. This is shown in Fig. 1(a) where we give $\alpha(k)$ for various atoms calculated in the first Born approximation with a Hartree-Fock-Slater (HFS) description of the target. As we have shown above, this parameter is zero at the ionization threshold for H targets. At 0.5 eV, which corresponds to the lowest energy measured in the experiments, we observe that the first Born approximation gives a significant asymmetry, which increases as a function of electron energy, for all targets except for Ne, which shows a very symmetric behavior. The accuracy of our results can be checked by noting that, in view of (3), the asymmetry in the limit $k\to 0$ is directly related to the additional phase shift $\sigma_\ell(0)$. The latter is related to the quantum defect μ_ℓ through the well known relation $\pi\mu_\ell=\lim_{k\to 0}\sigma_\ell(k)$ which allows the evaluation of $\sigma_\ell(0)$ from spectroscopic data [11]. Our calculated values with the HFS potential are in good agreement with those extracted from the spectroscopic data and the use of the latter in our calculations in place of the HFS ones does not change our results appreciably. As $\sigma_\ell(k)$ varies more slowly with k than $\delta^c_\ell(k)$, the dependence of the asymmetry on electron energy for small k is determined by the Coulomb phase shift. For these two reasons the results given in Fig. 1(a) with the HFS potential should be a reliable estimate of the asymmetry in the first Born approximation.

In addition to the previous source of asymmetry, we have to account, beyond the first Born approximation, for the two-center effect which is known to be very important for angular distributions. The two-center effect is due to the fact that the ionized electron is affected by the target potential and the Coulomb field of the projectile simultaneously. It enhances the electron yield in the forward direction and depletes it in the backward direction. In view of the previous discussion, it is clear that we must account at the same time for the two-center effect *and* for the deviation of the target potential from a pure Coulomb behavior. The continuum-distorted-wave–eikonal-initial-state (CDW-EIS) approximation of [12,13] satisfies this requirement (in contrast with the previous calculations of [14,15]).

In Fig. 1(b) we present the results of our CDW-EIS calculations of the asymmetry parameter $[\alpha(k)]$ using the same HFS potential as for the first Born calculations of Fig. 1(a). From the above discussion, it is clear that the case of H targets is a particular one since the asymmetry at threshold is entirely due to the two-center effect. The comparison be-

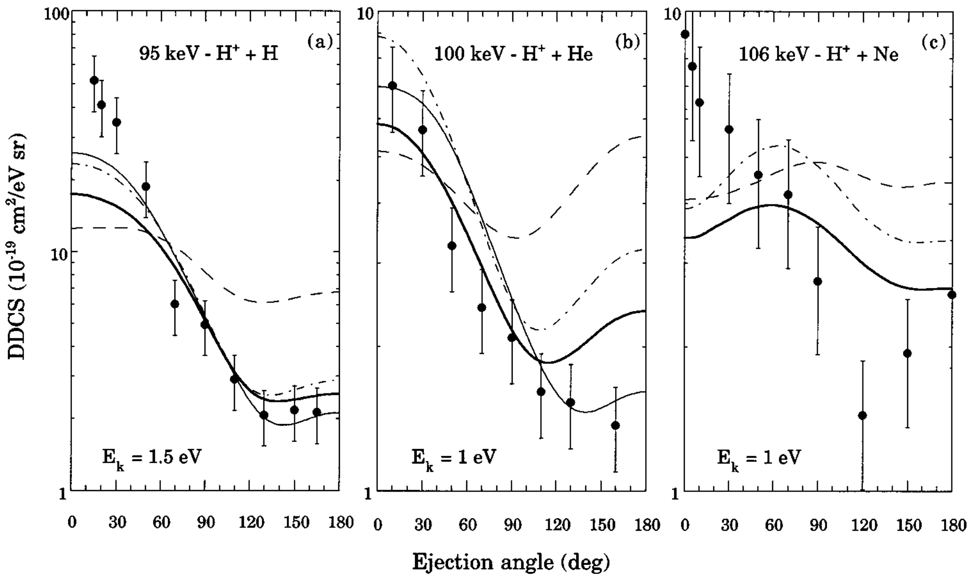

FIG. 2. Doubly differential cross section as a function of electron emission angle for proton impact on (a) H, (b) He, and (c) Ne. Theory: dashed line, first Born; thick line, CDW-EIS; dash-dot line, CDW; full line, close coupling. Experiments: (a) ●, from [17]; (b) ●, from [2]; (c) ●, from [7].

tween the CDW-EIS and first Born calculations shows that the two-center effect always increases the asymmetry. For all targets, it is already very important near the ionization threshold and gives a monotonically increasing asymmetry with increasing electron energy.

Before comparing our results with experiment, we would like to further assess the accuracy of our calculations. To this end we have also performed close-coupling calculations [16] of the doubly differential cross section for H and He targets. The calculations for He are based on an expansion over two-electron states of He including a discrete representation of the continuum. In the present work our basis sets include up to 123 one-center states with total angular momenta $L=0$–6. The same techniques as in [16] were used for the H calculations. The number of partial waves introduced at the given electron energy ensures convergence in the calculation of the doubly differential cross section (1). It has been shown in [16] that the close-coupling calculations account for the two-center effect. In addition, we have performed calculations with the CDW model that has been adapted for arbitrary targets in the same way as the CDW-EIS model through a HFS description of the target. The main difference between CDW-EIS and CDW lies in the distortion of the initial state which is an eikonal phase in the former and a Coulomb wave in the latter [1].

The results for H, He, and Ne targets are presented in Fig. 2 as a function of electron emission angle together with the experimental ones. It is remarkable that for H, the CDW-EIS, CDW, and close-coupling (CC) calculations are in good agreement in spite of the completely different status of the CC and CDW calculations (the latter being based on distorted-wave perturbation theory). The agreement is very good with experiments except in the forward direction for angles below 30°. For He the differences between theories, and between theory and experiment, is larger at backward angles although the three theoretical models show a similar asymmetry. We have done further comparisons between CDW-EIS, CDW, and CC at much higher impact energies (5 MeV/amu) for different projectiles impinging on He and obtained similar results: the agreement with the experiments from [5] is very good. For Ne we compare the results from the perturbative models with experiments. CDW-EIS and CDW give the same qualitative behavior and the same discrepancy with experiment appears at small ejection angles as for H targets. For Ne we compare in Fig. 1 the parameter $\alpha(k)$ from the CDW-EIS calculations with the experimental results [7]. Our results are in close agreement with experiment above 10 eV. Below this energy our results decrease with energy as expected for the two-center effect: the latter has always been observed to decrease when the difference in velocity between the projectile and electron increases. The nearly constant measured value is in clear contradiction with this expectation. Therefore the behavior of the experimental results can hardly be assigned to the two-center effect.

In conclusion, we have shown that the two-center effect is not the only source of forward-backward asymmetry in slow electron emission by ion impact, except for hydrogenic targets at threshold: the non-Coulomb character of the target potential induces an asymmetry even in a first Born calculation that does not include any two-center effect. Calculations in the first Born and CDW-EIS approximations including a Hartree-Fock-Slater description of the target allow extraction of information on the role of the two-center effect. The latter is very large even at threshold. The forward-backward asymmetry calculated with the CDW-EIS approximation is in fair agreement with results from a large scale one-center close-coupling calculation. Some unexplained discrepancies remain with experiment. The latter increase rapidly in the forward direction for H and Ne targets, inducing a very large asymmetry. We have shown that this result cannot be interpreted as a two-center effect and cannot therefore be assigned to any known effect.

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