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Sum rules and electron-electron interaction in two-center scattering

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The role of target-electron–projectile-electron interactions in projectile-electron loss is examined in the framework of the plane-wave-Born-approximation. The summation over target-electron states, which typically uses the closure approximation, is refined by using a sum rule for stopping power due to Bethe. The resulting expression for the cross section is compared with other modifications of the closure approximation and with the experimental H^0+H^0 electron-loss section.

I. INTRODUCTION

The ionization (or excitation) of the projectile in an ion-atom collision is, in the most frequently studied systems, due to the direct Coulomb interaction between the target nucleus and the projectile electrons. However, the target electrons can also contribute to the projectile-electron loss. The participation of the target electrons in the electron-loss process can take place in two ways: passive, when they stay in the ground state and their role in the process is restricted to screening the nuclear potential of the target; or active, when the target electrons are excited and become agents responsible for the projectile-electron loss.[1–3] These two effects of the target electrons on the projectile-electron loss have been called screening and antiscreening, respectively,[2,3] and, more recently, the active effect has been recognized as a two-center scattering correlation.[4] Experimentally these effects have been studied with interest.[5–10]

The calculation of the screening-antiscreening effects in ion-atom collisions has been carried out usually in the plane-wave-Born-approximation (PWBA) framework.[1–3,11] In this case, in the cross section, there occurs a product of two form factors, one connecting the initial and the final electron states of the projectile, and the other playing the same role for the target electrons. Because, in general, the final state of the target is not measured, it is necessary to consider all the possible target states which are excited by the projectile-electron–target-electron interactions. This is a complicated task to carry out for many electron targets. In this case, closure has been used for calculating the cross section summed over all the possible final states[2,3] to obtain manageable results.

Anholt[3] noted one defect of the closure approximation, namely that it does not take into account the threshold effect in the antiscreening (electron-electron) part of the cross section. If the target electrons were completely free, this threshold would be sharp and would be given by

$$\tfrac{1}{2}mv^2 > I_p \ ,$$

where v is the projectile velocity and I_p the excitation or ionization energy of the projectile. Essentially because of the momentum distribution in the target, the threshold is smeared out, as shown in the calculations of Ref. 1. To reintroduce the threshold in the closure approximation, Anholt proposed to multiply the antiscreening part of the cross section by $\sigma_e(v)/\sigma_p(v)$ where $\sigma_e(v)$ is the electron-induced and $\sigma_p(v)$ the proton-induced projectile excitation or ionization cross section. Although *ad hoc*, this procedure gives a good agreement with the Bates-Griffing calculations[1] away from the threshold which is artificially sharp.

Hartley and Walters[12] have proposed a different method for summing over the states of many-electron target atoms. In essence, they represent the initial target states by hydrogenic states with state-dependent effective nuclear charges (finally reduced to valence electron states in 1s orbitals with a common effective nuclear charge) and assume that target ionization is the predominant mode of excitation. The latter assumption makes their method especially applicable to rare-gas targets and indeed they obtain a good agreement with accurate calculations by Bell and co-workers[13,14] for H^0 excitation and electron loss in collision with He atoms.

II. THEORY

Within the PWBA, the use of the closure approximation to calculate projectile ionization is possible only if the summation over the final projectile states is interchanged with the integration over the momentum transfer. Unfortunately for this procedure, the minimum momentum transfer depends on the excitation energies of the target electrons. A usual approach to circumvent this difficulty is to take some kind of average over all the possible excitation energies;[2,3,12] this procedure, however, can lead to poor results, specially at energies below the cross-section maximum, as mentioned above (see Ref. 3).

The purpose of this paper is to consider more carefully this averaging procedure in order to obtain a consistent approximation for the projectile ionization (or excitation) cross section keeping the same philosophy as the closure method, which is to avoid the need for considering individually all the possible excited states of the target, as the Bates-Griffing method does.

Our starting point is the generalization of the theory of Ref. 1 developed by McGuire, Stolterfoht, and Simony[2] for He atoms as given by Anholt.[3] Assuming for simplicity that the projectile carries only one electron, the cross section for excitation or ionization of this electron is given by

$$\sigma_{sf}=\frac{8\pi}{(v/v_0)^2}\sum_n\int_{q_{\min}}^{\infty}dq\frac{1}{q^3}|F_{sf}(q)|^2 \times\left|\left\langle\phi_n\left|Z_2-\sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}\right|\phi_0\right\rangle\right|^2, \quad (1)$$

with

$$F_{sf}(q)=\langle\psi_f|e^{i\mathbf{q}\cdot\mathbf{r}}|\psi_s\rangle \quad (2)$$

and

$$q_{\min}=\frac{E_f-E_s+E_n-E_0}{\hbar v}\ . \quad (3)$$

In the above expressions $\psi_f(r)$ and $\psi_s(r)$ represent the final and initial states of the projectile, ϕ_n and ϕ_0 the final and initial states of the target, $\mathbf{r}_i$ is the coordinate of the ith target electron, E_f, E_s, E_n, and E_0 are, respectively, the corresponding energies of these states, Z_2 is the target atomic number, v is the projectile velocity, and $v_0=e^2/\hbar$ is the Bohr velocity, and q is the momentum transfer to the projectile electron. We are considering the case where the final target state is not observed and consequently the sum in Eq. (1) is over all possible target states n.

Let us define

$$q_0=\frac{E_f-E_s}{\hbar v}\ , \quad (4a)$$

$$q_n=\frac{E_n-E_0}{\hbar v}\ , \quad (4b)$$

and rewrite Eq. (1) as ($q_{\min}=q_0+q_n$):

$$\sigma_{sf}=\frac{8\pi}{(v/v_0)^2}\int_{q_0}^{\infty}dq\frac{1}{q^3}|F_{sf}(q)|^2\sum_n\left|\left\langle\phi_n\left|Z_2-\sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}\right|\phi_0\right\rangle\right|^2 -\frac{8\pi}{(v/v_0)^2}\sum_{n(\neq 0)}\int_{q_0}^{q_0+q_n}dq\frac{1}{q^3}|F_{sf}(q)|^2\left|\left\langle\phi_n\left|Z_2-\sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}\right|\phi_0\right\rangle\right|^2 . \quad (5)$$

The first term in Eq. (5) corresponds to the approximation of neglecting q_n as compared to q_0.[3,11] The sum over n was interchanged with the integral over q because q_0 does not depend on n and can be evaluated using closure and following the same steps as Ref. 3. In the second term of Eq. (5) the sum is over $n\neq 0$ because with $n=0$ the integral over q would vanish. We obtain

$$\sigma_{sf}=\frac{8\pi}{(v/v_0)^2}\int_{q_0}^{\infty}dq\frac{1}{q^3}|F_{sf}(q)|^2\left[\left|Z_2-\sum_i\langle\phi_0|e^{i\mathbf{q}\cdot\mathbf{r}_i}|\phi_0\rangle\right|^2\right] +\frac{8\pi}{(v/v_0)^2}\int_{q_0}^{\infty}dq\frac{1}{q^3}|F_{sf}(q)|^2\left[Z_2-\sum_i|\langle\phi_0|e^{i\mathbf{q}\cdot\mathbf{r}_i}|\phi_0\rangle|^2\right]-\frac{8\pi}{(v/v_0)^2}A\ , \quad (6)$$

where A represents the sum over $n\neq 0$ in the second term of Eq. (5),

$$A=\sum_{n(\neq 0)}\int_{q_0}^{q_0+q_n}dq\frac{1}{q^3}|F_{sf}(q)|^2\left|\left\langle\phi_n\left|\sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}\right|\phi_0\right\rangle\right|^2 . \quad (7)$$

This sum is usually approximated by a single term with q_n replaced by an average value when the closure method is adopted. It is our purpose to obtain a more accurate approximation for it. Before doing so, we note that the first term in Eq. (6) is the screening cross section and the remaining terms give the antiscreening cross section.

To simplify the notation, let us define

$$f(q)=\frac{|F_{sf}(q)|^2}{q^3}\ , \quad (8)$$

$$g_n(q)=\left|\left\langle\phi_n\left|\sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}\right|\phi_0\right\rangle\right|^2 . \quad (9)$$

Then, we have

$$A=\sum_{n(\neq 0)}\int_{q_0}^{q_0+q_n}dq\, f(q)g_n(q)\ , \quad (10)$$

where the following sum rules are associated with the function $g_n(q)$:

$$h(q)\equiv\sum_{n(\neq 0)}g_n(q) =Z_2-\sum_i|\langle\phi_0|e^{i\mathbf{q}\cdot\mathbf{r}_i}|\phi_0\rangle|^2\ , \quad (11)$$

$$\rho(q) \equiv \sum_{n(\neq 0)} q_n g_n(q) = \frac{1}{\hbar v} \sum_{n(\neq 0)} (E_n - E_0) \left| \left\langle \phi_n \left| \sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i} \right| \phi_0 \right\rangle \right|^2 = \frac{Z_2 \hbar q^2}{2mv} . \quad (12)$$

The last identity can be obtained using Bethe's sum rule for stopping power.[15]

Let us introduce some effective momentum transfer Δq, independent of n, which will be determined later. Equation (10) can be rewritten as

$$\begin{aligned} A &= \sum_{n(\neq 0)} \int_{q_0}^{q_0+\Delta q} dq\, f(q) g_n(q) + \sum_{n(\neq 0)} \int_{q_0+\Delta q}^{q_0+q_n} dq\, f(q) g_n(q) \\ &= \int_{q_0}^{q_0+\Delta q} dq\, f(q) h(q) + \sum_{n(\neq 0)} \int_{q_0+\Delta q}^{q_0+\Delta q+(q_n-\Delta q)} dq\, f(q) g_n(q) . \end{aligned} \quad (13)$$

Because of the negative sign in front of Δq, we consider that $q_n - \Delta q$ is small when compared with $q_0+\Delta q$, so that we can approximate Eq. (13) by

$$\begin{aligned} A &\cong \int_{q_0}^{q_0+\Delta q} dq\, f(q) h(q) + \sum_{n(\neq 0)} f(q_0+\Delta q) g_n(q_0+\Delta q)(q_n - \Delta q) \\ &= \int_{q_0}^{q_0+\Delta q} dq\, f(q) h(q) + f(q_0+\Delta q)[\rho(q_0+\Delta q) - \Delta q\, h(q_0+\Delta q)] , \end{aligned} \quad (14)$$

where advantage is taken of Eqs. (11) and (12).

To go further we choose Δq as

$$\Delta q \equiv \Delta q(q) \equiv \frac{\sum_{n(\neq 0)} q_n g_n(q)}{\sum_{n(\neq 0)} g_n(q)} = \frac{\rho(q)}{h(q)} . \quad (15)$$

Then, Eq. (14) can be rewritten as [if the argument is not specified, then $\Delta q = \Delta q(q_0)$]

$$A \cong \int_{q_0}^{q_0+\Delta q} dq\, f(q) h(q) + f(q_0+\Delta q) h(q_0+\Delta q)[\Delta q(q_0+\Delta q) - \Delta q] \quad (16a)$$

$$\cong \int_{q_0}^{q_0+\Delta q} dq\, f(q) h(q) + \int_{q_0+\Delta q}^{q_0+\Delta q+\mu} dq\, f(q) h(q) \quad (16b)$$

$$= \int_{q_0}^{q_0+\delta} dq\, f(q) h(q) , \quad (16c)$$

where $\mu = \Delta q(q_0+\Delta q) - \Delta q$ and $\delta = \Delta q + \mu$. Note that $\Delta q(q_0+\Delta q)$ means Δq *as a function of* $q_0+\Delta q(q_0)$. Then,

$$\delta = \Delta q(q_0 + \Delta q(q_0)) . \quad (17)$$

Substituting Eq. (16c) into Eq. (6) and using Eqs. (8), (9), and (11) we obtain

$$\begin{aligned} \sigma_{sf} = {} & \frac{8\pi}{(v/v_0)^2} \int_{q_0}^{\infty} dq \frac{1}{q^3} |F_{sf}(q)|^2 \left[\left| Z_2 - \sum_i \langle \phi_0 | e^{i\mathbf{q}\cdot\mathbf{r}_i} | \phi_0 \rangle \right|^2 \right] \\ & + \frac{8\pi}{(v/v_0)^2} \int_{q_0+\delta}^{\infty} dq \frac{1}{q^3} |F_{sf}(q)|^2 \left[Z_2 - \sum_i |\langle \phi_0 | e^{i\mathbf{q}\cdot\mathbf{r}_i} | \phi_0 \rangle|^2 \right] , \end{aligned} \quad (18)$$

with δ given by Eq. (17) and

$$\Delta q(q) = \frac{Z_2 \hbar q^2 / 2mv}{Z_2 - \sum_i |\langle \phi_0 | e^{i\mathbf{q}\cdot\mathbf{r}_i} | \phi_0 \rangle|^2} . \quad (19)$$

Equation (18) is our main result. The first term in this equation corresponds to the screening contribution and the second one to antiscreening. If δ is set equal to zero in Eq. (13), the results obtained using the closure approximation[3] are recovered.

In order to obtain some insight about the role played by δ in the integration limit, let us consider the low-velocity region, where $q_0 a > 1$ and where a is the target radius. In this case, a reasonable approximation for Δq can be obtained neglecting the scattering factor in Eq. (19). Thus,

$$\Delta q(q) \cong \frac{\hbar q^2}{2mv} \quad (20)$$

and, from Eq. (17),

$$\delta \cong \frac{\hbar}{2mv} \left[q_0 + \frac{\hbar q_0^2}{2mv} \right]^2 . \quad (21)$$

Using Eq. (4a), we obtain

$$q_0 + \delta \cong q_0 \left[1 + \frac{\Delta E}{2mv^2} \left[1 + \frac{\Delta E}{2mv^2} \right]^2 \right] , \quad (22)$$

where $\Delta E = E_f - E_s$.

From Eq. (22) it can be seen that when $\frac{1}{2}mv^2$ becomes

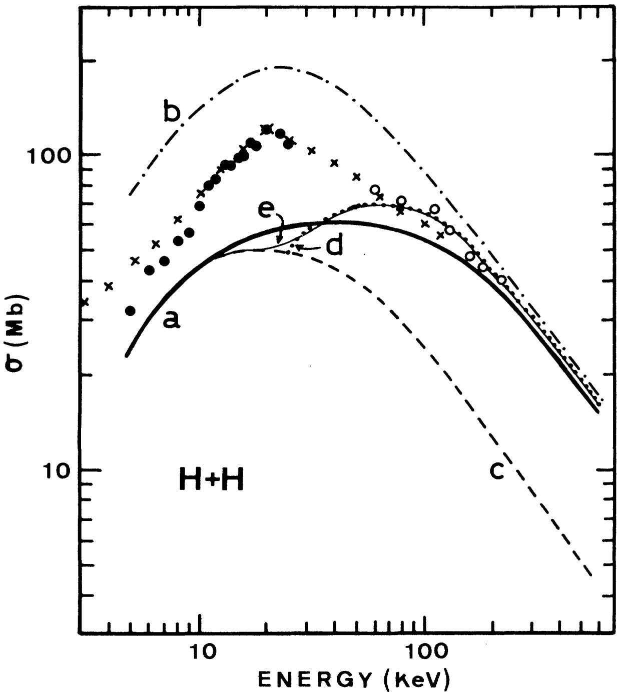

FIG. 1. Results from projectile ionization in H+H collisions. See text for the meaning of the various approximations. Thick solid curve (a) is the exact result (PWBA). Chain curve (b) is the closure approximation and the dashed curve (c) is the contribution due to screening. The dotted curve (d) is Anholt's calculation and the thin solid curve (e) shows the result from the present work [Eq. (18)]. Experiment: open circles, Ref. 16; solid circles, Ref. 17; crosses, Ref. 18. The two lowest energy points of Ref. 16 have been omitted because they appear to be incorrect (see Ref. 17).

smaller than ΔE, $q_0+\delta$ becomes significantly larger than q_0. The increase of $q_0+\delta$ reduces markedly the contribution due to the antiscreening term as the projectile velocity decreases below $\sqrt{2\Delta E/m}$. Considering the target electron as "free" in the projectile frame, the antiscreening contribution to the ionization is possible only if the target electron kinetic energy is larger than the ionization energy. Consequently, for projectile velocities such that $\frac{1}{2}mv^2 < \Delta E$, the contribution from antiscreening should be negligible. The parameter δ assures this behavior for the antiscreening term.

As an example of the above formulas and procedures, Fig. 1 displays the results for the H+H system.[1,3] In this case the exact PWBA result, Eq. (1), can be computed and it is shown by the thick solid curve. The closure approximation [Eq. (18) with $\delta=0$] is represented by the chain curve. The screening contribution [first term in Eq. (18)] is shown by the dashed curve. Comparison of the chain and dashed curves indicates that closure is a good approximation at high energies but is unable to reproduce the exact results at lower energies, which clearly comes only from the screening term. The dotted curve is Anholt's calculation showing the "kink"[10] artificially generated in this procedure. Finally, the thin solid line shows the results from the present calculations [Eq. (18)]. It can be seen that the present results are very similar to Anholt's but with a smooth transition to the region where the contribution from antiscreening is negligible. The experimental points are from Refs. 16–18. It should be noted that the data from Refs. 16 and 18 include the capture channel which partially contributes to the deviation from Bates and Griffing's calculations, specially for energies below 100 keV. Even so, the PWBA is not valid in the intermediate- and low-velocity range, below approximately 100 keV in this case.[18] The only reason we use the H_0+H_0 system is to illustrate the direct comparison with Ref. 3.

III. CONCLUSIONS

From the above results it is clear that the failure of the closure approximation at energies lower than the cross-section maximum comes from the averaging procedure of q_n adopted by this method. When a more discerning averaging procedure is considered, such as in Eq. (18), better results can be produced in all energy ranges with little computational effort and, more importantly, without the need of introducing additional terms which do not emerge naturally from the basic theory.

In the Appendix we also show that the lower limit $q_0+\delta$ found for the antiscreening term [see Eq. (18)] is nearly equal to the minimum momentum transfer for projectile electron loss by free electrons. The use of such a lower limit was suggested by Hartley and Walters[12] and, here, finds a natural explanation.

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APPENDIX

In this appendix it is shown that at high velocities ($\Delta E/2mv^2 \ll 1$) the proposed lower integration limit for the antiscreening term corresponds to the free-electron case.

The minimum momentum transfer for free-electron collisions is given by[15]

$$q_{\min}=\frac{\sqrt{2mE}}{\hbar}-\frac{\sqrt{2m(E-\Delta E)}}{\hbar}\;.$$

$$\cong\frac{\Delta E}{\hbar v}\left[1+\frac{\Delta E}{2mv^2}+\cdots\right]$$

$$\cong q_0\left[1+\frac{\Delta E}{2mv^2}+\cdots\right]\;. \tag{A1}$$

On the other hand, the approximation given by Eq. (A1) can be easily obtained from Eq. (22) by keeping only terms up to first order in $\Delta E/2mv^2$ inside the large parentheses.

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