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LETTER TO THE EDITOR

Quantal and classical correspondence of double scattering

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Abstract. Electron emission from atom–atom collisions is analysed within the framework of both quantal and classical dynamics. We examine the effect of explicit electron–electron (e–e) interactions on the ejected electron spectra in hard collisions involving simultaneous excitation and ionization in the collision of two structured atoms. A double scattering sequence represented by a second-order Born approximation has been shown to give a dominant contribution over the single scattering to projectile ionization. A classical simulation confirms the double scattering process is analogous to the Thomas two-step capture mechanism. We find good agreement between quantal and classical calculations, showing the convergence of the Born series to second order and the possibility of a classical treatment for e–e interactions in non-perturbative regimes. We also find that the shape of the ejected electron spectrum is very different from the usually assumed Lorentzian distribution.

Ionization in collisions between particles with internal atomic structures is an active field attracting considerable research interest. Many difficulties have prolonged a detailed understanding of the ionization process. In its simplest form (e.g. $H^0 \rightarrow H^0$), the collision is a four-body problem. A theoretical description faces the challenging task of treating the exit channels on both centres, including simultaneous excitation and ionization (Bates and Griffing 1954, McDowell and Coleman 1970). On the experimental side, separation of target and projectile ionization has proven to be very difficult and challenging (Heil *et al* 1991, DuBois and Manson 1986). A common practice is to extract cross sections by fitting to *a priori* distributions (such as the Lorentzian distributions).

There are two pathways leading to ionization by a structured particle impact (Wang *et al* 1991). One is the core interaction in which the electron(s) of the structured particle behave independently of the ejected electron with only 'passively' screening effects. Another one involves the explicit electron–electron interaction (correlation or two-centre electron–electron interaction, to be referred to simply as e–e interaction in this letter) (McGuire *et al* 1981, Stolterfoht 1992) which causes simultaneous excitation and ionization in a correlated fashion. While highly desirable, it is exceedingly difficult to build a theory which combines the two pathways to give a satisfactory explanation of the ejected electron spectrum over the entire angular and energy region. However, application of the core interaction alone to a subset of the spectrum produced by hard collisions has been very successful. This mechanism can explain qualitatively, sometimes quantitatively, such features like the splitting of binary encounter electron peak in the case of target ionization by partially stripped ions (Reinhold *et al* 1991), and the increasing intensity of electron loss for large angles in the backward direction for projectile ionization (Jakubassa 1980). But, as has been pointed out (Wang *et al* 1991), a component of the electron loss peak is poorly described without taking into account the e–e interaction. Subsequently, a double

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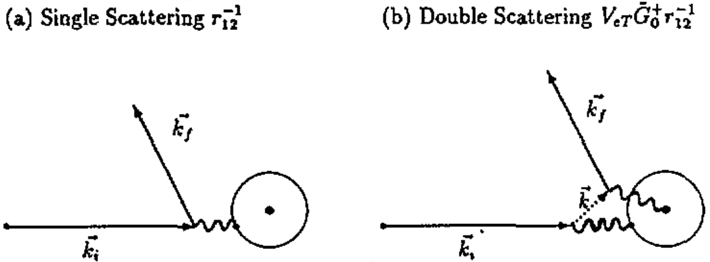
scattering (DS) mechanism has been proposed which substantially improves the agreement between theory and experiment (Wang *et al* 1992). However, accurate assessment of the DS mechanism is unavailable due to lack of direct experimental data for simple collision systems.

In this letter we present a combined study of the double scattering mechanism for electron loss in the simple system $H^0 \to H^0$ within the frameworks of quantal and classical dynamics. Our aim is to determine the importance of *e–e interaction in multiple scattering* along with how the electron spectrum is affected. We show the correspondence between quantal and classical treatment of the DS mechanism which resembles the Thomas two-step scattering originally proposed for capture in a classical picture. As will be shown below, the good agreement between the two approaches affords a direct test that the Born series has converged to second order. In addition, it also suggests the possibility of treating e–e interaction non-perturbatively in the regime where a Born series expansion criterion is violated or only marginally satisfied.

Ejection of a projectile electron to backward angles requires a large momentum transfer. For example, at a collision energy of 0.5 MeV u^{-1} ($v_p \sim 4.5$ au), a momentum transfer of $\Delta p \sim 2v_p = 9$ au is required to deflect an electron to 180°. This Δp is large compared to the typical orbital momentum width, of the order ~ 1 au. It is difficult to mediate such a large Δp involving two equal-mass electrons in a single step. In addition, in classical dynamics, an electron can be scattered only into the forward hemisphere by another electron at rest. Therefore, the contribution to the cross section in a single-step e–e scattering is expected to come from the extreme tail of the Compton profile of the target electrons that are energetic enough to scatter the projectile electron in the backward angles. As a result, the cross section is very small.


(a) Single Scattering r_{12}^{-1}

(b) Double Scattering $V_{eT}\bar{G}_0^+ r_{12}^{-1}$

Figure 1. Collision diagrams illustrating single and double scattering involving e–e interaction between the projectile electron and the target system. $\boldsymbol{k}_i$ and $\boldsymbol{k}_f$ denote respectively the initial and final momentum of the projectile electron. (*a*) Single scattering: the total momentum transfer $\boldsymbol{k}_f - \boldsymbol{k}_i$ is delivered in one step. (*b*) Double scattering: the same amount of momentum transfer is mediated via an intermediate step $\boldsymbol{k}$.

Consequently a multiple scattering approach has been proposed as the main source of the contribution to the cross section at backward angles involving e–e interaction (Wang *et al* 1992). In particular, a two-step double scattering mechanism was suggested as depicted in figure 1: the projectile electron suffers the first collision with the target electron which is excited or ionized, followed by another scattering at the target nucleus (or vice versa). The first collision slows down and deflects the electron, while the second collision is more effective in scattering the electron to large angles because of the much heavier mass of the target nucleus. Thus the momentum transfer can be achieved in two steps. This process is analogous to the Thomas double scattering (Thomas 1927) for capture where a large momentum mismatch (at high impact speeds) is better mediated via a two-step capture than a single-step direct capture. We note, however, that although the Thomas capture mechanism is proposed purely within classical mechanics and has been observed experimentally and interpreted in quantal calculations (McGuire *et al* 1982, Burgdörfer and Taulbjerg 1986), a direct confirmation of the mechanism using classical dynamics is unavailable and still attracts considerable interest (Schultz *et al* 1992). As we will show later, our study here represents a first attempt in establishing the quantal and classical correspondence of double scattering albeit for ionization.

The one- and two-step processes depicted in figure 1 can be expressed in terms of the Born series expansion

$$T_{B_1} = 1/r_{12} \tag{1}$$

and

$$T_{B_2} = T_{B_1} + 1/r_{12}G_0^+V_{eT} + V_{eT}G_0^+1/r_{12} + 1/r_{12}G_0^+1/r_{12} \tag{2}$$

where $1/r_{12}$ and V_{eT} are the interaction operators of the projectile electron with the target electron and with the target nucleus, respectively. G_0^+ is the Green's operator and r_{12} the relative coordinate between the projectile electron and the target electron. Equation (1) corresponds to the single scattering represented by the first Born approximation (B1), and equation (2) represents the double scattering in the second Born approximation (B2). Evaluation and restrictions of equations (1) and (2) can be found in Wang (1991) and Wang *et al* (1992).

For the treatment of the ionization process in classical dynamics, we use the classical trajectory Monte Carlo method (CTMC) (Abrines and Percival 1966, Olson and Salop 1977). The initial conditions are sampled randomly to resemble as closely as possible the corresponding quantal distributions in phase space. For the system under study, the classical initial momentum distributions are identical to those derived from quantum mechanics. The dynamical evolution of the four-body system is determined classically according to its Hamiltonian. At the end of evolution, the exit channels are analysed to determine what reaction has occurred.

In order to simulate the classical single and double scattering, we need to identify the characteristics of its quantal counterparts (equations (1) and (2)). For single scattering, it is straight forward to make a one to one correspondence by switching off the interaction between the projectile electron and the target nucleus ($V_{eT} = 0$) during evolution. In this case, only the e–e interaction can cause ionization. The identification of double scattering, however, can not be made in such a straightforward manner because one can not exclude either $1/r_{12}$ or V_{eT}. As we will show below, we need to examine the signature of double scattering by comparing the ejected electron spectra obtained both quantum mechanically and classically.

The calculated electron spectra of projectile ionization for simultaneous target excitation (or ionization) for $H^0 + H^0$ at 0.5 MeV u^{-1} are displayed in figure 2 for an ejection angle of 170°. The quantal results are calculated according to equations (1) and (2) for single and double scattering. Classical results are obtained within the framework of CTMC with two different procedures, as will be explained shortly. In order to take into account the contributions of various excited states of the target in the quantal calculation, a sum of the cross section over all final states of the target is performed with the closure approximation (Day 1981), excluding the ground state. Since the target excited states are continuous in the classical description, we adopt here in our CTMC results a well known procedure (Becker and MacKellar 1984) for quantization of the excited states of the target.

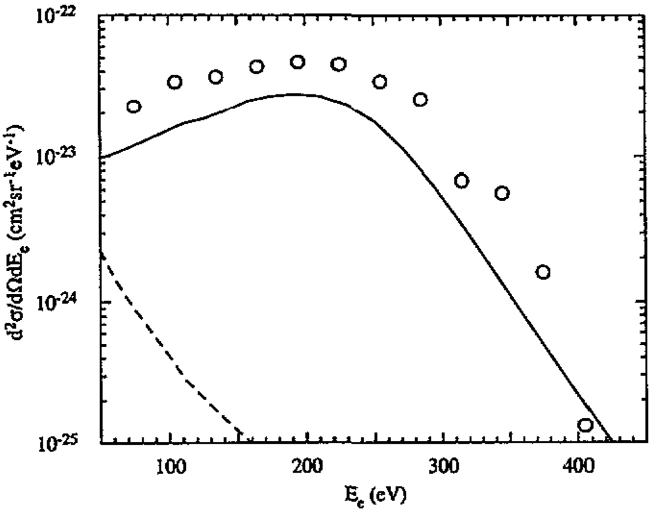


Figure 2. Cross sections of projectile ionization at 170° with simultaneous target excitation and ionization for 0.5 MeV u^{-1} $H^0 + H^0$ system. Full curve, quantal double scattering (B2); broken curve, quantal single scattering (B1); circle, four-body CTMC results.

The results in the Born approximations as shown in figure 2 have totally different behaviours for single and double scattering. The most striking feature is the large difference in the magnitude of the cross sections. The double scattering dominates over the single scattering as found previously for the H^0 + He system. It shows that the dominance is independent of the target, to be expected from the generic mechanism. The difference in magnitude increases with increasing ejection energy, which clearly demonstrates that in cases where a large momentum transfer is involved, a multiple scattering approach is preferred (Potapov 1972, Ascarelli and Tomellini 1988, Thumm 1989).

Another remarkable difference is illustrated in the shape of the emission spectrum. The double scattering curve (B2) displays a maximum. In contrast, the single scattering cross section decreases monotonically with increasing ejection energy. To understand this, we recall that the projectile electron has an initial momentum distribution given by its Compton profile centred near v_p. If we assume for a moment that the only role of the projectile nucleus is to provide the momentum distribution, we can regard the projectile electron as a wavepacket of free electrons. If the wavepacket scatters elastically on a rigid target core, we expect to see a peak around $v_e \sim v_p$ which resembles its Compton profile (Burch *et al* 1973). However, when the projectile electron must lose energy in order to excite the target, the peak structure will be skewed. This effect is especially evident for the single scattering case where no visible peak structure is present. The projectile electron loses much of its energy in a single collision with another electron in order to be deflected to large angles. But, the situation is different for double scattering in that the total momentum transfer can be delivered in two steps. In the first step the projectile electron can lose just enough energy to excite the target and be scattered in the second step by the target nucleus without further energy loss. As a result, the peak persists.

We now discuss the classical results as shown in figure 2. Due to the overall small cross sections in the backward direction, we have sampled 20 million trajectories in our CTMC calculation in order to achieve reasonable statistics. The circles are the results of a full four-body CTMC calculation. When we switch off the projectile electron–target nucleus interaction to simulate single scattering, no significant ionization events are detectable at this angle, confirming the extremely small cross sections by pure e–e scattering.

There is no ambiguity as to what operator causes the single scattering. But for double scattering, we need to be careful in making the comparison between the B2 curve and the full four-body CTMC curve. If we assume that at high impact speed, the Born series converges quickly enough so that third and higher order terms are negligible, then we can regard the full four-body CTMC results as containing contributions only up to second order. This assumption is very reasonable considering the large ratio of impact speed to the electronic orbital speed $v_p/v_{\text{orbital}} \sim 4.5$. Comparing the B2 curve with the CTMC curve, we find that both curves have a peak at about the same position. There is also good agreement in the shape which, as has been discussed above for quantal single and double scattering, is characteristic of the operator causing the ionization. In this case, contributions from higher processes must be small. Otherwise, one would expect a much different distortion of the spectrum. We conclude that the full four-body CTMC curve contains the signature of double scattering corresponding to the quantal operator (2).

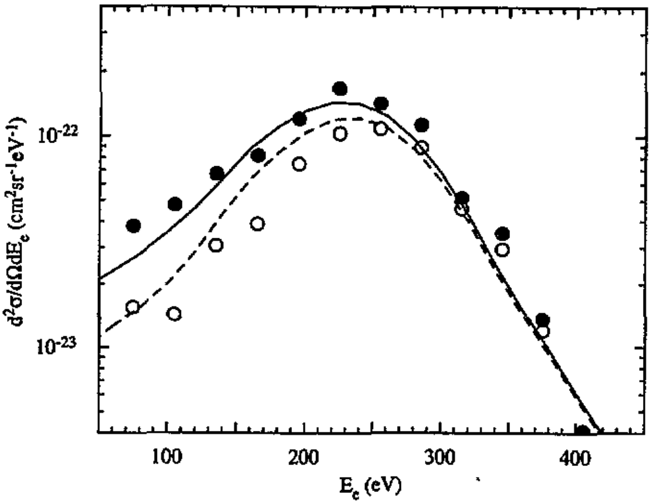


Figure 3. Total cross sections of projectile ionization at 170° in 0.5 MeV u^{-1} H^0+H^0 collisions. Full curve, quantal double scattering (B2 in figure 2) + core interaction (broken curve); broken curve, quantal results for core interaction; full circle, total classical cross section; open circle, classical results for core interaction (ground state).

To further test the convergence of the Born series, we show in figure 3 the total cross section which includes the sum of the contributions from the core interaction (when the target is in the ground state) and from e–e interaction (simultaneous excitation as displayed in figure 2). Apart from statistical fluctuations, the agreement between classical and quantal total cross sections is remarkable, especially considering the overall small magnitude of the cross sections. This directly confirms that the higher order Born terms are negligible. The good agreement may be understood as a result of hard collisions with large momentum transfers, conditions favourable to a classical description. The discrepancy between the total cross section and the cross section due to core interaction increases as the ejection energy decreases. The difference indicates how much the shape of the spectrum deviates from a Lorentzian distribution which would be predicted from the core interaction alone.

In summary, we have shown the correspondence between the classical and quantal single scattering and double scattering in projectile ionization at large ejection angles. Although e–e interaction is negligible in the first order, it contributes substantially in the second order. This suggests that in cases where e–e interaction is believed to play a role, higher order processes may also be important, especially when two electrons on two centres are involved. It is evident from figure 3 that the total ionization spectrum due to core interaction and e–e interaction has a very different shape than core interaction alone at lower ejection energies. When cross sections are to be extracted by fitting, one should modify the Lorentzian distribution which is often used in past experiments (Kövér *et al* 1988) to include the contributions from the e–e interaction.

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