

## LETTER TO THE EDITOR

# Charge transfer in asymmetric heavy-ion collisions

P A Amundsen and D H Jakubassa†

Institute of Physics, University of Oslo, Oslo, Norway

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**Abstract.** The impact parameter dependence of the capture of a target K-shell electron by a light projectile is calculated within the impulse approximation. Using a peaking approximation we show that the capture probability decreases monotonically with impact parameter. We evaluate the transfer probability in collisions of protons with C, Ne and Ar and compare with experiments.

Atomic rearrangement processes, such as charge transfer, have received much attention lately both theoretically and experimentally. It is well known that such processes cannot be adequately described by the (first-order) Brinkman-Kramers theory (McDowell and Coleman 1970 and references therein, Mott and Massey 1965). Although this theory in some cases reproduces experimental results quite well, it gives total cross sections systematically too large for large projectile velocities  $v$ . A study of the asymptotic behaviour shows that the second-order term of the Born series actually dominates at large velocities and partially compensates the first-order term (Dettmann and Leibfried 1969).

There have been several attempts to modify the Brinkman-Kramers theory by introducing second-order effects. These have been complicated by the fact that the wavefunctions of the initial and final states are not orthogonal, and thus one has to include overlap terms in the perturbation expansion (Bates 1958). This improves the agreement between theory and experiment for total cross sections (Mott and Massey 1965) at large  $v$ , but it introduces a zero in the impact parameter distribution of the transfer probability which is not observed experimentally (Cocke *et al* 1976, Horsdal Pedersen *et al* 1979).

An alternative approach to the description of charge transfer in atomic collisions is the impulse approximation (McDowell 1961, Bransden and Cheshire 1963, McDowell and Coleman 1970, Briggs 1977). In particular, in the semiclassical approximation, where the nuclear motion is treated classically, the impulse approximation may be derived as the first-order term in a systematic (Neumann) expansion of the time-dependent scattering Green's function after the weaker of the two nuclear potentials, taking care that the asymptotic behaviour of the wavefunctions remains correct. This result can be established by some minor modifications of Briggs' (1977) derivation. The theory can be formulated so that only matrix elements between eigenstates of the stronger potential occur in the calculations, without any spurious target-projectile overlap terms. Thus one can say that it is this approximation and not the Brinkman-Kramers theory that most closely corresponds to the first Born theory of ionisation.

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Consequently, this approximation should be valid not only for very swift collisions, but also for asymmetric ones, as long as molecular effects can be neglected. It should also be stressed that in a consistent semiclassical description the internuclear potential will not appear in the electronic Hamiltonian. Instead, the nuclei should follow classical trajectories of a given impact parameter. For the cases reported in this letter, this hyperbolic orbit is well approximated by a constant-velocity straight-line path.

Calculations of charge transfer within the impulse approximation have mostly been carried out for total cross sections (McDowell and Coleman 1970, Mott and Massey 1965). So far, the impact parameter dependence has only been reported for a symmetric system at rather low energies, where its validity may be doubtful (Coleman *et al* 1966). Recently, however, calculations using the method of continuum distorted waves (Cheshire 1964) have been carried out to obtain the impact parameter ( $b$ ) distribution for asymmetric systems (Belkić and Salin 1978). Also in these calculations one obtains a minimum in the  $b$  distribution, which is not present in the impulse approximation of Coleman *et al* (1966) and the physical origin of which is not clear.

In the present letter a different, and less restrictive, peaking approximation is used for the evaluation of the transition amplitude for charge transfer. In the prior form of the impact parameter formulation of the impulse approximation, which is appropriate for capture from heavy targets (charge  $Z_2$ ) by light projectiles ( $Z_1$ ), the transfer amplitude is given by (cf Briggs 1977)

$$a_{fi} = \frac{1}{i\hbar} \int dt \int d\mathbf{q} \exp[i/\hbar(\Delta E + \frac{1}{2}mv^2 + \hbar\mathbf{q}\mathbf{v})t] \times \psi_f^*(\mathbf{q}) \langle \psi_{\mathbf{q}+m\mathbf{v}/\hbar}(\mathbf{r}) | V_P(\mathbf{r}-\mathbf{R}) | \psi_i(\mathbf{r}) \rangle \exp(i\mathbf{q} \cdot \mathbf{b}). \quad (1)$$

Here, a straight line is used for the internuclear motion  $\mathbf{R}(t) = (b_x, b_y, T = vt)$ .  $\Delta E = E_f - E_i$  is the difference between the electronic energies in final and initial states  $\psi_f$  and  $\psi_i$ ,  $V_P$  is the interaction between electron and projectile and  $\psi_f(\mathbf{q})$  is the final-state wavefunction in momentum space in the projectile frame. The coupling to intermediate target continuum eigenstates  $\psi_{\mathbf{q}+m\mathbf{v}/\hbar}$  introduces an additional integral over momentum  $\mathbf{q}$ .

Using the Fourier representation of  $V_P$ , the time integral yields the  $z$  component of the momentum transferred to the electron as

$$q_z = -(\Delta E + \frac{1}{2}mv^2)/\hbar v + s_z \equiv q_0 \quad (2)$$

where  $s$  is the momentum transfer introduced by  $V_P$ . In order to carry out the  $\mathbf{q}$  integration we replace  $\mathbf{q}$  in  $\psi_{\mathbf{q}+m\mathbf{v}/\hbar}$  of equation (1) by  $q_0\mathbf{e}_z$ , making use of the fact that  $\psi_f^*(\mathbf{q})$  is strongly peaked at small  $\mathbf{q}$  especially for asymmetric systems, the oscillating behaviour of  $\exp(i\mathbf{q} \cdot \mathbf{b})$ , and further that equation (1) contains the same matrix element as occurs in ionisation theories, which is known to be mostly dependent on momentum transfer along  $\mathbf{v}$ . This peaking approximation should generally be valid when the impulse approximation itself is valid, i.e. when  $Z_1 \ll Z_2$  or for fast collisions. In particular for asymmetric systems, the weak potential  $V_P$  will not be able to change the transverse momentum components much, while  $\psi_f^*(\mathbf{q})$  will cut off all but its smallest values. For rapid collisions  $q_\perp$  will be small compared with  $m\mathbf{v}/\hbar$ .

Noting that the phase  $\exp(i\mathbf{q} \cdot \mathbf{b})$  contains only components of  $\mathbf{q}$  perpendicular to  $\mathbf{v}$  we can carry out the remaining  $\mathbf{q}$  integral:

$$\int d\mathbf{q} \psi_f^*(\mathbf{q}) \exp(i\mathbf{q} \cdot \mathbf{b}) \exp(i\mathbf{q} \cdot \mathbf{v}t) = (2\pi)^{3/2} \psi_f^*(\mathbf{R}). \quad (3)$$

We end up with the space representation of  $\psi_f$  taken at  $\mathbf{R}$ . Describing  $V_p$  by a Coulomb potential, the transition amplitude can thus be written as

$$a_{fi} = -\frac{Z_1 e^2}{i\hbar v} (2/\pi)^{1/2} \int \frac{ds}{s^2} \exp(-is \cdot \mathbf{b}) \langle \psi_{(q_0+mv/\hbar)\mathbf{e}_z}(\mathbf{r}) | \exp(is \cdot \mathbf{r}) | \psi_i(\mathbf{r}) \rangle \times \int dT \exp(-iq_0 T) \psi_f^*(\mathbf{R}). \tag{4}$$

For hydrogenic s states, the last integral can easily be performed, yielding, for example for the 1s state:

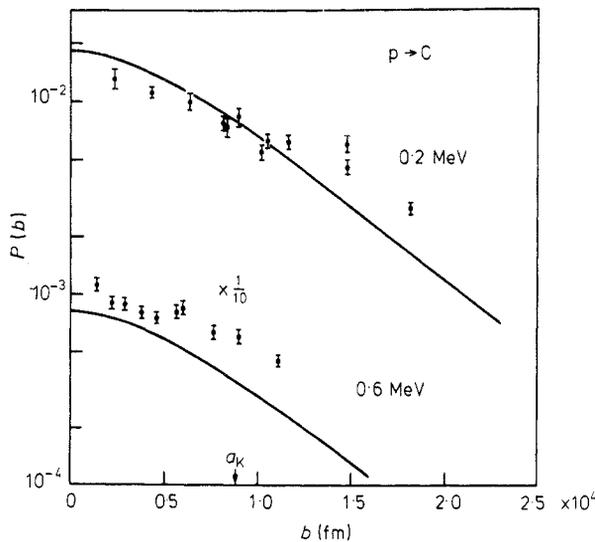
$$\int_{-\infty}^{\infty} dT \exp(-iq_0 T) \psi_f^*(\mathbf{R}) = \frac{2b\hat{Z}_1^{5/2}}{\pi^{1/2}(\hat{Z}_1^2 + q_0^2)^{3/2}} K_1(b\sqrt{\hat{Z}_1^2 + q_0^2}) \tag{5}$$

where  $K_1$  is a modified Bessel (Macdonald) function and  $\hat{Z} = Ze^2 m/\hbar^2$ . The matrix element can also be evaluated analytically (McDowell and Coleman 1970, p 364) if  $\psi_{q_0z\mathbf{e}_z}(\mathbf{r})$  is described by a Coulomb wave ( $q_{0z} = q_0 + mv/\hbar$ ). We get the final result as a two-dimensional integral

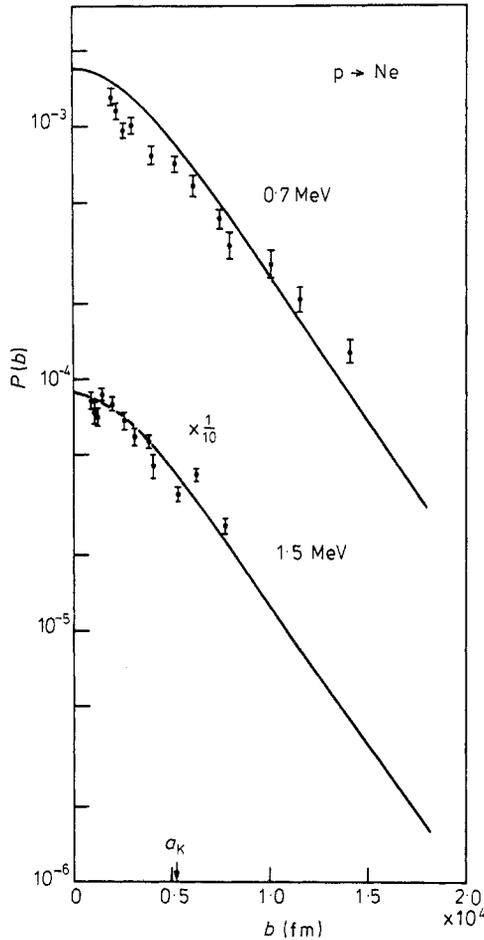
$$a_{fi} = \frac{16ie^2}{\pi\hbar v} bZ_1(\hat{Z}_1\hat{Z}_2)^{5/2} \int_0^\infty ds \int_{-1}^1 dx J_0(sx\sqrt{1-x^2}) \frac{K_1(b\sqrt{\hat{Z}_1^2 + q_0^2})}{(\hat{Z}_1^2 + q_0^2)^{3/2}} \exp(\frac{1}{2}\pi\eta)\Gamma(1-i\eta) \times \frac{[s^2 - (|q_{0z}| + i\hat{Z}_2)^2]^{-i\eta}}{N^{2-i\eta}} \left( (1+i\eta) \frac{N}{s^2 - (|q_{0z}| + i\hat{Z}_2)^2} + 1 - i\eta \right) \tag{6}$$

with  $N = \hat{Z}_2^2 + s^2 + q_{0z}^2 - 2sxq_{0z}$  and  $\eta = \hat{Z}_2/|q_{0z}|$ .

The probability  $P(b) = |a_{fi}|^2$  for charge transfer from the target K shell into the projectile 1s state is shown in figures 1-3 as a function of impact parameter  $b$ . The conversion of the measured cross section to impact parameter probabilities is performed by means of the classical relation between  $b$  and scattering angle which follows

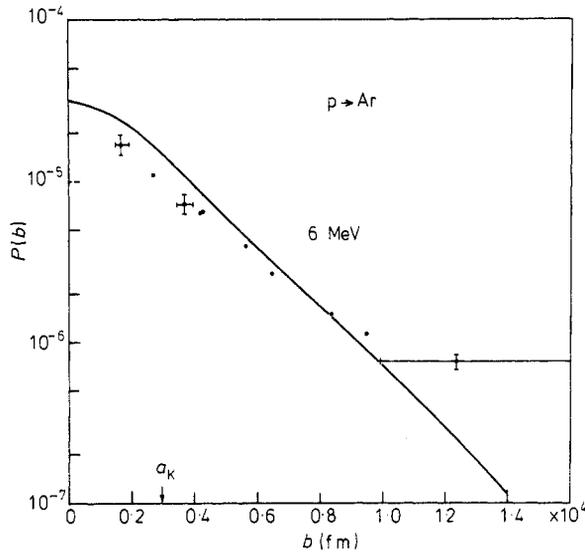


**Figure 1.** Capture probability of carbon K electrons by 0.2 and 0.6 MeV protons as a function of impact parameter. The experimental data are from Horsdal Pedersen *et al* (1979).



**Figure 2.** Capture probability of neon K electrons by 0.7 MeV and 1.5 MeV protons as a function of impact parameter. The data are from Horsdal Pedersen *et al* (1979).

from the internuclear potential, and by dividing the transfer cross section by the corresponding elastic scattering cross section. This simple procedure is valid as long as the calculated transfer amplitude does not vary rapidly with impact parameter and the corresponding angular momenta involved are large compared with  $\hbar$ . We find that  $P(b)$  decreases smoothly with  $b$  in agreement with experiment, and also the absolute values are well reproduced. Only for light targets, such as carbon, are deviations found. Partly, these are due to the use of Slater screened hydrogenic wavefunctions in our calculations. As equation (4) contains the same matrix element as occurs in ionisation theory, one can conclude from ionisation calculations (Aashamar and Amundsen 1979) that the use of more accurate wavefunctions may increase the K capture probability quite appreciably, in particular for large impact parameters and light target atoms. On the other hand, when the ratio  $Z_1/Z_2$  is not sufficiently small and the collision velocity below or comparable with the target K velocity, contributions beyond the first order in the expansion after  $V_p$  may become non-negligible, corresponding to the binding and polarisation corrections in ionisation theories (Basbas *et al* 1973, 1978). At the same time the peaking approximation also shows deviations from the full impulse approximation as may be seen from a comparison with the low-velocity calculations in symmetric systems by Coleman *et al* (1966).



**Figure 3.** Capture probability of argon K electrons by 6 MeV protons as a function of impact parameter. The data are from Cocke *et al* (1976).

The present formulation of the impulse approximation is readily extended to arbitrary  $s$ - $s$  transitions. The capture into higher shells is, however, expected to be small (Mapleton 1962, Belkić 1977).

A calculation of the  $1s \rightarrow 2s$  capture probability for the systems reported here shows a reduction by one order of magnitude compared with the  $1s$ - $1s$  transition, while the  $b$  dependence is very similar.

Finally we note that at asymptotically large impact parameters the transfer amplitude can be reduced to a double integral like equation (6) without making the peaking approximation. We found that  $P(b)$  calculated from equation (6) converges to this exact result for  $b$  very much larger than the target K-shell radius  $a_K$ . As a matter of fact, it seems quite feasible to generalise the present method to calculate  $P(b)$  with improved wavefunctions and without any peaking approximation for all  $b$ , although the calculations will be technically far more involved than those presented here.

We should like to thank E Horsdal Pedersen for directing our interest to this field and for supplying us with unpublished data.

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