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LETTER TO THE EDITOR

On the validity of the impulse approximation for electron capture in asymmetric collisions

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Abstract. For electron capture in asymmetric ion–atom collisions the projectile–target charge ratio is a natural expansion parameter. Recently Macek and Taulbjerg have claimed that the anomalies of the Coulomb T matrix introduce corrections to the impulse approximation which do not depend on this ratio. We show that this is due to the approximations they introduced, and that more accurate estimates lead to a dependence of their correction on the charge asymmetry. This correction may nevertheless be important even for rather asymmetric systems.

The problem of electron capture in asymmetric ion–atom collisions has received some attention lately, as it has become clear that this process may, after all, be quite well described by perturbation theory. If one carries out a systematic expansion of the scattering amplitude to the first order in the weaker of the two nuclear fields, retaining the stronger potential to all orders and also preserving the correct asymptotic behaviour of the initial- and final-state wavefunctions, one arrives at the so called 'second-order' Coulomb–Born (CB) approximation of Macek and Shakeshaft (1980). (The corresponding 'first-order' amplitude in their approach, which is the Brinkman–Kramers amplitude, is actually cancelled by a 'second-order' contribution.) If we consider the transfer from a heavy target (with charge Z_2) to a light projectile (charge (Z_1), the transfer amplitude can be written as an overlap between the matrix element for the target excitation to an intermediate off-shell continuum state and the (travelling) projectile final-state wavefunction. Since the amount the continuum state is off shell is proportional to the weaker potential, it is apparently consistent to replace the off-shell state by an on-shell one, which leads to the impulse approximation (IA) (McDowell 1961, Briggs 1977, Jakubassa-Amundsen and Amundsen 1980).

In the case of Coulomb potentials, however, Macek and Taulbjerg (1981) have pointed out that the replacement of the off-shell by an on-shell wavefunction may not necessarily be justified, because of the well known anomalies of the Coulomb amplitude at the energy shell (for a review see, for example, Chen and Chen 1972). By making a peaking approximation suggested by Briggs (1977), they found that there was a discrepancy between the CB and IA results which was independent of the lower nuclear charge Z_1, thus casting doubt on the consistency of the impulse approximation.

In the present letter we will investigate this problem further, making use of a less restrictive peaking approximation (Amundsen and Jakubassa 1980), which allows us to take into account both the discontinuous amplitude and the divergent phase of the

Coloumb T matrix more accurately. In the semiclassical (impact parameter) approximation (with a straight-line path for the internuclear motion, $\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}t$), the transfer amplitude at an impact parameter $\boldsymbol{b}$ and the collision velocity $\boldsymbol{v}(= v\boldsymbol{e}_z)$ can be written as

$$a_{fi}(b) = \frac{1}{\mathrm{i}\hbar} \int_{-\infty}^{\infty} \mathrm{d}t \int \mathrm{d}\boldsymbol{q}\, \exp[\mathrm{i}/\hbar(\Delta E + \tfrac{1}{2}mv^2 + \hbar \boldsymbol{q}\boldsymbol{v})t]\varphi_f^{*\mathrm{P}}(\boldsymbol{q})$$
$$\times \langle \psi^{\mathrm{T}}_{\boldsymbol{q}+m\boldsymbol{v}/\hbar}(\boldsymbol{r})|V_{\mathrm{P}}(\boldsymbol{r}-\boldsymbol{R})|\psi_i^{\mathrm{T}}(\boldsymbol{r})\rangle \exp(\mathrm{i}\boldsymbol{q}\boldsymbol{b}). \tag{1}$$

In this expression $|\psi_i^{\mathrm{T}}\rangle$ is the initial electronic state of energy E_i^{T}, $\varphi_f^{\mathrm{P}}(\boldsymbol{q})$ is the projectile final-state wavefunction in momentum space (energy E_f^{P}), $\Delta E = E_f^{\mathrm{P}} - E_i^{\mathrm{T}}$ and V_{P} is the projectile field. The only difference in (1) between the semiclassical Coulomb–Born (SCCB) and the corresponding impulse approximation (SCIA) lies in the choice of the state $|\psi_{\boldsymbol{k}}^{\mathrm{T}}\rangle$. For the SCCB this is an off-shell target continuum state with momentum $\hbar\boldsymbol{k}$ and energy

$$E_f(\boldsymbol{k}) = E_f^{\mathrm{P}} + \hbar\boldsymbol{k}\boldsymbol{v} - \tfrac{1}{2}mv^2$$

(Jakubassa-Amundsen and Amundsen 1980). In the SCIA this value is replaced by its on-shell value $E_f(\boldsymbol{k}) \to \hbar^2k^2/2m$.

While the amplitude (1) can be evaluated exactly in the SCIA theory (for final s states), the structure of the off-shell Coulomb waves makes the calculation of (1) within the SCCB rather unfeasible, and one has to resort to further approximations. In order to illustrate the difference between the peaking approximation applied by Macek and Taulbjerg (1981) and the present peaking approximation, we note that for capture into the K shell at $b = 0$ the transition amplitude can be written in both cases in a simple form

$$a_{fi}(b=0) = \frac{2^{3/2}\mathrm{i}e^2}{\hbar v} Z_1 \hat{Z}_1^{3/2} \int \frac{\mathrm{d}\boldsymbol{s}}{s^2} \langle \psi^{\mathrm{T}}_{q_0\boldsymbol{e}_z + m\boldsymbol{v}/\hbar}|\exp(\mathrm{i}\boldsymbol{s}\boldsymbol{r})|\psi_i^{\mathrm{T}}\rangle f(q_0)$$

where

$$q_0 = -(\Delta E + \tfrac{1}{2}mv^2)/\hbar v + s_z. \tag{2}$$

In this expression $\hat{Z}_i = Z_i e^2 m/\hbar^2$ and

$$\begin{aligned} f^{\mathrm{B}}(q_0) &= \delta(q_0) \\ f^{\mathrm{IP}}(q_0) &= \hat{Z}_1 \pi^{-1}(\hat{Z}_1^2 + q_0^2)^{-1} \end{aligned} \tag{3}$$

the superscripts denoting the Briggs' peaking (B) and the impulse peaking (IP), respectively. Physically Briggs' peaking essentially consists of neglecting the momentum distribution of φ_f^{P} entirely, while in our treatment only the transverse momentum transfer (with respect to $\boldsymbol{v}$) is neglected. The peaking applied by Macek and Taulbjerg is thus rather insensitive to the phase of the wavefunctions due to the simple structure of f^{B}, and they also loose the Z_1 dependence of a_{fi} that is introduced by the width of φ_f^{P} in momentum space. Both problems are, at least partially, amended by the IP approximation. Although the differences in these approximations are most easily seen for $b = 0$, the argument is actually valid for all b, as the difference between f^{B} and f^{IP} is qualitatively the same for all b.

For large momentum transfer, the ionisation matrix element will mainly depend on the short-range part of $\psi_{\boldsymbol{k}}^{\mathrm{T}}(\boldsymbol{r})$. The exact outgoing off-shell wavefunction at $\boldsymbol{r} = 0$ is given by (Okubo and Feldman 1960)

$$\psi_{\mathrm{ex}}(0)=(2\pi)^{-3/2}\int_0^1 \mathrm{d}u\left(\frac{(1-\beta+\beta/u)^{1/2}+1}{(1-\beta+\beta/u)^{1/2}-1}\right)^{-\mathrm{i}\eta_1} \tag{4}$$

where

$$\eta_1=\hat{Z}_2(2mE_f(\boldsymbol{k})/\hbar^2)^{-1/2}$$

and

$$\beta=\frac{2E_f(\boldsymbol{k})-\mathrm{i}\varepsilon-\hbar^2k^2/m}{2E_f(\boldsymbol{k})-\mathrm{i}\varepsilon}\qquad \varepsilon\to 0.$$

$\boldsymbol{k}=\boldsymbol{q}+m\boldsymbol{v}/\hbar$ and β measures the amount the wavefunction is off shell. The on-shell limit of this expression is

$$\begin{aligned}\psi_{\mathrm{ap}}(0)&=(2\pi)^{-3/2}|\Gamma(1+\mathrm{i}\eta_0)|^2(4/\beta)^{-\mathrm{i}\eta_0}\\ \eta_0&=\hat{Z}_2/k\end{aligned} \tag{5}$$

where Γ is the gamma function. We have compared (4) and (5) for values of the parameters that are relevant for the present discussion ($Z_1=1$, $\hbar v/e^2=Z_2=(10, 18)$) and found very good agreement in amplitude and a few per cent deviation in phase for the values of $\boldsymbol{q}$ that contribute significantly to the transfer amplitude. The phase agreement can be improved at the expense of the absolute value by replacing η_0 in (5) by η_1. The difference between (4) and (5) decreases as we approach the on-shell limit, i.e. as v or Z_2/Z_1 increases. Following Macek and Taulbjerg (1981) we can thus introduce

$$N_0=\psi_{\mathrm{ap}}(0)/\psi^{\mathrm{T}}_{\boldsymbol{q}+m\boldsymbol{v}/\hbar}(0)=(4/\beta)^{-\mathrm{i}\eta_0}\Gamma(1-\mathrm{i}\eta_0)\exp(-\tfrac{1}{2}\pi\eta_0) \tag{6}$$

as an off-shell correction factor for the $\psi^{\mathrm{T}}_{\boldsymbol{q}+m\boldsymbol{v}/\hbar}$ state. We note that there should be no further renormalisation of $\psi^{\mathrm{T}}_{\boldsymbol{q}+m\boldsymbol{v}/\hbar}$ as the *off-shell* Coulomb wavefunctions are well behaved (Okubo and Feldman 1960).

For the evaluation of the transition amplitude we follow closely Amundsen and Jakubassa (1980). When introducing the off-shell correction N_0 into (1) and making the peaking approximation which consists of replacing $\boldsymbol{q}$ by its z component in the continuum wavefunction one should, however, keep in mind that the neglect of the transverse components of $\boldsymbol{q}$ is not possible in the numerator of β,

$$2E_f(\boldsymbol{k})-\hbar^2k^2/m=-\hbar^2(q^2+\hat{Z}_1^2)/m$$

(for a 1s final state), as $\hat{Z}_1$ is of the same order. The $\boldsymbol{q}$ integration then gives

$$\int \mathrm{d}\boldsymbol{q}\,\varphi_f^*(\boldsymbol{q})(q^2+\hat{Z}_1^2)^{-\mathrm{i}\eta}\exp(\mathrm{i}\boldsymbol{qR})=4\pi^{1/2}\hat{Z}_1^2\frac{(2\hat{Z}_1)^{-\mathrm{i}\eta}}{\Gamma(2+\mathrm{i}\eta)}R^{1/2+\mathrm{i}\eta}K_{1/2+\mathrm{i}\eta}(\hat{Z}_1R) \tag{7}$$

where $\eta=\hat{Z}_2/|q_{0z}|$, $q_{0z}=q_0+mv/\hbar$, and K_ν is a modified Bessel function. After introducing the Fourier transform of the Coulomb field V_{P}, the time integral can also be carried out analytically

$$\begin{aligned}&\int_{-\infty}^{\infty}\mathrm{d}t\,\exp(-\mathrm{i}q_0vt)R^{1/2+\mathrm{i}\eta}K_{1/2+\mathrm{i}\eta}(\hat{Z}_1R)\\ &\qquad=\frac{(2\pi)^{1/2}}{v}\hat{Z}_1^{1/2+\mathrm{i}\eta}b^{1+\mathrm{i}\eta}(\hat{Z}_1^2+q_0^2)^{-1/2-\mathrm{i}\eta/2}K_{1+\mathrm{i}\eta}(b(\hat{Z}_1^2+q_0^2)^{1/2}).\end{aligned} \tag{8}$$

Thus the off-shell correction can easily be included in the transition amplitude which again can be written as a two-dimensional integral

$$
\begin{aligned}
a_{fi} = {} & \frac{16\mathrm{i}e^2}{\pi\hbar v} bZ_1(\hat{Z}_1\hat{Z}_2)^{5/2} \int_0^\infty \mathrm{d}s \int_{-1}^{1} \mathrm{d}x\, J_0(sb(1-x^2)^{1/2}) \\
& \times \frac{K_{1+\mathrm{i}\eta}(b(\hat{Z}_1^2+q_0^2)^{1/2})}{(\hat{Z}_1^2+q_0^2)^{1/2+\mathrm{i}\eta/2}} \frac{2\pi\eta}{1-\mathrm{e}^{-2\pi\eta}} [4m(E_i^{\mathrm{T}}+\hbar svx)/\hbar^2+\mathrm{i}\varepsilon]^{\mathrm{i}\eta} \\
& \times \frac{b^{\mathrm{i}\eta}}{\Gamma(2+\mathrm{i}\eta)} \frac{[s^2-(|q_{0z}|+\mathrm{i}\hat{Z}_2)^2]^{-\mathrm{i}\eta}}{N^{2-\mathrm{i}\eta}} \\
& \times \left((1+\mathrm{i}\eta)\frac{N}{s^2-(|q_{0z}|+\mathrm{i}\hat{Z}_2)^2}+1-\mathrm{i}\eta\right)
\end{aligned} \tag{9}
$$

with

$$N = \hat{Z}_2^2 + s^2 + q_{0z}^2 - 2sxq_{0z} \qquad x = \cos\vartheta_s.$$

Note that the singularity of the impulse approximation integrand at $q_{0z}=0$ has disappeared. On the other hand it is difficult to include the correction N_0 in the full SCIA theory (without peaking) as one of the angular integrals (over φ_s) can no longer be carried out analytically, and one would thus be left with four integrals that have to be done numerically.

In figures 1 and 2 the energy dependence of the capture cross section from the K shell of Ne and Ar into the hydrogen ground state is shown, and the present results are compared with the previous on-shell calculations. Also shown are the SCIA calculations in order to estimate the accuracy of the impulse peaking approximation. Again, Slater-screened hydrogenic wavefunctions and experimental binding energies were used. While for collision velocities higher than the target K-shell orbiting velocity the Coulomb–Born theory gives larger capture cross sections than the impulse approximation, they are reduced for lower velocities.

In figure 3 we compare the off-shell correction, i.e. the ratio of the cross sections calculated from (9) and from the corresponding on-shell theory, as a function of $\eta_2 = Z_2e^2/(\hbar v)$. We also show the analytic correction factor of Macek and Taulbjerg (1981)

$$|M|^2 = 2/\{(1+\eta_2^2)[1+\exp(-2\pi\eta_2)]\} \tag{10}$$

which only depends on the ratio Z_2/v, and not on the asymmetry Z_1/Z_2. It is seen that our results do indeed depend on Z_1/Z_2, and at high collision velocities the off-shell correction becomes less important for the more asymmetric system (p, Ar), which is consistent with the standard argument for the impulse approximation. The correction in this region appears, however, to be even larger than predicted by (10). Although the off-shell effect has the right sign for reducing the discrepancies between theory and experiment (see figures 1 and 2), it is rather large. Since the correction is dependent on Z_1/Z_2 it is, however, doubtful whether it makes sense to include this correction alone, without discussing other terms from the next order in the perturbation expansion. Furthermore, it is uncertain how much error is introduced by estimating the off-shell effects by $\psi_{\mathrm{ex}}(0)$ (or $\psi_{\mathrm{ap}}(0)$), as the off-shell wavefunctions are not proportional to the on-shell ones. Taking $\psi(r_{\mathrm{ad}})$, where the 'adiabatic' radius is defined by $r_{\mathrm{ad}} = \hbar v/(\Delta E + \frac{1}{2}mv^2)$, might be more appropriate, but even then the spatial variation of the off-shell wavefunction would be neglected.

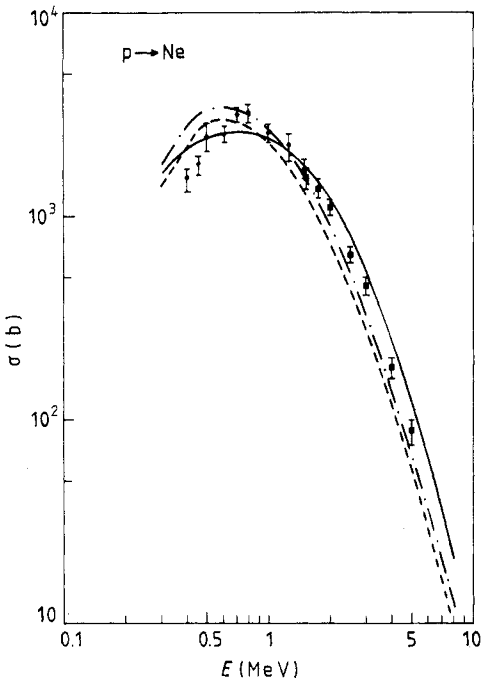

Figure 1. The cross section for the capture of Ne K-shell electrons by protons as a function of projectile energy. The full curve denotes the present SCCB result, the broken curve is the SCIA peaking approximation, and the chain curve shows the full SCIA. The data are from Rødbro *et al* (1979) (⧳) and from Cocke *et al* (1977)(▮).

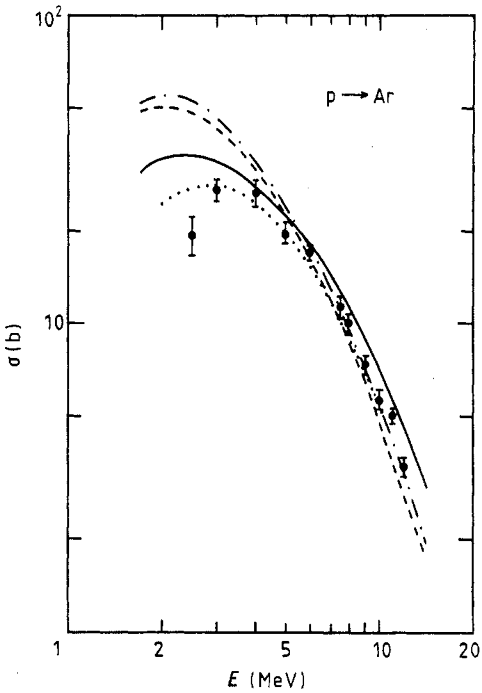

Figure 2. The cross section for the capture of Ar K-shell electrons by protons as a function of projectile energy. The full curve denotes the present SCCB result, the broken curve is the SCIA peaking approximation, the chain curve shows the full SCIA and the dotted curve is the CB result from Macek and Taulbjerg (1981). The data are from MacDonald *et al* (1974).

At lower collision velocities, around the maximum of the cross section, the off-shell corrections become smaller than predicted by the Macek–Taulbjerg formula (10). In this energy region that formula is, however, hardly applicable, as Briggs' peaking ceases to be valid (Jakubassa-Amundsen and Amundsen 1980). It is actually fortunate that

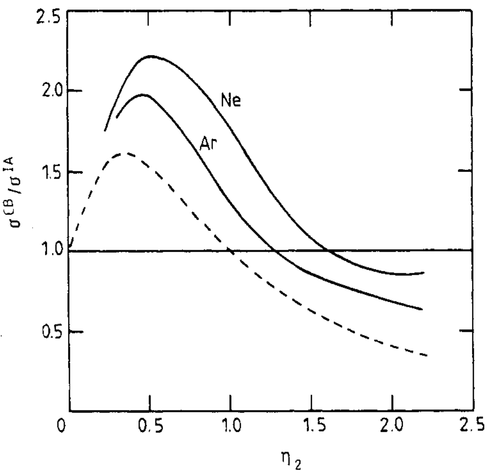

Figure 3. Ratio of capture cross sections calculated with the SCCB and the SCIA peaking theory, respectively, as a function of $\eta_2 = Z_2e^2/(\hbar v)$. The full curves are the present results for K-shell capture from Ne and Ar by protons, and the broken curve is the universal factor $|M|^2$ from Macek and Taulbjerg (1981).

the dependence on the continuum wavefunction seems to be so small in this region, because the approximations are rather crude at these collision velocities. The significance of the fact that the correction for Ar appears to be larger than for Ne in this region is thus hard to evaluate. Only the fact that the ratio of the SCCB and the SCIA is smaller than indicated by (10) seems to be assured.

We also studied the impact parameter dependence of the capture probability calculated with off-shell and on-shell wavefunctions, respectively. For all collision energies the difference in the shape of the impact parameter distributions was found to be small, with the off-shell calculations falling off somewhat more slowly at large b.

We conclude that although an improved wavefunction for the intermediate state may change the capture cross section by up to a factor of two in the energy range where the impulse approximation should be valid, it is not justified to consider the off-shell correction in isolation without taking other higher-order corrections into account, as they arise from a second-order expansion in terms of the weak field.

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