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Full first Born approximation for inner-shell pickup in heavy-ion collisions

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We have calculated K-shell pickup cross sections using the full first Born approximation developed by Jackson and Schiff for a number of heavy-ion collisions for which experimental data have recently become available. These include protons on argon at a range of velocities and fully stripped ions $Z = 1, 6, 7, 8, 9$, on argon at three velocities. The calculations attempted to include the effect of screening by target electrons with a crude effective potential. We conclude that the full first Born charge-exchange cross section gives nonphysical results for the systems examined, thus casting further doubt on the theoretical significance of the good agreement with experiment one obtains for protons on hydrogen.

Recent calculations[1] have shown that the anomalous projectile charge dependence of target K x-ray yields due to collisions with fast stripped ions could be explained by considering K-shell pickup to a bound state of the projectile as a competing process to ionization in K-vacancy formation. This conclusion is of particular interest not only because it explains the physical processes entering into the experimental vacancy formation rates but also because it affords another relatively simple testing ground for examining three-body rearrangement collisions. This is true because the relatively high nuclear charge of target atoms such as argon ensure that the K-shell electron wave function is nearly hydrogenic and that the effects of the other target electrons can be dealt with reasonably in terms of binding energy corrections, and a static screening potential for the projectile interaction. By sending in fully stripped projectiles we have a means of testing three-body rearrangement collisions over a wide choice of projectile and nuclear charges. Even for protons on argon, where ionization easily dominates the K-vacancy formation rate, pickup can be measured by means of coincidence techniques.[2]

Finding a good approximation for calculating three-body rearrangement collisions is still a major problem in atomic physics as witnessed by the continuing proliferation of such calculations for the simple case of protons on hydrogen,[3] a true three-body collision that has been the subject of intensive experimental study as well. Even as simple a calculation as the plane-wave first Born approximation is the subject of unresolved theoretical controversy. Brinkman and Kramers[4] (BK), arguing on physical grounds, used a truncated form of the Born approximation in which only the electron projectile interaction is retained in the "prior" (or "post") perturbing potential. The results overestimate the measured cross sections by a considerable amount although they give the energy dependence fairly well. Jackson and Schiff[5] (JS) have included the projectile–target-nucleus interaction in their first Born calculation, and due to an interference between this amplitude and that of Brinkman and Kramers, get good agreement with experiment for protons on hydrogen. The theoretical justification for keeping or omitting the projectile–target-nucleus interaction has been discussed by many authors over the years, from the point of view of high-energy limits,[6] distorted-wave formalisms,[7] variational derivation of a plane-wave approximation,[8] vanishing (to $\sim m/M$) of the exact amplitude if *only* the projectile–target-nucleus interaction is turned on,[9] and others. Calculations involving higher-order Born terms,[10] higher-order distorted-wave terms,[11] and time-dependent two-state techniques[12] have also been used to obtain better agreement with experimental total cross sections, and to help clarify the theoretical questions.

Thus the availability of essentially three-body systems involving projectiles and target nuclei with a variety of charges provides a new testing ground for all such approximations. In this paper we will demonstrate that the Jackson-Schiff "full" first-order plane-wave Born approximation can be eliminated as a meaningful lowest-order approximation for rearrangement collisions by comparing it to already available experiments in the high-charge domain.[13] In Sec. I we present briefly the theoretical development of the full first Born approximation; in Sec. II we compare numerical results with experiment, and present a scaling argument to explain these results. In Sec. III we present our conclusions.

I. THEORY

We consider a bare projectile of charge Ze impinging on a neutral atom of nuclear charge $Z_m e$ as shown in Fig. 1. The full first plane-wave Born amplitude can be written in the form

$$B_{if} = \int d^3R_{10}\, d^3R_{12} \exp(i\vec{R}_{10}\cdot\vec{A} - i\vec{R}_{12}\cdot\vec{B})\psi_f^*(\vec{R}_{12}-\vec{R}_{10}) \times\left[U_{02}(R_{02}) + W(R_{01}) + \int d^3R\, \rho'(\vec{R})U_{02}(\vec{R}-\vec{R}_{10})\right] \times \phi_i(\vec{R}_{12}), \quad \hbar = c = m_e = 1, \tag{1}$$

where U_{02} is the interaction potential of the active electron with the projectile, W is the interaction potential of the target nucleus with the projectile, ρ' is the electron charge density of the target atom less that of the active electron, and ϕ_i and ψ_f are the initial and final bound-state wave functions of the active electron. Also

$$\vec{A} = \vec{P} - \frac{M_0}{M_0+1}\vec{Q}, \quad \vec{B} = \frac{\vec{P}}{M_1+Z_m} + \frac{\vec{Q}}{M_0+1}, \tag{2}$$

where

$$P = \mu_i \vec{v} \tag{3a}$$

is the initial momentum of colliding system (c.m.),

$$Q = \mu_f \vec{v}' \tag{3b}$$

is the final momentum of colliding system,

$$\mu_i = \frac{M_0(M_1+Z_m)}{M_0+M_1+Z_m}, \quad \mu_f = \frac{(M_0+1)(M_1+Z_m-1)}{M_0+M_1+Z_m}, \tag{4}$$

and M_0 and M_1 are the projectile and target-nucleus masses, respectively.

Equation (1) is obtained in the following approximation, starting from a rigorous development: (a) independent-particle model used for target electron wave function, (b) momentum transfers of order A/M_1 neglected, (c) final state of residual atomic electrons not changed, (d) electron exchange terms in the pickup amplitude ignored. All the electron coordinates except those of the active electron (2) are integrated over. Equation (1) is just what one gets if one considers the problem to be a three-body interaction except that the projectile sees a screened target nucleus with screening density ρ', to account for the passive electrons.

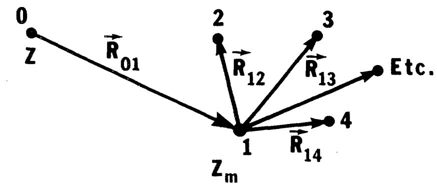

FIG. 1. Coordinate system for pickup. Z_m is the target-nucleus charge, Z is the projectile charge. Particles 0 and 1 are the projectile and target nucleus, respectively. Particle 2 is the active electron; the remaining target electrons are denoted by 3, 4, and "Etc."

B_{if} can be written as the sum of three terms: $B_{if}^{(1)} + B_{if}^{(2)} + B_{if}^{(3)}$ corresponding to the three interactions appearing in the brackets of Eq. (1). $B_{if}^{(1)}$ is thus the three-body Brinkman-Kramers amplitude, $B_{if}^{(2)}$ is the Jackson-Schiff amplitude, and $B_{if}^{(3)}$ is the additional screening amplitude. In momentum space these take on the familiar form

$$B_{if}^{(1)} = -\tilde{\phi}_i(\vec{\beta})(B_{02} + \tfrac{1}{2}\alpha^2)\tilde{\psi}_f^*(\vec{\alpha}), \tag{5}$$

$$B_{if}^{(2)} = \frac{ZZ_m e^2}{2\pi^2}\int \tilde{\phi}_i(\vec{\beta}-\vec{k})\tilde{\psi}_f^*(\vec{\alpha}-\vec{k})\frac{d^3k}{k^2}, \tag{6}$$

$$B_{if}^{(3)} = -\frac{Ze^2}{2\pi^2}\int \frac{d^3k}{k^2}\tilde{\rho}'(\vec{k})\tilde{\phi}_i(\vec{k})\tilde{\psi}_f^*(\vec{\alpha}-\vec{k}), \tag{7}$$

where

$$\vec{\alpha} = \vec{A} = \vec{P} - \frac{M_0\vec{Q}}{M_0+1},$$

$$\vec{\beta} = \vec{A} - \vec{B} = \left(\frac{M_1+Z_m-1}{M_1+Z_m}\right)\vec{P} - \vec{Q}, \tag{8}$$

and B_{02} is the final-state binding energy of the active electron.

Anticipating that most of the pickup occurs near the K shell, we can at least roughly approximate the screening of the projectile by a constant potential V_0. Then

$$B_{if}^{(3)} \approx V_0\tilde{\phi}_i(\vec{\beta})\tilde{\psi}_f^*(\vec{\alpha}). \tag{9}$$

We will use this latter approximation, which is adequate for our purposes. Finally, noting that we will consider only cases where $Z < Z_m$, we restrict ourselves to capture from the target K shell into the ground state of the projectile, noting that capture to higher projectile states contributes substantially less to the total pickup cross section.

After some work, and following the development of JS, we get

$$B_{if} = 32\pi(ZZ_m)^{5/2}a_0^2e^2\left[-\frac{1}{\Delta_1^2\Delta_0} + ZZ_m\int_0^1 x(1-x)\left(\frac{2}{\Delta^3(\Delta-q^2)^{1/2}} + \frac{1}{\Delta^2(\Delta-q^2)^{3/2}} + \frac{3/4}{\Delta(\Delta-q^2)^{5/2}}\right)dx + \frac{V_0}{\Delta_1^2\Delta_0^2}\right], \tag{10}$$

where

$$\Delta = \left(\frac{Z_m'^2 + Z^2}{2} + \frac{v^2}{4v_0^2} + \frac{(Z^2 - Z_m'^2)^2}{4}\,\frac{v_0^2}{v^2} + \mu^2 \frac{v^2}{v_0^2}\,\theta^2\right) + (Z_m^2 - Z_m'^2)x, \tag{11}$$

$$(\Delta - q^2) = Z^2 + \left((Z_m^2 - Z^2) + \frac{v^2}{v_0^2}\right)x - \frac{v^2}{v_0^2}x^2, \tag{12}$$

$$\Delta_1 = \Delta(x=1), \quad \Delta_0 = \Delta(x=0), \tag{13}$$

and $v_0 = 1/a_0 = e^2$ is the hydrogen ground-state velocity, V_0 is the constant potential in units of Rydbergs, Z_m' is defined so that $Z_m'^2$ Ry equals the binding energy of target K electron (this is the binding correction mentioned earlier), θ is the scattering angle, and $\mu \approx \mu_i \approx \mu_f$ is the reduced mass of the colliding system.

The differential scattering cross section is then

$$\frac{d\sigma}{d\Omega} = 2\left(\frac{\mu_f}{2\pi\hbar^2}\right)^2 \frac{v'}{v}\,|B_{if}|^2, \tag{14}$$

and using $v' \approx v$, $\mu_f \approx \mu$ and the fact that scattering is very sharply peaked in the forward direction:

$$\sigma = 2\pi \int_0^\infty \frac{d\sigma}{d\Omega}\,\theta\,d\theta = \frac{4\pi}{(2\pi\hbar^2)^2}\int_0^\infty |B_{if}(y)|^2 y\,dy, \tag{15}$$

where

$$y \equiv \mu\theta, \tag{16}$$

and as expected the total cross section is independent of masses of heavy particles. If we keep only the first term in the bracket of Eq. (10) in Eq. (15) we get the BK cross section σ_{BK}. If we keep the first two terms we get the JS cross section, σ_{JS}, and if we include the last term (screening term) we get the total first Born cross section, σ_T.

II. NUMERICAL RESULTS

As a first case we consider protons on argon. The results are in Table I. The experimental values are those of Ref. 2. As can be seen σ_{BK} overestimates the experimental cross sections by a factor of 2–3, comparable to what happens with protons on hydrogen. σ_{JS}, on the other hand, varies from 750 down to 60 times the experimental cross sections as the proton energy varies from 2.5 up to 12 MeV. As can be seen the effect of screening with a reasonable value of V_0 is not sufficient to change this effect. We varied V_0 over a wide range of values and found that even at $V_0 = -200$ Ry the cross section dropped by only 3%, and furthermore the $B_{if}^{(3)}$ amplitude was more than an order of magnitude lower than $B_{if}^{(2)}$ at all angles.

As a second case we consider fully stripped ions scattered off argon at three velocities. The results are in Table II. The experimental results are obtained by subtracting a Z^2-scaled ionization cross section normalized to protons on argon from the data of Ref. 14. This is somewhat crude, especially in light of the experimental uncertainties and is not meaningful at some points, which are omitted. As can be seen σ_{BK} gives roughly the

TABLE I. K-shell to $n=1$ level charge exchange calculations. Protons on argon; $Z=1$, $Z_m=18$, $Z_m'=15.34$; all cross sections in units of 10^{-22} cm^2.

E (MeV)	v/v_0	σ_{BK}	σ_{JS}	σ_T [a]	σ_{expt} [b]
2.5	10.00	0.390	150.	147.	0.192
3.0	10.96	0.428	110.	107.	0.272
4.0	12.65	0.435	62.	60.	0.262
5.0	14.15	0.392	36.	35.	0.196
6.0	15.49	0.336	22.	21.	0.168
7.5	17.32	0.252	11.	10.	0.110
8.0	17.89	0.228	8.9	8.4	0.099
9.0	18.98	0.186	5.9	5.5	0.072
10.0	20.00	0.151	4.0	3.7	0.056
11.0	20.98	0.123	2.8	2.6	0.050
12.0	21.91	0.100	1.9	1.8	0.034

[a] V_0 here was chosen as −88 Ry. As V_0 varied from −40 Ry to −200 Ry, $\sigma_T(10^{-22}$ cm$^2)$ varied from 148 to 144. For $V_0 = -200$ Ry, $B_{if}^{(3)} < \frac{1}{15}B_{if}^{(2)}$ at all angles.
[b] Data from Ref. 2 (K-shell pickup to all states).

TABLE II. K-shell to K-shell pickup calculations. Fully stripped ions on argon; $Z_m=18$, $Z_m'=15.34$; all cross sections in units of 10^{-20} cm^2.

Z	σ_{BK}	σ_{JS}	σ_{expt} [a]
	(1) $v/v_0 = 6.504$ (1.05 MeV/amu)		
1	0.115×10^{-2}	3.86	...
6	19.3	23 530.	...
7	54.9	48 340.	...
8	144.7	92 720.	~2.
9	359.6	170 100.	12.
	(2) $v/v_0 = 7.777$ (1.50 MeV/amu)		
1	0.222×10^{-2}	2.84	...
6	30.7	19 770.	4.0
7	80.8	40 880.	5.7
8	194.5	78 240.	15.0
9	434.9	141 600.	30.7
	(3) $v/v_0 = 8.713$ (1.88 MeV/amu)		
1	0.302×10^{-2}	2.20	...
6	37.1	16 930.	5.1
7	93.1	35 140.	12.8
8	212.4	67 040.	22.9
9	446.8	120 000.	43.3

[a] Data from Ref. 14 (pickup to all states). Pickup extracted from K-vacancy rate by assuming Z^2 scaling for ionization.

correct Z dependence and velocity dependence but is over an order of magnitude too large. σ_{JS} is too large by well over 10^3 and exhibits the wrong velocity dependence as well. Checks on the V_0 term show that, as before, it is incapable of significantly changing the above result.

One way of understanding the anomalous behavior of σ_{JS} (and σ_T) is to use a scaling argument. For simplicity let us assume that we are dealing with a one-electron target so that $Z'_m = Z_m$. Then under the transformation

$$Z \to aZ, \; Z_m \to aZ_m,$$

and projectile velocity $v \to av$, we get

$$B_{if}^{(1)} \to (1/a)B_{if}^{(1)}, \quad B_{if}^{(2)} \to B_{if}^{(2)}.$$

So for example in considering (a) $p + He^+ \to H + He^{++}$ as compared to (b) $F^{+9} + Ar^{+17} \to F^{+8} + Ar^{+18}$, we would have $a = 9$, and scaling the velocities accordingly we would have $\sigma_{BK}(b) = \frac{1}{81}\sigma_{BK}(a)$ while $\sigma_{JS}(b) \approx \sigma_{JS}(a)$.

In a real scattering situation there are many electrons in the target atom and $Z'_m \neq Z_m$. Unfortunately Z'_m does not scale the same way Z_m does. Nonetheless, we can calculate σ_{BK} and σ_{JS} for $p + He$ and for $F^{+9} + Ar$, and compare the calculations and experimental results for fluorine velocities nine times those of the protons. The results are shown in Table III. The $F^{+9} + Ar$ data are taken from Ref. 14, while $p + He$ data are those of Stier and Barnett.[15] As can be seen, σ_{BK} scales down by a factor of about 10^3 in going from the proton to the fluorine case, as do the experimental numbers. σ_{JS} stays the same order of magnitude for both cases, as predicted. The reason for the factor of 1000 rather than 81 is due mainly to the fact that $Z'_m = 1.34 \ll 2$ in He, and $B_{if}^{(1)}$ is extremely sensitive to Z'_m.

TABLE III. Test of scaling: scale factor of 9.

v/v_0	σ_{BK} [a]	σ_{JS} [a]	σ_{expt} [a]
$F^{+9} + Ar$: $Z = 9$, $Z_m = 18$, $Z'_m = 15.34$. Cross sections are in units of 10^{-20} cm^2			
6.5	360	170 100.	12
7.8	435	141 600.	31
8.7	447	120 000.	43
$p + He$: $Z = 1$, $Z_m = 1.7$ [b], $Z'_m = 1.34$. Cross sections are in units of 10^{-17} cm^2			
v/v_0	σ_{BK} [c]	σ_{JS} [c]	σ_{expt} [d]
0.72	245	185	12
0.87	184	116	18
0.97	146	80	19

[a] From Table II.
[b] Except in potential in matrix element where $Z_m = 2$.
[c] K-shell to K-shell calculation.
[d] Data from Ref. 15 (K pickup to all states).

III. CONCLUSIONS

We have seen that σ_{JS} (and σ_T) are quite nonphysical for protons on argon, and for $C^{+6}, N^{+7}, O^{+8}, F^{+9}$ on argon, and that indeed σ_{JS} scales the wrong way with increasing charge of projectile and target. Thus the delicate cancellation between $B_{if}^{(1)}$ and $B_{if}^{(2)}$ that leads to good agreement between σ_{JS} and experiment for protons on hydrogen does not hold for Z and/or Z_m much different from 1. One is thus led to the conclusion that keeping the projectile–target-nucleus interaction in the plane-wave Born approximation gives good results in the case of protons on hydrogen for fortuitous, or at least not understood, reasons. One could argue that since the interaction is proportional to the product ZZ_m, it gets sufficiently large for high Z and Z_m that the criteria for validity of the Born approximation no longer hold in the velocity domains considered. That is certainly a valid argument for high Z, but for protons on argon, at velocities 18 times those for which σ_{JS} gives good results for protons on hydrogen, we should expect comparable validity of first Born, and, as we have shown, this is just not the case.

Thus, since the best first-order plane-wave amplitude is that of Jackson and Schiff, we must conclude that either the use of plane waves for the projectile is just not good enough, or ignoring such effects as electron polarization is just not good enough. Judging from calculations already performed,[7,11] it is projectile distortion that is the dominant effect. The authors are presently performing a projectile distortion calculation using an eikonal approximation for proton-hydrogen charge exchange as well as the other systems considered here.

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