Inversion relations for exclusive and inclusive cross sections within the independent electron approximation

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(Received 6 March 1998)

Inversion relations expressing inclusive cross sections as linear combinations of exclusive cross sections are derived within the independent electron approximation without exchange. Both binomial and multinomial probability distributions are used. No particular model is used for $P(\vec{b})$. A criterion for applicability of the multinomial probability distribution to describe second-order transitions for the different collision channels, also independent of $P(\vec{b})$, is presented. The coupling of ionization and capture of outer-shell electrons is discussed and the inversion relations derived are applied to the analysis of coincidence measurements of projectile and target charge states. Parametrization and scaling laws for single and double ionization of outer-shell electrons of many-electron atoms are considered by studying the influence of the electron capture channel. [S1050-2947(98)09809-6]

PACS number(s): 34.10.+x, 34.50.−s, 34.70.+e

I. INTRODUCTION

Collisions involving many-electron targets can lead to transitions of one or more target electrons to various final states. In collisions with highly charged projectiles, several such channels are not only important but also strongly coupled among themselves, resulting in relatively complex collision systems. The independent electron approximation (IEA) has been used as a useful starting point for the analysis of total cross sections involving many-electron transitions [1–5]. In the IEA the collision is seen as a product of independent interactions between the projectile and the target electrons. By treating the motion of the projectile classically, ignoring electron correlation and exchange and choosing common transition probabilities, the cross sections describing many-electron transitions can be expressed as integrals over the impact parameter of binomial or multinomial distributions of single-electron probabilities [5,6]. The simplified binomial IEA (BIEA) and multinomial IEA (MIEA) allow a relatively simple analysis of cross sections for many-electron transitions using probabilities for effective one-electron transitions. In the IEA first-order perturbation theory [5] or semiclassical approximations [7] are often used.

Even for strongly correlated systems, the IEA can have a role in defining the dynamical correlation since the correlation is defined generally as the difference between exact or experimental quantities and uncorrelated quantities [5]. For example, Ford and Reading [8] proposed a definition for correlation in a collision as the difference between an exact collision calculation and calculations carried out within the IEA, although they pointed out that this definition is not unique because the results of the IEA depend on the single-electron potential used.

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II. BINOMIAL INDEPENDENT ELECTRON APPROXIMATION

In the simple BIEA, the cross section for a collision in which m out of a total of N equivalent electrons undergo transitions with the same probability $P(\vec{b})$ is given by

$$\sigma_m^{(N)}=\binom{N}{m}\int P(\vec{b})^m[1-P(\vec{b})]^{N-m}d\vec{b}, \qquad (1)$$

with $m=0,1,2,\ldots,N$. This approximate expression for $\sigma_m^{(N)}$ contains information both on the dynamics of the collision with one single electron of the target and on the statistics of several equivalent electrons in the target. The collision dynamics are carried by the choice of a particular $P(b)$, which is dependent on the single-electron potential used, and the statistics are binomial [5]. The $\sigma_m^{(N)}$ are called exclusive cross sections [1,5,9].

Several theories predict useful scaling laws for the dependences of $P(\vec{b})$ on v_p, Z_p, and Z_t for different collision processes. In the case of one-electron target, scaling laws for the integrated cross sections can be obtained directly from those for $P(\vec{b})$. On the other hand, exclusive cross sections for collisions with many-electron atoms have more complex dependences on v_p, Z_p, and Z_t, partially due to the statistical effect of the presence of many electrons on the target. Within the BIEA, the inclusive cross sections [5,9] for m

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transitions out of N equivalent electrons, regardless of the final states of the remaining $N-m$ electrons, are expressed as

$$s_m^{(N)} = \binom{N}{m} \int P(\vec{b})^m d\vec{b}, \qquad (2)$$

with $m=0,1,2,\ldots,N$. The exclusion of the term $[1-P(\vec{b})]^{N-m}$, associated with the electrons that have a passive role in the collision, makes more evident the effect of the single interaction potential used and makes $s_m^{(N)}$ a better candidate for universal parametrizations than the $\sigma_m^{(N)}$. However, the usually measured cross sections are the exclusive cross sections, obtained through the observation of target and projectile final states.

DuBois and Toburen [10] pointed out that for the ionization of He by different projectiles, the role of correlation is better studied by comparing the double ionization cross section $\sigma_2^{(2)}$ to the ''total ionization cross section,'' defined as $\sigma_T^{(2)} = \sigma_1^{(2)} + 2\sigma_2^{(2)}$, because this linear combination of the exclusive cross sections $\sigma_1^{(2)}$ and $\sigma_2^{(2)}$ results in the inclusive cross section $s_1^{(2)} = \sigma_T^{(2)}$. For multiple ionization in proton-atom collisions, DuBois and Manson [11] used a different approach, choosing a particular form for $P(\vec{b})$ and comparing the exclusive cross sections thus obtained. In order to obtain some information about the interaction between the projectile and each of the active electrons, these authors modeled the ionization probability by the expression $P(\vec{b}) = P(b) = P(0)\exp(-b/R)$ to obtain the scaling parameter R in terms of the measured exclusive cross sections. This kind of model calculation, with different choices for $P(b)$, has been widely used [10,12–15] for the analysis of the ionization and the electron capture collision channels in multielectronic targets.

Using the binomial inverse pair relations [16–19], we show in Sec. III that for any number of equivalent target electrons N, the inclusive cross sections $s_m^{(N)}$ can be expressed as linear combinations of the exclusive cross sections $\sigma_m^{(N)}$ corresponding to different numbers of electrons undergoing transitions. The coefficients of the linear combinations are determined in a simple closed form. No hypothesis is made about the impact parameter dependence of $P(\vec{b})$ and these relations can be applied to the ionization as well as to the electron capture or any other inelastic collision process. However, for the remainder of this paper we replace $\int d\vec{b} = \int d\phi\, b\, db$ by $\int 2\pi\, b\, db$, which is a little simpler. This assumes that $P(\vec{b})$ is isotropic in the azimuthal angle ϕ, i.e., $P(\vec{b}) = P(b,\phi) \to P(b)$. When the scattering is not isotropic in ϕ (e.g., aligned targets), then $P(b)$ and $\int 2\pi\, b\, db$ may be generally replaced by $P(\vec{b})$ and $\int d\vec{b}$, respectively.

In Sec. IV a generalization for multinomial distributions is also presented and a criterion for applicability of the MIEA to describe second-order transitions, using measured total cross sections, is derived based on the Schwarz inequality and without any hypothesis on the behavior of the probabilities involved. Finally, in Sec. V some applications of the relations developed are explored. The coupling of ionization and capture of outer-shell electrons are discussed. Applications to the analysis of coincidence measurements of projectile and target charge states are examined. Parametrization and scaling laws for ionization and double ionization of outer-shell electrons of many-electron atoms are studied.

III. INVERSION FOR THE BINOMIAL PROBABILITY DISTRIBUTION

Although Eq. (1) describes cross sections for collision channels involving only m electronic transitions, the constraint of having another $N-m$ passive electrons to be described makes $\sigma_m^{(N)}$ dependent on $P(b)$ in all orders between m and N. This dependence becomes explicit when the integrand in Eq. (1) is expanded in powers of $P(b)$. The binomial term in the integral of Eq. (1) can be expanded to give

$$(1-P)^{N-m} = \sum_{i=0}^{N-m} (-1)^{N-m-1} \binom{N-m}{i} P^{N-m-i}. \qquad (3)$$

Substituting this result into Eq. (1), changing the order of the sum and the integral, and introducing the index $j=N-i$, we have

$$\sigma_m^{(N)} = \sum_{j=m}^{N} (-1)^{j-m} \binom{j}{m} \binom{N}{j} \int P(b)^j 2\pi\, b\, db. \qquad (4)$$

This equation expresses the set of $\sigma_m^{(N)}$ as linear combinations of integrals of powers of $P(b)$. Thus, if $P(b)$ has a simple dependence on some parameter, e.g., Z_p^2, the cross sections for collisions with atoms with N equivalent electrons turns out to be a sum of terms in powers of this dependence, i.e., Z_p^{2j}, with j varying from m to N, and the original simplicity is lost. Moreover,

$$s_j^{(N)} = \binom{N}{j} \int P(b)^j 2\pi\, b\, db$$

is the expression, within the BIEA, for the inclusive cross section $s_j^{(N)}$ for j electrons undergoing transitions. Thus Eq. (4) expresses the set of exclusive cross sections as linear combinations of the set of inclusive cross sections. While the $\sigma_m^{(N)}$ are cross sections for exactly m electrons undergoing transitions, the $s_m^{(N)}$ are cross sections for at least m electrons undergoing transitions while the other electrons may or may not be undergoing transitions. This becomes clearer by writing $s_m^{(N)}$ as

$$s_m^{(N)} = \binom{N}{m} \int P(b)^m \{P(b) + [1-P(b)]\}^{N-m} 2\pi\, b\, db.$$

With the inversion of the linear set of equations represented by Eq. (4) it is possible to express $s_m^{(N)}$ as a sum of exclusive cross sections involving different numbers of active electrons. The coefficient matrix [20] of the system of N linear equations, described by Eq. (4), is nonsingular. Thus the system is invertible using Cramer's rule [20] and can be solved for the inclusive cross sections. For a general matrix, this solution is expressed in terms of the cofactors of the system of equations, with each cofactor written in terms of a sum of several elements of the original coefficient matrix. For the present system we show, using the inverse pair relations [16–19], that the elements of the inverse matrix can be written in a closed form and therefore each of the integrals of the $s_m^{(N)}$ can be written as a simple sum over the exclusive cross sections $\sigma_j^{(N)}$.

The basic binomial inverse pair relations [17] states that if the coefficients $a_0, a_1, \ldots, a_n$ and $b_0, b_1, \ldots, b_n$ are such that

$$b_n = \sum_{i=0}^{n} \binom{n}{i} a_i, \tag{5}$$

then

$$a_n = \sum_{i=0}^{n} (-1)^{n-i} \binom{n}{i} b_i. \tag{6}$$

Introducing the indices $j=N-i$ and $m=N-n$, we obtain the inverse pair relations

$$a_{N-m}\binom{N}{m} = \sum_{j=m}^{N} (-1)^{j-m}\binom{j}{m}\binom{N}{j} b_{N-j} \tag{7a}$$

and

$$b_{N-m}\binom{N}{m} = \sum_{j=m}^{N} \binom{j}{m}\binom{N}{j} a_{N-j}. \tag{7b}$$

Comparing Eq. (4) with Eq. (7a), we can make the identification of the coefficients a_{N-m} and b_{N-j} in Eq. (7a) and obtain from Eq. (7b)

$$b_{N-m} = \int P(b)^m 2\pi\, b\, db \tag{8a}$$

and

$$a_{N-j} = \frac{\sigma_j^{(N)}}{\binom{N}{j}}. \tag{8b}$$

From Eqs. (7b), (8a), and (8b) it follows that

$$s_m^{(N)} \equiv \sum_{j=m}^{N} \binom{j}{m} \sigma_j^{(N)} = \binom{N}{m} \int P(b)^m 2\pi\, b\, db, \tag{9}$$

with $m=0,1,2,\ldots,N$.

Equation (9) is one of the main results of this paper. Together with Eq. (1) it forms a pair of relations that have the same conditions of applicability to the description of inelastic collisions with multielectronic targets and emphasize different aspects of these collisions. While the exclusive cross sections $\sigma_m^{(N)}$ include the statistical effect of constraining the interaction with $N-m$ of the target electrons elastic, the inclusive cross sections $s_m^{(N)}$ make more evident the dynamics of the inelastic interaction with each electron, described by $P(b)$.

The case $m=1$ in Eq. (9) is of particular interest. In this case Eq. (9) reduces to

$$\sum_{j=1}^{N} j\sigma_j^{(N)} = N \int P(b) 2\pi\, b\, db. \tag{10}$$

Equation (10) provides an example of an inclusive cross section that can be directly measured [1,5]. The sum $\Sigma j \sigma_j^{(N)}$ is a quantity directly obtained from experiments where the total current produced by all different ionization events is measured, without the knowledge of any particular $\sigma_j^{(N)}$. This inclusive cross section has also been called an apparent cross section for positive ion production [21]. For ionization by electron impact, where the electron capture channel does not exist, or for ionization by high-velocity projectiles, where capture is negligible, it is also called a net ionization cross section [22,23], gross ionization cross section [24], or simply total ionization cross section [10].

The symmetry between inclusive $s_m^{(N)}$ and exclusive $\sigma_m^{(N)}$ cross sections can be made more explicit by rewriting Eqs. (4) and (9) as

$$\sigma_m^{(N)} = \sum_{j=m}^{N} (-1)^{j-m} \binom{j}{m} s_j^{(N)} \tag{11a}$$

and

$$s_m^{(N)} = \sum_{j=m}^{N} \binom{j}{m} \sigma_j^{(N)}, \tag{11b}$$

which is a pair of equations very similar to the basic binomial inverse-pair relations. The simple mutual transformation relations connecting $\sigma_m^{(N)}$ and the $s_m^{(N)}$ allow one to take advantage of both exclusive and inclusive cross sections to reach a better understanding of a collisions process. In the first step, the measured exclusive cross sections can be combined, according to Eq. (9), to determine one or more of the $N+1$ inclusive cross sections. In the next step, the inclusive cross sections for different collision systems can be compared with each other and with the theory. This comparison can include not only collision systems with different projectiles but also targets with different number of equivalent electrons. Finally, once a satisfactory description of the inclusive cross sections $s_m^{(N)}$ is achieved, the theoretical predictions for the exclusive cross sections $\sigma_m^{(N)}$ can be obtained by either Eq. (1) or (11a).

The inversion relations can also be written for the exclusive probabilities [5]

$$\mathcal{P}_m^{(N)}(b) = \binom{N}{m} P(b)^m [1-P(b)]^{N-m} \tag{12}$$

and the inclusive probabilities, resulting in the pair of equations

$$\mathcal{P}_m^{(N)}(b) = \sum_{j=m}^{N} (-1)^{j-m} \binom{j}{m}\binom{N}{j} P(b)^j \tag{13a}$$

and

$$\binom{N}{m} P(b)^m = \sum_{j=m}^{N} \binom{j}{m} \mathcal{P}_j^{(N)}(b). \tag{13b}$$

The particular case of $m=0$ in Eq. (13b) is the unitarity condition for $\mathcal{P}_j^{(N)}$ in the binomial probability distribution.

The validity of Eq. (9), derived in this section using binomial inverse pair relations, is also demonstrated in Appendix A using a simple proof by substitution. We proceed, in the next section, to generalize these results when several collision channels need to be considered.

IV. MULTIPLE CHANNELS AND THE MULTINOMIAL PROBABILITY DISTRIBUTION

The inversion relations between exclusive and inclusive cross sections, derived in Sec. III for a single inelastic collision channel, can be generalized using multinomial probability distributions [5] to any number of collision channels. In Appendix B it is shown that in the case of two inelastic collision channels, represented by α and β, the multinomial probability distribution gives, for N equivalent electrons,

$$\sigma_{m,n}^{(N)}=\frac{N!}{m!n!(N-m-n)!}\int P_\alpha(b)^m P_\beta(b)^n[1-P_\alpha(b)-P_\beta(b)]^{N-m-n}2\pi\, b\, db, \tag{14}$$

$$\sum_{i,j}\binom{i}{m}\binom{j}{n}\sigma_{i,j}^{(N)}=\frac{N!}{m!n!(N-m-n)!}\times\int P_\alpha(b)^m P_\beta(b)^n 2\pi\, b\, db, \tag{15}$$

where the sum of the indices i and j is over $i+j\leqslant N$ with $i\geqslant m$ and $j\geqslant n$. The probabilities $P_\alpha(b)^m$ and $P_\beta(b)^n$ may represent, for example, the ionization and capture probabilities in collisions of bare projectiles with an atom with N equivalent electrons. Target excitation may be included with ionization and electron capture to the continuum by defining $P(b)=(\Sigma_n+\int d\vec{k})P(\vec{b},n,\text{ or }\vec{k})$, which sums over both bound and continuum final states.

The generalization presented in Appendix B gives, for M inelastic collision channels α_i,

$$\sigma_{n_1,\ldots,n_M}^{(N)}=\frac{N!}{n_1!\cdots n_M!(N-n_1-\cdots-n_M)!}\times\int P_{\alpha_1}(b)^{n_1}\cdots P_{\alpha_M}(b)^{n_M}[1-P_{\alpha_1}(b)-\cdots-P_{\alpha_M}(b)]^{N-n_1-\cdots-n_M}2\pi\, b\, db, \tag{16}$$

$$\sum_{i_1,\ldots,i_M}\binom{i_1}{n_1}\cdots\binom{i_M}{n_M}\sigma_{i_1,\ldots,i_M}^{(N)}=\frac{N!}{n_1!\cdots n_M!(N-n_1-\cdots-n_M)!}\times\int P_{\alpha_1}(b)^{n_1}\cdots P_{\alpha_M}(b)^{n_M}2\pi\, b\, db, \tag{17}$$

where the sum of the indices $i_1,i_2,\ldots,j$ is over $i_1+i_2+\cdots+i_M\leqslant N$ with $i_1\geqslant n_1$, $i_2\geqslant n_2,\ldots,i_M\geqslant n_M$. With $s_{n_1,\ldots,n_M}^{(N)}$ the inclusive cross sections for the M inelastic collision channels $\alpha_1,\alpha_2,\ldots,\alpha_M$,

$$s_{n_1,\ldots,n_M}^{(N)}\equiv\frac{N!}{n_1!\cdots n_M!(N-n_1-\cdots-n_M)!}\times\int P_{\alpha_1}(b)^{n_1}\cdots P_{\alpha_M}(b)^{n_M}2\pi\, b\, db, \tag{18}$$

it follows that

$$\sigma_{n_1,\ldots,n_M}^{(N)}=\sum_{i_1,\ldots,i_M}(-1)^{i_1+\cdots+i_M-n_1-\cdots-n_M}\times\binom{i_1}{n_1}\cdots\binom{i_M}{n_M}s_{i_1,\ldots,i_M}^{(N)} \tag{19a}$$

and

$$s_{n_1,\ldots,n_M}^{(N)}=\sum_{i_1,\ldots,i_M}\binom{i_1}{n_1}\cdots\binom{i_M}{n_M}\sigma_{i_1,\ldots,i_M}^{(N)}. \tag{19b}$$

Equations (19a) and (19b) relate the exclusive and inclusive cross sections in the MIEA.

Criterion for applicability of the MIEA in multiple transitions

Several collision systems have been studied using multinomial probability distributions with equivalent electrons [3]. Although good general agreement with the experimental data is often obtained for single-electron transitions, it has been noted that double-electron transitions frequently present poor agreement with experiment [3].

Using Schwarz's inequality [25] and the expressions for inclusive cross sections of Sec. IV, it will be shown that the hypothesis of equivalent electrons in the MIEA implies an inherent limitation on the agreement between theory and experimental data for double-electron transitions, independently of the $P(b)$ used for each collision channel.

Schwarz's inequality [25,26] leads to

$$\int P_\alpha(b)P_\beta(b)2\pi\, b\, db\leqslant\left[\int P_\alpha(b)^2 2\pi\, b\, db\right]^{1/2}\times\left[\int P_\beta(b)^2 2\pi\, b\, db\right]^{1/2}. \tag{20}$$

Note that the above inequality is valid for arbitrary probabilities $P_\alpha(b)$ and $P_\beta(b)$ with different impact parameter dependences. On the other hand, the particular case of the equality in Eq. (20) holds only if $P_\alpha(b)$ and $P_\beta(b)$ have the same impact parameter dependence, i.e., $P_\alpha(b)/P_\beta(b)$ is independent of b.

In terms of the sums $s_{m,n}^{(N)}$ given by Eq. (18), for two inelastic channels, the integrals in Eq. (15) are written as

$$\int P_\alpha(b)P_\beta(b)2\pi\, b\, db=\frac{1}{N(N-1)}s_{11}^{(N)}, \tag{21}$$

$$\int P_\alpha(b)^2 2\pi\, b\, db=\frac{2}{N(N-1)}s_{20}^{(N)}, \tag{22}$$

and

$$\int P_\beta(b)^2 2\pi\, b\, db = \frac{2}{N(N-1)} s_{02}^{(N)}. \tag{23}$$

Thus, as a consequence of Schwarz's inequality, we have

$$R_S \equiv \frac{s_{11}^{(N)}/2}{\sqrt{s_{20}^{(N)} s_{02}^{(N)}}} \leqslant 1. \tag{24}$$

While R_S calculated within the MIEA with equivalent electrons has to be less than or equal to 1, independently of the energy and the collision system, the same does not happen with the values of R_S obtained from the experimental data. Applications of the criterion described above are presented in Sec. V.

The use of different probabilities $P_1(b)$ and $P_2(b)$ for the same collision channel to describe two independent events occurring in a double-electron transition eliminates the restriction from Schwarz's inequality [25], but does not allow the use of binomial or multinomial probabilities to describe simultaneously all the collision channels. The version of the IEA using the different probabilities $P_1(b)$ and $P_2(b)$ is also called the independent event model (IEV) [27–29].

V. IONIZATION AND CAPTURE BY BARE PROJECTILES

A. Ionization and capture on a He target by bare projectiles

The He atom is the simplest atom for which multiple transitions can occur. The coupling between the ionization, excitation, and capture channels in collisions of bare projectiles with He has been extensively studied both theoretical and experimentally. Theoretical approaches involving the MIEA are often used [3,4,9,13,30].

Neglecting excitation, the inelastic channels involved in the collision are single ionization, single capture, double ionization, double capture, and transfer ionization, with the corresponding exclusive cross sections represented by σ_I, σ_C, σ_{DI}, σ_{DC}, and σ_{TI}, respectively. In this simple case, the inclusive and exclusive cross sections are the same [9,13] for the channels involving two-electron transitions and

$$s_{02}^{(2)} = \int P_I(b)^2 2\pi\, b\, db, \tag{25}$$

$$s_{20}^{(2)} = \int P_C(b)^2 2\pi\, b\, db, \tag{26}$$

$$s_{11}^{(2)} = 2\int P_I(b) P_C(b) 2\pi\, b\, db. \tag{27}$$

The application of Schwarz's inequality [25] results in the criterion

$$R_S = \frac{\sigma_{TI}/2}{\sqrt{\sigma_{DI}\sigma_{DC}}} < 1. \tag{28}$$

In Fig. 1 the experimental data of Shah and Gilbody [31] for double ionization, double capture, and transfer ionization of H^+, He^{2+}, and Li^{3+} projectiles incident on He are combined to give R_S as a function of projectile energy. Region II

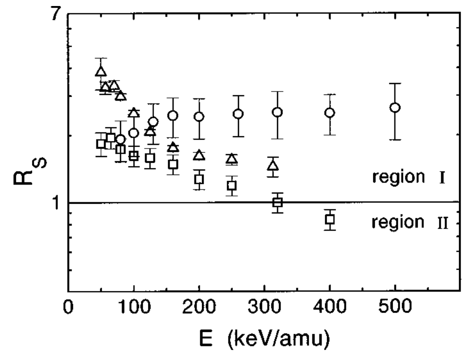

FIG. 1. Criterion for applicability of the MIEA. R_S (see the text) is shown for different projectiles incident on He as a function of projectile energy. The experimental data are from Ref. [31]: circles, H^+; squares, He^{2+}; triangles, Li^{3+}. The Schwartz inequality of Eq. (20), corresponding to $R_S < 1$, is violated in region I, indicating a breakdown of the MIEA.

is the region of the plot where calculations of R_S based on the MIEA with equivalent electrons can, in principle, reproduce simultaneously double ionization, double capture, and transfer ionization. In region I this is forbidden by Schwarz's inequality. In the range of velocities shown, almost all the experimental data lie in region I. For the points in region I, an expression for $P_I(b)$ and another for $P_C(b)$ can, in principle, be found to describe two of the cross sections among σ_{DC}, σ_{DI}, and σ_{TI}, but not all three of them. In Fig. 1 the behavior for the H^+ projectile is qualitatively different from that of He^{2+} and Li^{3+} projectiles. When the projectile energy increases, the values of R_S for He^{2+} and Li^{3+} projectiles approach region II, indicating improvement for the conditions of applicability of the MIEA. This behavior, with the improvement of the MIEA with increasing velocities, has been observed for most collision systems [5]. For H^+ projectiles, on the other hand, R_S increases with the velocity and reaches a constant value between 2 and 3, independently of the projectile energy.

Theoretical conditions for the validity of the MIEA used above are the neglect of electron correlation (including exchange) and the equivalence of transition probabilities (i.e., P_I is the same for both electrons and so is P_C). In reality, electronic relaxation can occur during the collision. The relaxation of the second electron before its transition depends on the projectile velocity. However, this effect is expected to have the same importance for the double ionization by the three projectiles. For double capture and transfer ionization the case of H^+ projectile may be qualitatively different from the others. In an idealized situation in which the electron captured in the first event has enough time to fully relax, the capture in the second event will take place by the neutral projectile H^0. In the case of the He^{2+} and Li^{3+} projectiles, the dressed relaxed projectile will still be charged when the second event occurs.

The role of electron relaxation in single and double removal of helium by protons is discussed by Ford *et al.* [27]. They pointed out that an aspect of electron correlation that can cause deviation from the MIEA and IEV calculations is the screening of the projectile from the second electron by the first electron if the first electron follows closely the projectile after it has been released from the target [27]. They show that the inclusion of projectile screening effects in the second interaction of the H^+ projectile, if the first electron is captured, improves significantly the agreement with experiment at intermediary energies. The results in Fig. 1 are consistent with these arguments indicating that using the same target wave function for both target electrons causes significant deviations from the uncorrelated MIEA for all collision systems studied. The results in Fig. 1 show that the MIEA tends to improve at high energies except for $Z_p = 1$.

B. Scaling for many-electron atoms: Single ionization

In collisions of heavy charged projectiles with many-electron atoms at intermediate velocities, ionization and capture are often collision channels that must both be considered. Outer-shell ionization [32] dominates the total ionization cross sections and the exclusive cross section for single ionization (neglecting excitation) within the MIEA is

$$\sigma_{01}^{(N)} = N \int P_I(b)[1 - P_I(b) - P_C(b)]^{N-1} 2\pi\, b\, db, \tag{29}$$

while the corresponding inclusive cross section can be written, according to Eq. (15), as

$$s_{01}^{(N)} \equiv \sum_{j=0}^{N} \sum_{i=1}^{N-j} i\,\sigma_{i,j}^{(N)} = N \int P_I(b) 2\pi\, b\, db, \tag{30}$$

which is independent of $P_C(b)$.

Equation (30) is similar to the cross section for ionization of simple one-electron atoms. Scaling laws based on one-electron atom transitions have been used [5,33] to search for common patterns for different systems. A typical analysis searching for scaling laws can be illustrated by the work of Krishnamurthi *et al.* [23], which used the BIEA to study the dependence of the ionization of molecular targets with Z_p. The form of Eq. (30) suggests the possible application of the parametrization used for K-shell ionization [5,33] to search for scaling laws for inclusive cross sections for ionization of outer target electrons. Because in the cross sections presented in this section there is no selection of the shell of the ionized electrons, we make the hypothesis that the ionized electrons are from the outer shell for each target, thus involving the subshells $1s$ for atomic hydrogen and He, $2s$ and $2p$ for Ne, $3s$ and $3p$ for Ar, and $4s$ and $4p$ for Kr. A mean binding energy $\overline{u_b}$ for subshells s and p is taken as the harmonic mean [25]

$$\overline{u_b} = \frac{N}{N_s/u_s + N_p/u_p}, \tag{31}$$

with $N = 8$, $N_s = 2$, and $N_p = 6$. Here the mean velocity of the outer-shell electrons, in atomic units, is $\overline{v} = \sqrt{\overline{u_b}}$, where $\overline{u_b}$ is written in rydbergs. Since $u = k/r$, this corresponds to choosing a common $\overline{r} = N_s r_s + N_p r_p/(N_s + N_p)$ for all electrons within each shell. This choice of $\overline{u_b}$ in Eq. (31) gives the expected result in the Bethe limit and heightens the weight of electrons with lower binding energy. Numerically, for the atoms mentioned above, the difference between $\overline{u_b}$ given by Eq. (31) and a simple arithmetic weighted mean is small. Values for u_n for all subshells were taken from Ref. [34]. In the semiclassical approximation, the probability for ionization of a single electron with binding energy of modulus $\overline{u_b}$, in rydbergs, by a projectile of charge Z_p at a velocity v_p can be written as [5,33]

$$P_I(Z_p, \overline{u_b}, v_p; b) = \frac{Z_p^2}{\overline{u_b}} P_I(1,1,v_p/\overline{v}; \overline{v}b) \tag{32}$$

or

$$P_I(b) = \frac{Z_p^2}{\overline{u_b}} P_I^{(1)}(\overline{v}b), \tag{33}$$

with $P_I^{(1)}(b)$ being the ionization probability for a proton incident on atomic hydrogen, with velocity $v_p/\overline{v}$.

With the above parametrization, the exclusive and inclusive cross sections are reduced, respectively, to the integrals

$$N \frac{Z_p^2}{\overline{u_b}} \int P_I^{(1)}(\overline{v}b) \left(1 - \frac{Z_p^2}{\overline{u_b}} P_I^{(1)}(\overline{v}b) - P_C(b) \right)^{N-1} 2\pi\, b\, db, \tag{34}$$

and

$$s_{01}^{(N)} = N \frac{Z_p^2}{\overline{u_b}} \int P_I^{(1)}(\overline{v}b) 2\pi\, b\, db. \tag{35}$$

With the change of the integration variable to $x = \overline{v}b$, Eq. (35) can be written as

$$s_{01}^{(N)}(v_p) = N \frac{Z_p^2}{\overline{u_b}^2} \sigma_I^{\mathrm{H}}(v_p/\overline{v}). \tag{36}$$

Thus Eq. (36) expresses the inclusive cross sections for single ionization of outer-shell electrons at a velocity v_p as a function of N, Z_p, $\overline{u_b}$, and the ionization cross section for the H target at a velocity $v_p/\overline{v}$.

In the high-energy limit, the Bethe approximation provides useful analytical expressions for both $P_I(b)$ [12],

$$P_I(b) = c_1 \frac{Z_p^2}{\overline{u_b}} \frac{\exp\left(-\dfrac{c_2}{v_p/\overline{v}} \overline{v}b \right)}{(v_p/\overline{v})^2 (\overline{v}b)^2}, \tag{37}$$

and the integrated inclusive cross section [12,24,35]

$$s_{01}^{(N)} = N c_1 \frac{Z_p^2}{\overline{u_b}^{\,2}} \frac{\ln\left(\dfrac{v_p/\overline{v}}{c_2} \right)}{(v_p/\overline{v})^2}, \tag{38}$$

where c_1 and c_2 are dimensionless numbers, independent of N, Z_p, and $\overline{u_b}$.

In Figs. 2(a) and 2(b) the parametrized cross sections for exclusive and inclusive one-electron ionization of few- and many-electron targets by He^{2+} projectiles are shown. For the atomic hydrogen target the definitions of exclusive and in-

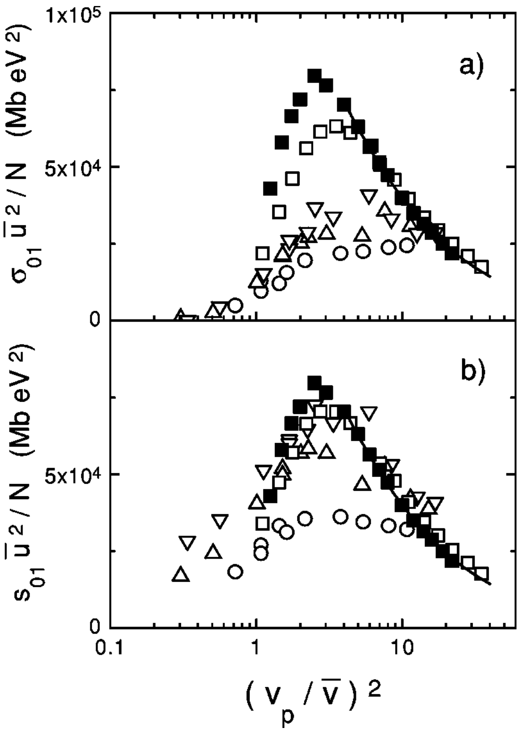

FIG. 2. Single ionization of several targets by He^{2+} projectiles for (a) exclusive and (b) inclusive cross sections. Closed squares, H, Ref. [36]; open squares, He, Ref. [31]; circles, Ne, Ref. [37]; up triangles, Ar, Ref. [37]; down triangles, Kr, Ref. [37]. Theory: full line, Bethe limit of the PWBA for H (see the text).

clusive cross sections are the same. The continuous line is the Bethe theory [24] for ionization of atomic hydrogen, which coincides with the high-energy limit of the plane-wave Born approximation (PWBA). The excellent agreement between Bethe's prediction and experimental data has to be considered with caution because the experimental data [36] themselves were normalized by the PWBA in the high-energy limit. Despite that, the agreement of velocity dependence between Bethe theory and experiment is remarkable. In Fig. 2(b), for projectile velocities higher than the mean velocity of the target electron, all but the Ne data coalesce with the H ionization data. Even for Ne, the curve of experimental data has a shape different from the exclusive cross sections [Fig. 2(a)] and assumes a maximum at the same position as the other curves. One possible explanation for the Ne points being low is that, for this target, exclusive cross sections for ionization up to only four electrons were measured, while for Kr, for example, up to eight electrons were measured. Thus the sum

$$s_{01}^{(N)}=\sum_{j=0}^{N}\sum_{i=1}^{N-j} i\sigma_{i,j}^{(N)} \tag{39}$$

was truncated with fewer terms in Ne than in Kr. Although the cross sections for high-order processes were not measured because they are small, their relative importance for the sum of Eq. (39) increases with the order of the processes. In addition, the mean binding energy of outer electrons is higher for Ne than for any other of the studied targets [34] and because the scaled cross section is proportional to $\overline{u_b}^{\,2}$, the effect of the unmeasured cross sections for Ne is enhanced.

For $v_p/\overline{v_n}>3$ the differences between inclusive and exclusive cross sections become small because the probabilities involved are all small, typically less than 5%. Therefore,

$$[1-P_I(b)-P_C(b)]^{N-1}\approx 1 \tag{40}$$

and $\sigma_1^{(N)}\approx s_1^{(N)}$. For $(v_p/\overline{v_n})<1$ the parametrization used increases the dispersion of the inclusive when compared to the exclusive cross sections, suggesting that a theoretical description based on the statistical energy deposition model [5,38] or on the IEV, taking into account relaxation of electrons, should be more appropriate.

C. Scaling for many-electron atoms: Double ionization

The IEA has been broadly used to study two-electron transitions in collisions with a He target [3,4]. Although the MIEA presents limitations to the analysis of this problem, as discussed in Sec. V A, the use of the MIEA by several groups [3,4] clearly leads to a better understanding of the problem. To analyze the applicability of multinomial probability distributions to collisions involving two-electron transitions in *many-electron targets*, the criterion derived in Sec. IV A for R_S, neglecting the excitation channel,

$$R_S=\frac{s_{11}^{(N)}/2}{\sqrt{s_{02}^{(N)}s_{20}^{(N)}}}<1, \tag{41}$$

is applied to He^{2+} projectiles incident on He, Ne, Ar, and Kr. The inclusive cross sections for two-electron transitions in targets with N equivalent electrons are, according to Eq. (15),

$$s_{02}^{(N)}\equiv\sum_{j=0}^{N}\sum_{i=2}^{N-j}\frac{i(i-1)}{2}\sigma_{i,j}^{(N)}=\binom{N}{2}\int P_I(b)^2 2\pi\, b\, db, \tag{42}$$

$$s_{20}^{(N)}\equiv\sum_{j=2}^{N}\frac{j(j-1)}{2}\sum_{i=0}^{N-j}\sigma_{i,j}^{(N)}=\binom{N}{2}\int P_C(b)^2 2\pi\, b\, db, \tag{43}$$

and

$$s_{11}^{(N)}\equiv\sum_{j=1}^{N} j\sum_{i=0}^{N-j} i\sigma_{i,j}^{(N)}=2\binom{N}{2}\int P_C P_I(b)2\pi\, b\, db, \tag{44}$$

corresponding to double ionization, double capture, and transfer ionization, respectively. Note that this analysis of R_S is independent of any estimate of the number of target electrons N accessible to the transitions. The results are shown in Fig. 3.

We first consider the close grouping of data in Fig. 3. The experimental data for all targets, including He, are in general good agreement. This suggests that the effect of correlation in many-electron atoms is not more important than for the

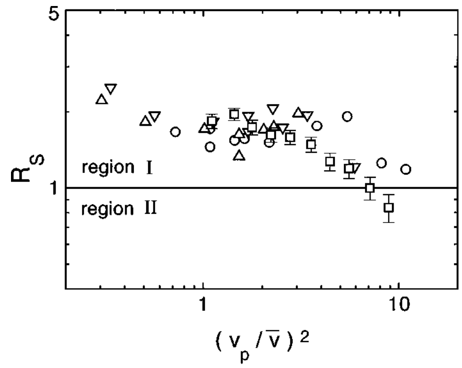

FIG. 3. Criterion for applicability of the MIEA. R_S (see the text) is shown for He^{2+} incident on several targets. Squares, He, Ref. [31]; circles, Ne; up triangles, Ar; down triangles, Kr, Ref. [37]. The Schwartz inequality of Eq. (20), corresponding to $R_S<1$, is violated in region I, indicating a breakdown of the MIEA.

He target. Thus the MIEA with equivalent electrons may, in principle, give useful information about two-electron transitions in collisions with more complex targets than He for relatively fast highly charged projectiles. Next we consider the violation of the Schwartz inequality evident in Fig. 3, which indicates a breakdown in the MIEA. That the MIEA has limited validity for small Z_p is not totally unexpected for outer-shell electrons. Shah *et al.* [39] have shown that transfer plus ionization of outer-shell electrons in Fe targets is fit by the IEA within uncertainties of about 20%, which is, however, not inconsistent with Fig. 3. On the other hand, in the case of protons, antiprotons, electrons, and positrons on helium [40], it would be difficult to argue that the IEA is better than 30% or so at any velocity. A sensible simple validity criterion for the IEA is that the interaction V_I with the projectile is large compared to the electron correlation V_{corr}. That is, $\int V_I dt \gg \int V_{\mathrm{corr}} dt$. This is often satisfied for large Z_p at moderate to moderately large V_{corr}.

For the double ionization of a target with N equivalent electrons, with the same parametrization used for single ionization, the exclusive and inclusive cross sections are, respectively,

$$\sigma_{02}^{(N)} = \binom{N}{2} \frac{Z_p^4}{\overline{u_b}^{\,2}} \int P_I^{(1)}(\overline{v}b)^2 \times \left(1 - \frac{Z_p^2}{\overline{u_b}} P_I^{(1)}(\overline{v}b) - P_C(b)\right)^{N-2} 2\pi\, b\, db \tag{45}$$

and

$$s_{02}^{(N)} = \binom{N}{2} \frac{Z_p^4}{\overline{u_b}^{\,2}} \int P_I^{(1)}(\overline{v}b)^2 2\pi\, b\, db. \tag{46}$$

From Eqs. (45) and (46) we note that the MIEA predicts $s_{02}^{(N)}\overline{u_b}^{\,3}/\binom{2}{N}$ to be constant for all targets, but not $\sigma_{02}^{(N)}\overline{u_b}^{\,3}/\binom{2}{N}$. In Figs. 4(a) and 4(b) experimental data from Refs. [31] and [37] for $\sigma_{02}^{(N)}$ and $s_{02}^{(N)}$, respectively, are plotted with the parametrization suggested by the MIEA and semiclassical approximation. The dispersion of the points is larger than that obtained for single ionization with the same parametrization, but the overall behavior is quite similar (compare Figs. 2 and 4). In Fig. 4(a) the scaled exclusive cross sections for the three heaviest targets Ne, Ar, and Kr have a similar energy dependence, but with the maximum located at a different energy and a factor of 3 smaller than for He. In Fig. 4(b) all scaled inclusive cross sections present their maxima at the same energy and with approximately the same magnitude, except for Ne. The underestimated values for Ne can be explained in the same way as in the single ionization: the truncation with few terms in the sum of the experimental exclusive cross sections giving $s_{02}^{(N)}$. For $v_p/\overline{v_n}<1$ the relaxation of the target electrons seems to cause the breakdown of the MIEA with equivalent electrons. In the limit of high velocities, only the Kr target does not converge to the values of the cross sections for the other gases. The high-energy behavior can be further analyzed by considering the ratio between double and single ionization. This ratio has been extensively used to analyze double ionization in He by several projectiles [3,4]. In order to compare different targets we show in Figs. 5(a) and 5(b) the ratios between the scaled exclusive and inclusive cross sections defined as

$$\rho_{21} \equiv \frac{\sigma_{02}^{(N)}}{\sigma_{01}^{(N)}} \overline{u_b} \frac{2}{N-1} \tag{47}$$

and

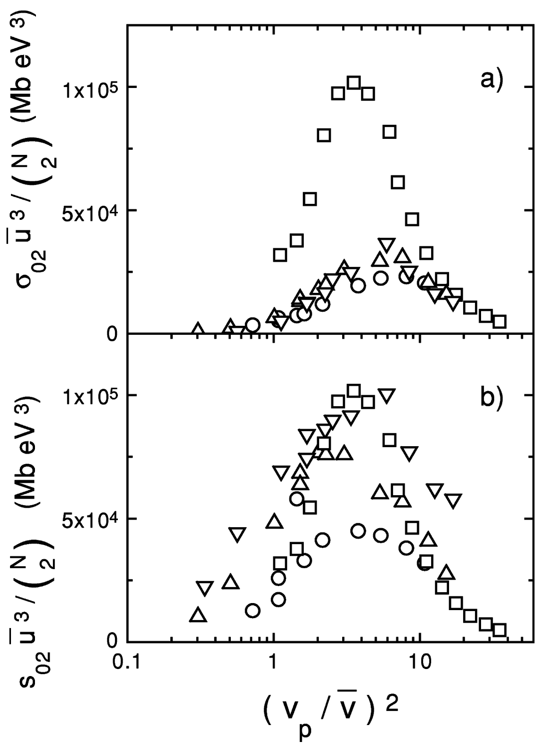

FIG. 4. Double ionization of several targets by He^{2+} projectiles for (a) exclusive and (b) inclusive cross sections. The data are from Ref. [31] (squares, He) and from Ref. [37] (circles, Ne; up triangles, Ar; down triangles, Kr).

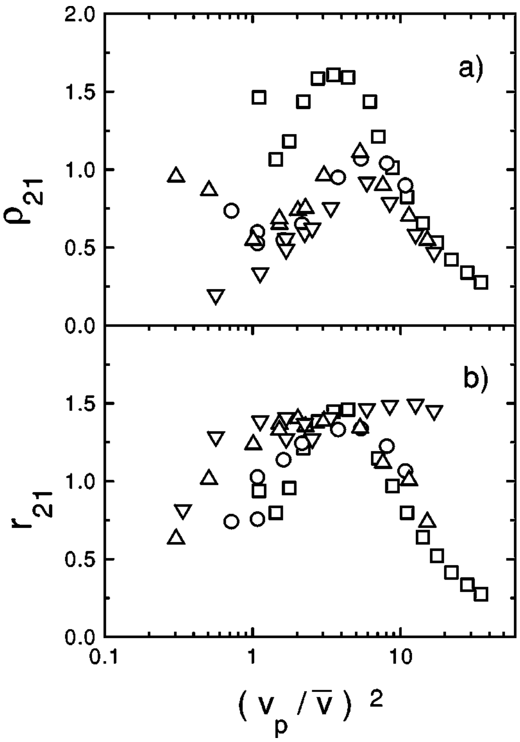

FIG. 5. Ratio of double to single ionization by He^{2+} incident on several targets. The ratio between exclusive cross sections is shown in (a) and between inclusive cross sections in (b). The data are from Ref. [31] (squares, He) and from Ref. [37] (circles, Ne; up triangles, Ar; down triangles, Kr).

$$r_{21}\equiv\frac{s_{02}^{(N)}}{s_{01}^{(N)}}\,\overline{u_b}\,\frac{2}{N-1}, \tag{48}$$

respectively.

In Fig. 5(b), at velocities corresponding to the maximum of the He double ionization, $v_p/\overline{v}\approx 2$, the experimental results for all targets coalesce. For $v_p/\overline{v}>2$, the r_{21} data for He, Ne, and Ar present the same energy dependence, but the data for Kr are almost constant with v_p. In other words, s_{02}^{Kr} has the same energy dependence as s_{01}^{Kr}. This means that s_{02}^{Kr} is dominated, for high velocities, by some postcollisional effect leading to multiple ionization. The fact that this effect appears for r_{21} but not for ρ_{21} indicates that for $v_p/\overline{v}>2$ ionization channel for three or more electrons by postcollisional effects can be a relevant ionization mechanism for Kr, the only target studied with d-shell electrons.

VI. CONCLUSIONS

The binomial and multinomial independent electron approximations are quite simple and may be easily applied to the analysis of many-electron transitions in relatively complex atomic systems without the use of intricate (but more detailed) computer codes. The BIEA and MIEA express the difficult N-electron quantum amplitude in terms of much simpler one-electron amplitudes without exchange. The BIEA and MIEA are valid when the electron correlation and exchange are small. This often occurs when the interaction of the electrons with an external potential is larger than the fluctuations in the mean field of the electron-electron interactions and exchange effects are small. For inner-shell target electrons the BIEA and MIEA tend to work because the nuclear charge of the target is relatively strong. For outer-shell target electrons considered in this paper the MIEA tends to work at intermediate collision velocities, especially for highly charged projectiles where the influence of the projectile charge dominates. At high velocity, the electron correlation tends to dominate since there is more time for the correlations to affect the collision process than the fast, weakly interacting projectile. At low velocity both electron correlation and exchange can be significant. Therefore, in this paper we have considered intermediate velocities for our many-electron targets with active outer electrons. At these intermediate velocities the cross sections and corresponding reaction rates tend to be large, so this is an important regime.

We have presented a way to express physically measurable inclusive cross sections and $\int P(\vec{b})d\vec{b}$. This is a major result of this paper. This provides a more direct connection between experiment and the effective one-electron transition probability $P(\vec{b})$ than exclusive cross sections, which specify which electrons make transitions and which do not. If the probabilities are small, i.e., $P(\vec{b})\ll 1$, then $\int P(\vec{b})d\vec{b}$ reduces to the inclusive total cross section.

Using the Schwartz inequality $\int P_\alpha P_\beta d\vec{b} \leqslant[\int P_\alpha d\vec{b}]^{1/2}[\int P_\beta d\vec{b}]^{1/2}$, we have tested the consistency of the observed cross sections in systems with active outer-shell electrons with the MIEA. In many cases considered in this paper Schwarz's inequality can be violated by a factor of 2–3, suggesting that the MIEA is not sufficient to consistently describe the observed data with high precision. The Schwartz inequality is most strongly violated when the projectile in the final state is neutral. We recommend that other data be tested in this manner.

Also we have used our inclusive cross sections to test scaling behavior based on the high-energy PWBA and Bethe scaling for $P(\vec{b})$. The PWBA and Bethe scaling hold approximately at moderately high velocities for the data considered here. Although in theory our analysis is not consistent to higher orders in Z_p^2, we do observe some consistency in practice. It is not unusual for the PWBA results to hold in regions that exceed somewhat the expected range of theoretical validity. At moderately low velocities, the MIEA could hold without following the Bethe or PWBA scaling since the MIEA can be valid for interactions of arbitrary strength. However, for strongly interacting systems we are not aware of any simple scaling properties for $P(\vec{b})$. Nevertheless, specific theories for $P(\vec{b})$ could be tested using our analysis in cases where the MIEA is valid.

ACKNOWLEDGMENTS

This work was partially supported by the Conselho Nacional de Desenvolvimento Científico e Tecnológico, Financiadora de Estudos e Projetos, Fundação de Amparo à Pesquisa do Estado do Rio de Janeiro, and MCT (PRONEX), Brazil, and partially by the Division of Chemical Sciences, Office of Basic Energy Sciences, Office of Energy Research, U.S. Department of Energy.

APPENDIX A: PROOF BY SUBSTITUTION OF THE INVERSE PAIR RELATION FOR EXCLUSIVE AND INCLUSIVE CROSS SECTIONS

In Sec. III the correspondence between the pair of equations

$$\sigma_m^{(N)} = \binom{N}{m} \int P(b)^m [1-P(b)]^{N-m} 2\pi\, b\, db, \quad \text{(A1a)}$$

$$\sum_{j=m}^{N} \binom{j}{m} \sigma_j^{(N)} = \binom{N}{m} \int P(b)^m 2\pi\, b\, db. \quad \text{(A1b)}$$

was derived by making use of the binomial inverse pair relation [16–19]. In this appendix a simpler alternative proof by substitution is presented. Taking the sum of the product of Eq. (A1a) (with the index m replaced by j) and the binomial coefficient $\binom{j}{m}$,

$$\sum_{j=m}^{N} \binom{j}{m} \sigma_j^{(N)} = \sum_{j=m}^{N} \binom{j}{m}\binom{N}{j} \times \int P(b)^j [1-P(b)]^{N-j} 2\pi\, b\, db \quad \text{(A2)}$$

$$= \int \frac{N!}{m!} \sum_{j=m}^{N} \frac{1}{(N-j)!(j-n)!} \times P(b)^j [1-P(b)]^{N-j} 2\pi\, b\, db \quad \text{(A3)}$$

$$= \int \frac{N!}{m!(N-m)!} P(b)^m \times \sum_{j=m}^{N} \frac{(N-m)!}{(j-m)!(N-j)!} P(b)^{j-m} \times [1-P(b)]^{(N-m)-(j-m)} 2\pi\, b\, db. \quad \text{(A4)}$$

In terms of binomial coefficients and with the change in the indices $j-m \equiv i$, one has

$$\sum_{j=m}^{N} \binom{j}{m} \sigma_j^{(N)} = \int \binom{N}{m} P(b)^m \sum_{i=0}^{N-m} \binom{N-m}{i} P(b)^i \times [1-P(b)]^{(N-m)-i} 2\pi\, b\, db. \quad \text{(A5)}$$

However, by the binomial expansion theorem

$$\sum_{i=0}^{N-m} \binom{N-m}{i} P(b)^i [1-P(b)]^{(N-m)-i} = 1. \quad \text{(A6)}$$

Thus

$$\sum_{j=m}^{N} \binom{j}{m} \sigma_j^{(N)} = \binom{N}{m} \int P(b)^m 2\pi\, b\, db. \quad \text{(A7)}$$

APPENDIX B: PROOF OF MULTINOMIAL INVERSION RELATIONS

For two inelastic collision channels, the multinomial probability distribution gives, for N equivalent electrons,

$$P_{m,n}^{(N)}(b) = \frac{N!}{m!n!(M-m-n)!} P_\alpha(b)^m P_\beta(b)^n \times [1-P_\alpha(b)-P_\beta(b)]^{N-m-n}, \quad \text{(B1)}$$

with

$$\sum_{m,n} P_{m,n}^{(N)}(b) = 1, \quad \text{(B2)}$$

where the sum extends over all the possible non-negative values of m and n with $n+m \leqslant N$. The cross sections are expressed in the MIEA as

$$\sigma_{m,n}^{(N)} = \frac{N!}{m!n!(N-m-n)!} \int P_\alpha(b)^m P_\beta(b)^n \times [1-P_\alpha(b)-P_\beta(b)]^{N-m-n} 2\pi\, b\, db. \quad \text{(B3)}$$

Looking at Eqs. (A1a) and (A1b) we can try the ansatz

$$s_{m,n}^{(N)} \equiv \sum_{i,j} \frac{i!j!}{m!n!(i-m)!(j-n)!} \sigma_{i,j}^{(N)}, \quad \text{(B4)}$$

where the domain of the indices of the sum will be chosen later. Thus

$$s_{m,n}^{(N)} = \sum_{i,j} \frac{i!j!}{m!n!(i-m)!(j-n)!} \frac{N}{i!j!(N-i-j)!} \times \int P_\alpha(b)^i P_\beta(b)^j [1-P_\alpha(b) - P_\beta(b)]^{N-i-j} 2\pi\, b\, db, \quad \text{(B5)}$$

$$s_{m,n}^{(N)} = \int \frac{N!}{m!n!} \sum_{i,j} \frac{1}{(i-m)!(j-n)!(N-i-j)!} \times P_\alpha(b)^i P_\beta(b)^j [1-P_\alpha(b)-P_\beta(b)]^{N-i-j} 2\pi\, b\, db, \quad \text{(B6)}$$

and

$$s_{m,n}^{(N)} = \int \frac{N}{m!n!(N-m-n)!} P_\alpha(b)^m P_\beta(b)^n \sum_{i,j} \frac{(N-m-n)!}{(i-m)!(j-n)![(N-m-n)-(i-m)-(j-n)]!} \times P_\alpha(b)^{i-m} P_\beta(b)^{j-n} [1-P_\alpha(b)-P_\beta(b)]^{(N-m-n)-(i-m)-(j-n)} 2\pi\, b\, db. \quad \text{(B7)}$$

Introducing the indices $k\equiv i-m$ and $l\equiv j-n$ ($i\equiv k+m$ and $j\equiv l+n$), we obtain

$$s_{m,n}^{(N)}=\int \frac{N!}{m!n!(N-m-n)!}P_{\alpha}(b)^{m}P_{\beta}(b)^{n} \times\sum_{k,l} \frac{(N-m-n)!}{k!l![(N-m-n)-k-l]!}P_{\alpha}(b)^{k}P_{\beta}(b)^{l} \times[1-P_{\alpha}(b)-P_{\beta}(b)]^{(N-m-n)-k-l}2\pi\ b\ db. \tag{B8}$$

If we choose this sum to extend over all the possible nonnegative values of k and l with $k+l\leqslant N-m-n$,

$$\sum_{k,l} \frac{(N-m-n)!}{k!l![(N-m-n)-k-l]!}P_{\alpha}(b)^{k}P_{\beta}(b)^{l} \times[1-P_{\alpha}(b)-P_{\beta}(b)]^{(N-m-n)-k-l}=1 \tag{B9}$$

and

$$\sum_{i,j} \frac{i!j!}{m!n!(i-m)!(j-n)!}\sigma_{i,j}^{(N)} =\int \frac{N!}{m!n!(N-m-n)!}P_{\alpha}(b)^{m}P_{\beta}(b)^{n}2\pi\ b\ db, \tag{B10}$$

where, to be consistent with the choice for the domain of k and l, the sum over i and j must extend over $i+j\leqslant N$ with $i\geqslant m$ and $j\geqslant n$. In terms of binomial coefficients and cross sections we can write

$$\sigma_{m,n}^{(N)}=\frac{N!}{m!n!(N-m-n)!}\int P_{\alpha}(b)^{m}P_{\beta}(b)^{n} \times[1-P_{\alpha}(b)-P_{\beta}(b)]^{N-m-n}2\pi\ b\ db, \tag{B11}$$

$$\sum_{i,j}\binom{i}{m}\binom{j}{n}\sigma_{i,j}^{(N)}=\frac{N!}{m!n!(N-m-n)!} \times\int P_{\alpha}(b)^{m}P_{\beta}(b)^{n}2\pi\ b\ db. \tag{B12}$$

The generalization of this result for any number of collision channels M is straightforward

$$\sigma_{n_1,\ldots,n_M}^{(N)}=\frac{N!}{n_1!\cdots n_M!(N-n_1-\cdots-n_M)!} \times\int P_{\alpha_1}(b)^{n_1}\cdots P_{\alpha_M}(b)^{n_M}[1-P_{\alpha_1}(b)-\cdots -P_{\alpha_M}(b)]^{N-n_1-\cdots-n_M}2\pi\ b\ db, \tag{B13}$$

$$\sum_{i_1,\ldots,i_M}\binom{i_1}{n_1}\cdots\binom{i_M}{n_M}\sigma_{i_1,\ldots,i_M}^{(N)} =\frac{N!}{n_1!\cdots n_M!(N-n_1-\cdots-n_M)!} \times\int P_{\alpha_1}(b)^{n_1}\cdots P_{\alpha_M}(b)^{n_M}2\pi\ b\ db, \tag{B14}$$

where the sum over $i_1,i_2,\ldots,j$ must extend over $i_1+i_2+\cdots+i_M\leqslant N$ with $i_1\geqslant n_1$, $i_2\geqslant n_2,\ldots,i_M\geqslant n_M$.

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