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SEVERAL MANIFESTATIONS OF PAULI CORRELATIONS IN ENERGETIC ION-ATOM COLLISIONS*

Richard L. Becker
Physics Division, Oak Ridge National Laboratory
Oak Ridge, TN 37831-6373, USA

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Richard L. Becker
Physics Division, Oak Ridge National Laboratory
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1. INTRODUCTION

The most usual foundation of atomic structure theory is an independent particle model (IPM) in which the electron-electron interactions are treated in a mean field approximation. When the Pauli Exclusion Principle is enforced by employing an anti-symmetric wave function, we refer to an independent Fermi particle model (IFPM). The IFPM contains correlations between electrons. These "statistical" or Pauli correlations are most simply exhibited by the pair-correlation function (PCF). For the model system (called "jellium") of an electron gas embedded in a uniform, charge neutralizing, background of positive charge the IFPM gives a PCF which remains constant with r_{12} for spin singlets, but which goes to zero as $r_{12} \rightarrow 0$ for spin-triplet pairs. This decrease is referred to as the Fermi hole.¹ For the exact pair-correlation function, which includes the residual electron-electron interactions, the spin singlet PCF goes to zero as $r_{12} \rightarrow 0$ (the Coulomb hole) and the triplet PCF goes to zero even more rapidly (Coulomb plus Fermi hole). The correlations which result from the residual electron-electron interaction² are usually called dynamical electron-electron correlations. The physical observables of an atomic system can be written as the sum of an IFPM part and a remainder, referred to as the (dynamical) correlation part, which arises from the residual interactions.

The magnitudes of the statistical (Pauli) and dynamical (residual interaction) correlations depend on the prescription used for the mean field. A change in the mean field clearly requires a compensating change in the value of the dynamical-correlation part of any observable. The problem of optimizing the mean field arises. For static atomic structure, one traditionally minimizes the IFPM energy (subject to taking the electron-electron interactions only to first order) and obtains the Hartree-Fock (HF) mean field. It has the very desirable feature (Koopmans' theorem³) that the HF energy eigenvalue of an occupied spin-orbital is equal to its removal energy (ionization potential). However, the HF choice is not unique. If, following K. Brueckner, one allows ladders of electron-electron interactions in the definition of the mean field, one obtains an independent-pair model which contains the pair (or

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geminal) wave functions of Bethe and Goldstone, which display along with the Fermi hole a good approximation to the Coulomb hole. The residual correlation energy is greatly reduced. The Brueckner approximation loses the Koopmans' property, but it is regained in the propagator-renormalized Brueckner-Hartree-Fock (RBHF) approximation.⁴

In our discussion of Pauli correlation effects in collisions, we shall limit consideration to a fixed basis of spin-orbitals of the target, given by the static HF approximation, together with hydrogenic orbitals for electrons captured by the projectile. Moreover, we shall restrict attention to closed shell cases or to the case with one half-occupied s-shell, so that the mean field has spherical symmetry. The case of more general open shells requires multiplet theory which, strictly speaking, goes beyond the IPM by involving a linear combination of determinants. In the case discussed here we can use the m-scheme in which many-electron states are specified by the quantum numbers $k = (n, l, m_l, m_s)$ of each occupied spin-orbital. The initial state of an F-electron system will be specified by the spin-orbital labels $h_1, \dots, h_F$. Reactions will be described in terms of occupancies and vacancies of spin-orbitals.

For our application of the IPM to collisions an important preliminary notion is the description of reactions on a scale of inclusiveness from fully exclusive to fully inclusive.^{5,6} A fully exclusive reaction is one which leads to a uniquely specified final state, $(k_1, \dots, k_F)$. At a given value, b , of the impact parameter the probability of the exclusive reaction $(h_1, \dots, h_F) \rightarrow (k_1, \dots, k_F)$ will be denoted by

$$P^{k_1 \dots k_F}(b; h_1 \dots h_F) = \left| A^{k_1 \dots k_F}(b; h_1 \dots h_F) \right|^2. \quad (1)$$

Final state occupancies will always be written as superscripts and vacancies as subscripts; initial state occupancies, if needed, will be written on line within parentheses. Any experimental set-up for which more than one final states are accepted will be said to measure a partially inclusive reaction. There are two commonly occurring ways of introducing inclusiveness. The first is for the state k_i of an electron not to be uniquely specified, but rather to be restricted only to some set of states, such as a shell, or the continuous spectrum (for direct ionization), or to states of the projectile (for charge transfer to the projectile). Here we speak of hyperinclusive reactions. The second way is for the final situation to be specified only in terms of fewer than the total number of electrons (F) in the system. Thus, $P_k(h_1 \dots h_F)$, which specifies only that the final state contains a vacancy (hole) in the spin-orbital k , is an inclusive-single-vacancy probability. It includes (i.e. is more inclusive than) the inclusive-double-vacancy probability, $P_{k,k}$.

An important class of reactions is defined by those in which only the number of final occupancies (and hence the number of final vacancies) in a shell (or in each of several shells) is specified. We call these number-exclusive hyperinclusive (NEHI) reactions.⁶ The simplest case is for a shell with only two states. Consider the example in which the NEHI probabilities are given by the binomial distribution

$$p_v^{2-v} = \binom{2}{v} p^v (1-p)^{2-v}, \quad v = 0, 1, 2, \quad (2)$$

where p is the vacancy probability per electron, and therefore $Q_1 \equiv 2p$ is the inclusive-single-vacancy expected value. Then

$$p_0^2 = (1-p)^2, \quad p_1^1 = 2p - 2p^2, \quad p_2^0 = p^2 \quad (3)$$

and

$$Q_1 = p_1^1 + 2p_2^0, \quad (4a)$$

i.e. the inclusive-single-vacancy expected value ($0 < Q_1 < 2$) is equal to the exclusive-single-vacancy probability ($0 < p_1^1 < \frac{1}{2}$) plus twice the double-vacancy probability. Similarly,

$$Q^1 = 2(1-p) = p_1^1 + 2p_0^2 = 2 - Q_1 \quad (4b)$$

Consider the slightly more general case of the K-shell without assuming a binomial distribution. There are four particular inclusive probabilities which refer to the occupancy or vacancy of the two spin-orbitals of the K-shell, namely, $p_{1s\uparrow, 1s\uparrow}^{1s\uparrow}$, $p_{1s\uparrow, 1s\downarrow}^{1s\uparrow}$, and $p_{1s\downarrow, 1s\downarrow}^{1s\downarrow}$. Two of these are NEHI probabilities,

$$p_{K0}^{K2} = p_{1s\uparrow, 1s\uparrow}^{1s\uparrow}, \quad p_{K2}^{K0} = p_{1s\downarrow, 1s\downarrow}^{1s\downarrow}. \quad (5)$$

(If there are only two electrons in the system, p_{K0}^{K2} is not inclusive.) The third NEHI probability is

$$p_{K1}^{K1} = p_{1s\uparrow, 1s\downarrow}^{1s\uparrow} + p_{1s\downarrow, 1s\uparrow}^{1s\downarrow}. \quad (6)$$

We have the particular inclusive-single-occupancy probabilities

$$p^{1s\uparrow} = p_{1s\uparrow, 1s\uparrow}^{1s\uparrow} + p_{1s\downarrow, 1s\uparrow}^{1s\downarrow}, \quad p^{1s\downarrow} = p_{1s\uparrow, 1s\downarrow}^{1s\uparrow} + p_{1s\downarrow, 1s\downarrow}^{1s\downarrow} \quad (7)$$

and, hence, the hyperinclusive single-K-occupancy expected value

$$Q^{K1} \equiv p^{1s\uparrow} + p^{1s\downarrow} = p_{K1}^{K1} + 2p_{K0}^{K2}. \quad (8a)$$

Similarly,

$$Q_{K1} \equiv p_{1s\uparrow} + p_{1s\downarrow} = p_{K1}^{K1} + 2p_{K2}^{K0}. \quad (8b)$$

Since

$$P_{1s\downarrow} = 1 - P^{1s\uparrow} \text{ and } P_{1s\uparrow} = 1 - P^{1s\downarrow}, \quad (9)$$

it follows that Q^{K1} and Q_{K1} are not probabilities because

$$Q^{K1} + Q_{K1} = 2. \quad (10)$$

For this reason we have called them "expected values" and have used for them a symbol other than P. Since the inclusive-double probabilities in a $j=1/2$ shell are the same as the exclusive-double ones, i.e.

$$Q^{K2} \equiv P_{K0}^{K2}, \quad Q_{K2} \equiv P_{K2}^{K0}, \quad (11)$$

we can write the inverses of Eqs. (8a) and (8b) as

$$P_{K1}^{K1} = Q^{K1} - 2Q^{K2} = Q_{K1} - 2Q_{K2}. \quad (12)$$

Whether to use a NEHI probability or a number-nonexclusive expected value in describing an experiment depends on the experimental conditions. For example, if an experiment to measure K-hole production does not distinguish between the K X rays (or the Auger electrons) from the K^{-1} and K^{-2} configurations, then Q_{K1} is relevant because the K^{-2} configuration gives rise to two X rays (or two Auger electrons) in the limit in which the fluorescence yield is 1 (or 0). If the two configurations are distinguished, then $P_{K1}^{K1} + 1 \cdot P_{K2}^{K0}$ is relevant for K^{-1} and P_{K2}^{K0} for K^{-2} .

The formalism has been extended⁶ to shells with an arbitrary number of spin-orbitals and to two or more shells (or subshells). For the investigation of Pauli correlations, we must deal with cases where two or more occupancies, two or more holes, or where at least one occupancy together with at least one vacancy are specified. In the past we have studied in some detail the case of K_α satellites and hypersatellites, where one or two K vacancies are produced along with one or more vacancies in the L-shell. (See especially Refs. 7 and 8.) If one ignores the Pauli exchange terms (PETs), one obtains^{9,6} at a given value of the impact parameter a binomial distribution over the L-shell vacancies, or, if one distinguishes the subshells, a multinomial distribution. These distributions had been postulated earlier,¹⁰ and have been widely and successfully used. We found^{7,8} that the PET terms tend to be small because of a tendency toward random phases in the transition amplitudes. Consequently, the PET terms result in only a slight change in the mean L-shell vacancy probability per electron, $\bar{p}_L$, and a slight narrowing of the distribution relative to the binomial.

Here we shall discuss reactions in which vacancies in the K or L shell of the target are measured in coincidence with the change of charge of the projectile. When the number of electron captures is >1 , we are studying coincidences of the particle-hole sort, in contrast to the multiple-hole case discussed above. We begin in Section 2 with a description of the PETs in the IFPM. Section 3 discusses K-vacancies in coincidence with exclusively single electron transfer to the projectile

for the case of $\text{He}^{2+} + \text{Ne}$. Section 4 treats multiple L-shell vacancies in coincidence with 0, 1, or 2 electron transfers, again for the example of $\text{He}^{2+} + \text{Ne}$. In Section 5 we consider the attempt to isolate K-to- $\bar{\text{K}}$ transfer (the bar designates a shell of the projectile) by taking linear combinations of K-vacancy cross sections obtained with projectiles initially having 0, 1, or 2 $\bar{\text{K}}$ electrons. An important issue faced there is the extent to which the projectile's $\bar{\text{K}}$ electrons can be treated as inert (passive).

2. THE PAULI EXCHANGE TERMS IN THE IFPM

All the PETs can be expressed in terms of the single-electron transition-density matrix elements^{9,6}

$$a_{k,k'}^{(2)}(b) = \sum_h^{\text{occ}} a_{kh}^* (b) a_{k'h}(b), \quad (13)$$

which provide a mechanism for the coherent enhancement or suppression of otherwise incoherent independent-electron transitions. Because the Coulomb interaction does not involve the intrinsic spin of the electrons, $a_{k,k'}^{(2)} \approx 0$ unless the intrinsic spins of k and k' have the same magnetic quantum number ($\sigma = \sigma'$), and only those initially occupied spin-orbitals, h , contribute which have this spin projection.

If we specify one occupancy and one vacancy, the particular inclusive probability is

$$p_{k,k'}^k = p^k p_{k'}^{k'} + \delta_{\alpha_k, \alpha_{k'}} \left| a_{k,k'}^{(2)} \right|^2. \quad (14)$$

When the PETs are neglected one obtains what we call the single-particle model (SPM).^{6,8} In Eq. (14)

$$p^k = \sum_h^{\text{occ}} \left| a_{kh} \right|^2 \quad (15a)$$

and

$$p_{k,k'}^{k'} = 1 - p^{k'} = 1 - \sum_h^{\text{occ}} \left| a_{k'h} \right|^2 \quad (15b)$$

where occ stands for the F initially occupied spin-orbitals. Thus, $p^k p_{k'}^{k'}$ contains unphysical Pauli-violating terms of the form $-\sum_h^{\text{occ}} \left| a_{kh} a_{k'h} \right|^2$. These are cancelled by the terms with $h' = h$ in

$$\left| a_{k,k'}^{(2)} \right|^2 = \sum_h^{\text{occ}} \left| a_{kh} a_{k'h} \right|^2 + 2\text{Re} \sum_{h < h'} a_{kh}^* a_{kh'} a_{k'h} a_{k'h'}^* \quad (16)$$

Hence

$$P_k^k = P^k - \sum_h^{\text{occ}} \left| a_{kh} \right|^2 \sum_{h'(\neq h)}^{\text{occ}} \left| a_{k'h'} \right|^2 + 2\text{Re} \sum_{h < h'} a_{kh}^* a_{kh'} a_{k'h} a_{k'h'}^* \quad (17)$$

For the case where the vacancy is specified in one of the initially occupied states, say $k' = h_1$, then $|a_{k,h_1}^{(2)}|^2$ contains the term

$$|a_{k,h_1}|^2 |a_{h_1,h_1}|^2 = |a_{k,h_1}|^2 [1 - (1 - |a_{h_1,h_1}|^2)].$$

When the projectile only weakly perturbs a target, the probability that the electron in the target state h_1 remains there, $|a_{h_1,h_1}|^2$, is nearly unity. The remaining factor, $|a_{k,h_1}|^2$, represents the probability that the coincident occupancy of spin-orbital k and vacancy in h_1 were produced by the single-electron transition (SET) from h_1 to k . This SET contribution,

$$\text{SET } P_{h_1}^k \equiv |a_{k,h_1}|^2 \quad (18)$$

is often the dominant term in $P_{h_1}^k$. The SPM term, $P^k P_{h_1}$, contains $|a_{k,h_1}|^2$, but it is multiplied by the usually small factor

$$P_{h_1} = 1 - |a_{h_1,h_1}|^2 - \sum_{h \neq h_1} |a_{h_1,h}|^2. \quad (19)$$

Thus, $P_{h_1}^k$ is a coincidence probability in which the exchange (PET) contribution is sometimes much larger than the direct (SPM) contribution. We shall see this quantitatively in the next section. We also note here that $P_{h_1}^k$ can be decomposed into a SET term and a double-electron-transition term (DET) where

$$\text{DET } P_{h_1}^k = P^k P_{h_1} + \left[|a_{k,h_1}^{(2)}|^2 - |a_{k,h_1}|^2 \right] \quad (20)$$

or, symbolically, $\text{DET} = \text{SPM} + (\text{PET-SET})$.

Following my talk at the IXth International Symposium on Ion-Atom Collisions (ISIAC) last July in Bad Soden, West Germany, Jim McGuire raised the question whether one could experimentally determine a PET. My answer is that there is no (single) experiment in which the SPM term is absent. However, one could do two or more related experiments to determine the more inclusive factors (like P^k and $P_{k'}$ in Eq. (14)) which appear in the SPM term. Then one could subtract the measured SPM term to obtain the PET term. A related question, with a similar answer, is whether one can isolate a particular SET contribution. Experimentalists have been trying for some time to determine the SET part of K to $\bar{K}$ charge transfer by varying the ionic charge of the projectile and taking differences of the K -vacancy cross sections. This procedure involves the assumption that the initial one or two $\bar{K}$ electrons affect the cross section only by what I call "Pauli blocking", a striking effect of Pauli correlations. We discuss this effect in Section 5.

3. Ne K-VACANCIES IN COINCIDENCE WITH SINGLE ELECTRON TRANSFER TO He^{2+}

Röddbro et al.¹¹ have measured the cross section for producing a Ne K Auger electron in coincidence with He^+ in $\text{He}^{2+} + \text{Ne}$ collisions for impact energies (~ 0.5 to 1.4 MeV/amu) near the peak in the K-vacancy cross section. We calculate cross sections semiclassically (impact-parameter method) from

$$\sigma = 2\pi \int db \cdot b [P(b) \text{ or } Q(b)] \quad (21)$$

We show in Fig. 1a the experimental data together with coupled channels calculations. The older calculations,¹² (short-dashed curve), above 0.4 MeV/amu, are of the quantity $1.2 \sigma_{\bar{K}^1 K^1}^{\bar{K}^1}$ calculated with a single-center-expansion (SCE) employing pseudoeigenstates of the Ne HF field. The Oppenheimer factor 1.2 includes approximately the charge transfer into excited states of the projectile.¹³ The cross section $\sigma_{\bar{K}^1 K^1}^{\bar{K}^1}$ is inclusive of both double transfer and double K-vacancy production. The three other curves were calculated with the unitary version of the one-and-a-half-center expansion method (OHCEU)¹⁴ in coupled-channels theory. The long-dashed curve is again for $1.2 \sigma_{\bar{K}^1 K^1}^{\bar{K}^1}$; the full curve is for $1.2 \sigma_{\bar{K}^1 K^1}^{\bar{K}^1, K^1}$, which involves purely single charge transfer to the $\bar{K}$ shell; and the long- and short-dashed curve represents $1.2 \sigma_{\bar{K}^1 K^1}^{\bar{K}^1 K^1}$, which involves exclusively single charge transfer to the $\bar{K}$ shell and exclusively single K-vacancy production. As a generalization of Eqs. (8a) and (8b), one has^{15, 8}

$$Q_{K^1}^{\bar{K}^1} = Q_{\bar{K}^1 K^1}^{\bar{K}^1 K^1} + 2 \left(Q_{\bar{K}^0 K^1}^{\bar{K}^2 K^1} + Q_{\bar{K}^1 K^2}^{\bar{K}^1 K^0} \right) + 4 Q_{\bar{K}^0 K^2}^{\bar{K}^2 K^0} \quad (22)$$

Fig. 1. Cross section for a single K-vacancy in Ne in coincidence with single electron transfer to He^{2+} . a) Experimental data from Ref. 11 and coupled-channels calculations described in the text. b) Components of the theoretical $\sigma_{\bar{K}^1 K^1}^{\bar{K}^1}$ (full curve). The SPM, PET, and SET contributions are identified in the text.

For He^{2+} projectiles the double K-vacancy terms are negligibly small. The double transfer also is rather small, but it causes $\sigma_{K1}^{\bar{K}1}$ to overestimate $\sigma_{K1K1}^{\bar{K}1\bar{K}1}$ by about 25% for E/A below 100 keV/amu.

Figure 1b shows the decomposition of

$$\sigma_{K1K1}^{\bar{K}1} = \sigma_{K1K1}^{\bar{K}1\bar{K}1} + 2\sigma_{K1K2}^{\bar{K}1\bar{K}0} \quad (23)$$

(full curve) into its SPM part (long- and short-dashed curve) and its PET part (long- and double short-dashed curve). The PET part is much larger than the SPM part both at large and small impact energies. However, the SPM part becomes as much as twice the PET part for intermediate energies where both the L-shell contribution to electron transfer and the K-shell vacancy production are appreciable, so that the product $P_L \sigma_K$ is large. The SET contribution to the PET part is shown as the dashed curve. It lies above the full PET curve at all energies and, in fact, provides a rather good approximation to $\sigma_{K1K1}^{\bar{K}1}$ except at intermediate energies. Without knowledge of the IFPM theory Rødbro et al.¹¹ discussed their measured coincidence cross section, which they called R, as the sum of our SET contribution (their σ_{CK}) and a "double step (DS)" contribution, $P_L \sigma_{VK}$, where their P_L represents the probability for electron transfer from the L-shell at a small value of the impact parameter appropriate for K-vacancy production and where their σ_{VK} stands for the (inclusive-single) K-vacancy production cross section. Thus, their $P_L \sigma_{VK}$ is a close approximation to our SPM contribution. They found that their estimated DS contribution was "much too large to be consistent with the present experimental finding for 0.5 MeV [per amu] He^{2+} on neon. ...We do not at present have an explanation for the failure of the...analysis". I believe the explanation lies in Eq. (20), which shows that the DET (or DS) contribution contains not only the SPM term, but also a term PET-SET, which we have seen to be negative. At 0.5 MeV/amu our OHCEU calculation gives DET/SPM = 24%. At lower energies this ratio increases to about 50%, but at higher energies it decreases steadily, becoming only 5% at E/A = 1.25 MeV/amu.

Our OHCEU calculations also yield cross sections for K-vacancies in coincidence with 0 or 2 electron transfers to the alpha particle. Instead of showing these we turn to cross sections for multiple vacancies in the L-shell of neon in coincidence with 0, 1, or 2 transfers from the L-shell, for which very recent experimental data are available.

4. Ne L-VACANCIES IN COINCIDENCE WITH 0, 1, OR 2 ELECTRON TRANSFERS TO He^{2+}

R. DuBois¹⁶ has measured the final charges on both the projectile and target for He^{2+} collisions with Ne in the energy range from about .01 to .5 MeV/amu. Cross sections for reactions with up to four vacancies were obtained. The shells in which the holes are produced were not identified experimentally, but in this fairly low energy region the K-vacancy production is known to be much less than the L-vacancy

production. We have performed OHCEU, coupled-channels calculations of $\sigma_{K^{2-n}L^v}^{K\alpha}$ for $n = 0, 1$, and 2 and $v = 1, 2, 3$, and 4 , using the IFPM. As in the preceding sections the expressions for these cross sections can be written as the sum of an SPH and a PEL part. Whereas in Section 3 the double K-vacancy contribution was negligible, here the multiple vacancy cross sections are appreciable. For a collision which produces v vacancies the dominant terms involve v electron transitions. They appear in the PETs. The other terms involve more than v electron transitions. A detailed discussion of the relative magnitudes of these components will be given elsewhere. Here we show in Fig. 2 the quality of the agreement between the calculations and the

Fig. 2. Experimental¹⁶ and OHCEU, coupled-channels calculations for v vacancies in (the L-shell of) neon in coincidence with $n = 0, 1$, or 2 electron transfers to He^{2+} . Experimental points: ∇ , $v = 1$; $\blacksquare$, $v = 2$; $\times$, $v = 3$; and $\blacktriangle$, $v = 4$. Theoretical curves: long-dash-short dash, $v = 1$; long-dash-two-short-dashes, $v = 2$; medium-sized-dash, $v = 3$; short-dash, $v = 4$. a) No electron transfer (purely direct ionization). The curves for $v = 3$ and 4 have been scaled down by factors of $2/3$ and $1/5$, respectively. b) Single electron transfer. c) Double electron transfer. The curves for $v = 3$ and 4 have been scaled by $1/2$ and $1/3$, respectively.

data. For $v = 1$ and 2 the calculated cross sections have about the same magnitudes as the experimental ones. It is quite common that, as the number of vacancies increases, the IFPM gives cross sections which are too large because it fails to take into account that the second and higher ionization potentials are greater than the first.⁷ The present calculations are no exception, so we have scaled down some of the cross sections for $v = 3$ and 4 in order to make it easier to compare the theoretical and experimental energy dependences.

One aspect of the greater sensitivity of the coincidence experiment in comparison with "singles" experiments on vacancy production is shown in Fig. 3. This shows that the mean L-shell vacancy probability per electron, beyond that implied by the constraint of n electron transfers, is a function of n . It is less likely that an

additional L-shell electron is removed "after" two transfers than "after" one transfer, and less likely "after", one transfer than "after" no transfer. We believe this is the first time such an effect has been calculated. The effect should be enhanced if one could employ more accurate second- and higher-ionization potentials.

Fig. 3. Mean L-shell vacancy probability per electron in Ne reduced by $n/8$, where n is the number of L-shell electrons transferred to He^{2+} , as calculated by the IFPM-OHCEU-coupled-channels method, versus the impact parameter in units of the Bohr radius divided by Z_{Ne} . Full curve, $n = 0$; short-dash, $n = 1$; two short dashes, $n = 2$.

5. COMPARISON OF PREDICTIONS FOR K TO $\bar{K}$ TRANSFER BY THE IFPM, AND BY PASSIVE- $\bar{K}$ -ELECTRON APPROXIMATIONS TO IT, WITH DATA FOR $\text{Cl}^{17+}, 16+, 14+ + \text{Ti}$

In several papers,¹⁷ James Hall, Pat Richard and collaborators have sought to measure the SET part of K to $\bar{K}$ electron transfer, generated (see Eq. (21)) by

$$2 \left| a_{\bar{1}S, 1S} \right|^2 \equiv 2P(1s+ - \bar{1}S+) \equiv Q(K^1 + \bar{K}^1) \quad (24)$$

in the nearly symmetric system $^{17}\text{Cl} + ^{22}\text{Ti}$ at high impact energies. They assumed that, in our notation,¹⁸ $\sigma(K^1 + \bar{K}^1) = \sigma_{K^1}^{K^1} - 2\sigma_{K^1}^{\bar{K}^1}$, where the superscript labels the number of $\bar{K}$ electrons initially on the projectile (0 corresponds to Cl^{17+} and 2 corresponds to Cl^{15+}).

In the IFPM the sums over initially occupied spin-orbitals include those centered on the projectile, if any, and thus

$$\bar{1}S^+_p{}_{1s+} = {}^{op}{}_{1s+} - \left| \bar{1}S^+_p{}_{1s+, \bar{1}S+} \right|^2, \quad (25a)$$

provided that

$${}^{op}{}_{1s+} \equiv 1 - \sum_{h_T}^{\text{occ}} \left| {}^0a_{1s+, h_T} \right|^2 = 1 - \sum_{h_T}^{\text{occ}} \left| \bar{1}S^+_p{}_{1s+, h_T} \right|^2. \quad (25b)$$

This assumption may be violated statically by the screening of the projectile nucleus

by the $\overline{1s\uparrow}$ electron, and dynamically if the $\overline{1s\uparrow}$ electron is "active" (i.e., makes transitions other than to the $1s\uparrow$ state) and if its transitions indirectly affect the elements $a_{1s\uparrow, h_T}$. But if (25a) holds, then the IFPM predicts that

$$Q(K^1 - \overline{K}^1) = 2(^0Q_K - ^1Q_K) = ^0Q_K - ^2Q_K, \quad (26)$$

which is the same as that assumed by Hall et al. except that (26) relates to the inclusive single K-vacancy cross section (see (8b) or (4a)) rather than to the exclusively single one. From the completeness relation for the pseudostates in our coupled-channels basis, which contains only one orbital centered on the projectile ($\overline{1s}$), we can write an alternative expression for the vacancy probabilities, namely,

$$^0p_{1s\uparrow} = \sum_{k_T}^{\text{unocc}} \left| ^0a_{k_T, 1s\uparrow} \right|^2 + \left| ^0a_{\overline{1s\uparrow}, 1s\uparrow} \right|^2 \quad (27a)$$

and

$$\overline{1s\uparrow}p_{1s\uparrow} = \sum_{k_T}^{\text{unocc}} \left| \overline{1s\uparrow}a_{k_T, 1s\uparrow} \right|^2. \quad (27b)$$

This shows that (25a) holds provided that

$$\left| ^0a_{\overline{1s\uparrow}, 1s\uparrow} \right|^2 = \left| \overline{1s\uparrow}a_{\overline{1s\uparrow}, 1s\uparrow} \right|^2 \quad (28a)$$

and

$$\sum_{k_T}^{\text{unocc}} \left| ^0a_{k_T, 1s\uparrow} \right|^2 = \sum_{k_T}^{\text{unocc}} \left| \overline{1s\uparrow}a_{k_T, 1s\uparrow} \right|^2. \quad (28b)$$

Equation (25b) can be obtained directly from (28a,b) by the completeness relation.

We show in Fig. 4 the comparison between the experimental data¹⁷ and the IFPM-OHCEU calculations¹⁸ (full curves) for the inclusive-single K-vacancy production. In Fig. 4c there are no data for $^{17}\text{Cl}^{15+}$ because this beam contained some ions in the metastable $1s2s\ ^3S$ configuration. Moreover, the ionic charge actually used varied from 14 at $E = 15$ MeV/amu down to 5 at $E = 0.5$ MeV/amu. Consequently, the data are lower than the data which would have been obtained for $\text{Cl}^{15+}(1s^2)$ ions. The last equality in Eq. (26) implies that the open circles in Fig. 4c should agree with the unavailable data from $\text{Cl}^{15+}(1s^2)$ and, hence, should lie above or be nearly equal to the closed circles. This is not the case at several energies. Some of the values of

$$\sigma_K^{17+} - 2(\sigma_K^{17+} - \sigma_K^{16+}) = \sigma_K^{16+} - (\sigma_K^{17+} - \sigma_K^{16+})$$

(open circles) are actually negative. Even though the error bars on the open circles are very large, it appears that the simple Pauli blocking effect, which leads to Eq. (26), is not the whole story.

The theoretical IFPM inclusive-single K-vacancy cross section for bare chlorine

ions in Fig. 4a lies below the data by from 30 to 50 per cent. This suggests that the charge transfer to the $\bar{K}$ -shell as calculated with the OHCEU method, for this strongly interacting system, is too small. This is confirmed in Fig. 5, which compares the calculated (see Eq. (24) $\sigma(K^1 + \bar{K}^1)$) (full curve) with differences of experimental of cross sections (see Eq. (26)).

Also shown in Figs. 4b, 4c, and 5 are curves calculated from two models which are approximations to the full IFPM. The first, which gives the long-dashed curves, contains the assumption that the channels for electron transfer between the $\bar{K}$ -shell and all the target-centered states are closed when the $\bar{K}$ state is initially occupied, i.e. the $\bar{K}$ -electron is inert. The second approximate model is based on a decomposition of the K-vacancy cross section into parts with 0, 1, and 2 electron transfers. Thus, in the IFPM we can write

Fig. 4. Inclusive-single ^{22}Ti K-vacancy cross sections produced by $^{17}\text{Cl}^{19+}$ ions. (a) $^0\sigma_K$, $q = 17$. (b) $^1\sigma_K$, $q = 16$. (c) Theory, $^2\sigma_K$ ($q = 15$). Experiment: $^{17}\text{Cl}^{19+}$ closed circles, $^2\sigma_K$, $q < 14$; open circles, $\sigma_K^{17+} - 2(\sigma_K^{17+} - \sigma_K^{16+})$. Full curves, IFPM. Dashed curves, results of two models which are approximations to the IFPM as described in the text.

$${}^0\sigma_K = {}^0\sigma_{\bar{K}^0, K} + {}^0\sigma_{\bar{K}^1, K} + {}^0\sigma_{\bar{K}^2, K} \quad (29)$$

and similar expressions when the projectile has initially one or two $\bar{K}$ electrons. The second passive- $\bar{K}$ -electron model, which gives the short-dashed curves, is defined by the assumption that

$${}^1\sigma_K = {}^0\sigma_{\bar{K}^0, K} + \frac{1}{2} {}^0\sigma_{\bar{K}^1, K} \quad (30a)$$

and

$${}^2\sigma_K = {}^0\sigma_{\bar{K}^0, K} \quad (30b)$$

One sees from Figs. 4 and 5 that these models give results rather close to that of the full IFPM. A detailed discussion is given in Ref. 18, which also treats double K to K transfer. Much more work, both experimental and theoretical, is needed in order to distinguish the effects of Pauli correlations, screening, and projectile-electron excitations in energetic collisions involving incident projectiles which carry electrons. Pauli blocking is also beginning to be studied¹⁹ in inner shell excitation with high resolution 0° projectile Auger electron spectroscopy.

Fig. 5. Differences of inclusive-single Ti K-vacancy cross sections from $Cl^{q+} + Ti$ collisions: — Experiment: 17 full circles, $\sigma_K^{17+} - \sigma_K^{14+}$ (q varies with E); full squares, $2(\sigma_K^{17+} - \sigma_K^{16+})$. Theory: full curve, IFPM inclusive-single K to $\bar{K}$ transfer cross section, which equals ${}^0\sigma_K - {}^2\sigma_K = 2({}^0\sigma_K - {}^1\sigma_K)$; long-dashed curve, the same but with closed channels for transfer to the $\bar{K}$ -shell when an initial $\bar{K}$ -electron is present; short-dashed curve, ${}^0\sigma_{\bar{K}^1, K} + {}^0\sigma_{\bar{K}^2, K}$.

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