(INVITED PAPER - 8th Conference on the Application of Accelerators in Research and Industry, Nov. 12-14, 1984, Denton, TX 76203)

CONF-841117--32

THEORY OF K^nL^v MULTIPLE VACANCY PRODUCTION BY HEAVY IONS

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CONF-841117--32

DE85 004443

ABSTRACT

Observation of intensities of K_α x-ray or Auger satellites and hypersatellites together with fluorescence yields provides knowledge of KL^v and K^2L^v vacancy distributions produced by ion-atom collisions. The traditional theory used since ~1972 employs a single-particle model and a weak-coupling ionization approximation. We review our recent extensions of the theory to include Pauli correlations in the independent Fermi particle model, a unitary collision theory in the first Magnus and coupled-channels approximations, electron transfer to the projectile, and contributions from shakeoff which interfere with the collision-induced amplitudes.

*Research sponsored by U.S. Department of Energy, Division of Basic Energy Sciences, under Contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

†Research supported by the National Science Foundation under Grant No. PHY-79-09146.

1. Introduction

A fundamental theoretical interest in collisions of heavy projectile ions ($Z_p >> 1$) with atomic systems arises from the fact that the Coulomb interaction between the projectile nucleus and the target electrons can become so strong that low order perturbation theory fails. The need arises for the development of unitary, strong-coupling collision approximations. Although inclusive single-vacancy cross sections grow with Z_p, they are not so interesting a probe of strong interactions as multiple vacancy production, which grows more rapidly. For ion impact, as opposed to electron impact [1], it is usually adequate to use a semiclassical theory in which the relative motion of the projectile and target is treated classically. In this "impact-parameter method" one can distinguish "close" from "distant" collisions as precisely as one desires. For a given projectile, the average interaction is larger the closer the collisions. For this reason, multiple-vacancy production is largest in very close collisions. Experimentally, the close collisions can be singled out either by detecting the projectile at relatively large scattering angles or by detecting a vacancy in the K shell of the target through its decay by Auger or x-ray emission. The latter technique is particularly useful because with moderate energy resolution the satellite emission lines correspond (to good approximation) to the various numbers v of collisionally produced vacancies in the L shell accompanying the K-shell vacancy (KL^v hole configurations). If both the K-shell electrons are knocked out, one speaks of hypersatellites (K^2L^v configurations). The energies of the K satellites and hypersatellites are given quite well by the Hartree-Fock theory of hole configurations. The intensity distributions of Auger electrons or x-rays can be converted (see [2]) to probabilities of various numbers of L-shell vacancies, provided that the fluorescence yields (x-ray branching ratios) are known for the various hole configurations. It is the multiple-vacancy distributions, denoted here by $P_{K,L^v}^{K,L^{I-v}}$ for satellites and by $P_{K^2,L^v}^{K^0,L^{I-v}}$ for hypersatellites (I = initial number of L-shell electrons), which are of primary interest.

Experimentally, the distributions almost always have a nearly binomial distribution. This distribution follows directly from what we have called [3,4] the single-particle model (SPM), discussed in sect. 2, which contains the assumption of statisticaly independent hole production. More generally, it has been shown [5] that the binomial distribution is the most likely distribution in the sense of Bayesian probability theory, given only the known constraints. The independence of the holes is somewhat surprising in view of the known importance of correlations in other collision processes. In order to understand the relative importance of correlations in various reactions, we have developed [3,4] the theory of multiple-vacancy production and of other "number-exclusive, hyperinclusive" (NEHI) processes [4] in the independent Fermi particle model (IFPM), which contains Pauli correlations. In sect. 3, we include a new, simpler derivation [6] of the main formal relation in this theory, and show the way [6,1] in which the Pauli exchange terms (PET's) make possible the non-binomial distributions which occur in some coincidence measurements involving electron transfer to the projectile. In sect. 4, we describe how [7] a tendency of the PET's to have random phases in the case of K^nL^v

vacancies leads to nearly binomial distributions. Sect. 5 describes our unified treatment of shakeoff and of ion-impact contributions to multiple vacancy production, and sect. 6 reviews recent "unitary" calculations of the mean L-shell vacancy probability per electron, $\overline{p}_L$, as a function of the projectile speed and charge.

2. The single-particle model

The traditional semiclassical theory of multiple vacancy production [8] employs what we call, following standard terminology in the nuclear shell model, the single-particle-model (SPM) version of the independent particle model, even though it deals with arbitrarily many target electrons. The assumptions embodied in this model [6] have not been fully explicit in the literature. One begins by considering a single-electron system with the electron in spin-orbital h, and calculates scattering amplitudes $a_{kh}(B)$, at impact parameter B, to states k. The probabilities ρ^k and ρ_k that the single-particle state k is occupied or not occupied after the collision are given by

$$\rho^k(h) = |a_{k,h}|^2 = 1 - \rho_k(h) . \tag{1}$$

For an F-electron system in the SPM one does not introduce many-electron wave functions or amplitudes, but rather forms probabilities directly from the probabilities of the one-electron system. Clearly, one thereby loses quantal interference effects. Many-electron inclusive probabilities will be denoted by $\rho^{k_1,k_2,\ldots}_{v_1,v_2,\ldots}$, where the superscripts label specified occupancies and the subscripts label specified vacancies. The Pauli exclusion principle is introduced in an ad hoc manner in the SPM by assuming

$$\rho^{\ldots k \ldots k \ldots}_{\ldots} = 0. \tag{2}$$

The complementarity of occupancy and vacancy corresponds to

$$\rho^{k_1 \ldots k_m}_{v_1 \ldots v_n} = \rho^{k_1 \ldots k_m}_{v_1 \ldots v_n k} + \rho^{k_1 \ldots k_m k}_{v_1 \ldots v_n} \tag{3}$$

The SPM is completed by requiring that

$$\rho^k(h_1,\ldots,h_F) = \sum_{i=1}^{F} \rho^k(h_i) \tag{4}$$

and by the statistical-independence hypothesis

$$\rho^{k_1 \ldots k_m} = \prod_{j=1}^{m} \rho^{k_j}, \quad m \leq F,\ k_i \neq k_j. \tag{5}$$

Eq. (5) lacks exchange terms, so that unphysical factors of the form

$$\rho^k(h)\ \rho^{k'}(h)$$

are included. Eq. (5) together with eq. (3) implies

$$\rho^{k_1 \ldots k_m}_{v_1 \ldots v_n} = \prod_{i=1}^{m} \rho^{k_i} \prod_{j=1}^{n} \rho_{v_j}, \quad m + n \leq F \tag{6}$$

provided that no two states are the same.

For multiple vacancy production in a shell or subshell containing I electrons initially, one wants the NEHI probabilities ($v = 0,\ldots,I$)

$$P^{I-v}_{v}(B) \equiv \sum_{\lambda_1 < \ldots < \lambda_v} \rho^{\lambda_{v+1} \ldots \lambda_I}_{\lambda_1 \ldots \lambda_v}(B), \tag{7}$$

where the sum is over the different combinations of v states selected from the I states initially occupied, and ($\lambda_{v+1} < \ldots < \lambda_I$) is the complementary combination. If the I states of the shell all have the same final inclusive vacancy probability, $\rho_{\lambda_i}(B) = p(B)$, then

$$P_v^{I-v}(B) = \binom{I}{v} \quad (1 - p)^{I-v} \, p^v \, , \tag{8}$$

the binomial distribution. For $K^n L^v$ vacancy production one has

$$\sigma_{K^n,L^v}^{K^{2-n},L^{I-v}} = 2\pi\int_0^\infty dB \; B\binom{2}{n} \, p_K(B)^n[1 - p_K(B)]^{2-n} \, \binom{I}{v} \, p_L(B)^v[1 - p_L(B)]^{I-v} \tag{9}$$

$$\approx \binom{I}{v} \, \overline{p}_L{}^v \, (1 - \overline{p}_L)^{I-v} \, \sigma_{K^n}^{K^{2-n}} \tag{9a}$$

The approximation (9a) is a good one because $p_K(B)$ falls off much more rapidly than does $p_L(B)$; and $\overline{p}_L \approx p_L(a_k) \approx p_L(0)$, where a_K is the radius of the K-shell. The binomial distribution, or its generalization [8] to allow subshells to have different $\overline{p}$'s, has been extremely successful in describing the data.

3. The independent-Fermi-particle model (IFPM) [3,4]

In the IFPM, one works with an antisymmetric F-electron wave function with the form of a Slater determinant. Thus Pauli, but not dynamical, correlations are included. The multiple-occupancy probabilities are defined by

$$\rho^{k_1,\ldots,k_m} \equiv \sum_{k_{m+1}<\ldots<k_F}{}' \rho^{k_1,\ldots,k_F}, \quad m \leq F-1. \tag{10}$$

We refer to $\rho^{k_1\ldots k_m}$ as a <u>particular</u> <u>inclusive</u> probability; it is inclusive because it includes all possibilities for the remaining F-m electrons, whose final states are not specified, and it is particular because it specifies particular final spin-orbitals, not merely the final shells. From eqs. (10) and (3), we obtain probabilities $\rho_{v_1\ldots v_n}^{k_1\ldots k_m}$.

We want to calculate the number-exclusive, hyperinclusive (NEHI) probabilities, P_v^{I-v} (B), defined by eq. (7). We call them hyperinclusive because they involve sums over particular inclusive probabilities, and number-exclusive because the total number of specified vacancies and occupancies equals the number of initially occupied states of the shell or shells under consideration. Because particular inclusive probabilities in which all the specified states are occupied (or in which all are vacant) have especially simple expressions [9,4], we have developed the "occupancy formalism" and the "vacancy formalism" in which the NEHI's are expressed, respectively, in terms of multiple-occupancy or multiple-vacancy probabilities. Our original derivation of the basic formulas involved an inversion. Here, we give a new, simpler, and direct derivation [6], in the vacancy formalism. We simply lower all superscripts in (7) by using (3), and repeat the process I-v-1 times. This gives

$$\rho_{\lambda_1\ldots\lambda_v}^{\lambda_{v+1}\ldots\lambda_I} = \rho_{\lambda_1\ldots\lambda_v}^{\lambda_{v+2}\ldots\lambda_I} - \rho_{\lambda_1\ldots\lambda_{v+1}}^{\lambda_{v+2}\ldots\lambda_I} = \ldots$$

$$= \rho_{\lambda_1\ldots\lambda_v} - \sum_{\lambda_{v+1}}{}' \rho_{\lambda_1,\ldots,\lambda_{v+1}} + \sum_{\lambda_{v+1} < \lambda_{v+2}}{}' \rho_{\lambda_1\ldots\lambda_{v+2}} - \ldots \quad (11)$$

where the λ_i's in the sums $\neq \lambda_1,\ldots,\lambda_v$. Then

$$P_v^{I-v}(B) = \sum_{\lambda_1<\ldots<\lambda_v} \Big\{ \rho_{\lambda_1,\ldots,\lambda_v} - (v+1) \sum_{(\lambda_v<)\lambda_{v+1}}{}' \rho_{\lambda_1\ldots\lambda_{v+1}} + \frac{(v+2)(v+1)}{2} \sum_{(\lambda_v<)\lambda_{v+1} < \lambda_{v+2}}{}' \rho_{\lambda_1\ldots\lambda_{v+2}} - \ldots \Big\} . \quad (12)$$

Thus,

$$P_{v}^{I-v}(B) = \sum_{j=0}^{I-v} (-)^j \binom{v+j}{v} Q_{v+j}(B) \tag{13}$$

in terms of "hyperinclusive expected values"

$$Q_v \equiv \sum_{\lambda_1<\ldots<\lambda_v} \rho_{\lambda_1\ldots\lambda_v} . \tag{14}$$

In the SPM

$$Q_{v+j} = \binom{I}{v+j} p^{v+j} , \tag{15}$$

so one regains the binomial distribution. Conversely to eq. (13), one finds [3,4]

$$Q_n = \sum_{v=n}^{I} \binom{v}{n} P_v^{I-v} , \quad Q^n = \sum_{j=n}^{I} \binom{j}{n} P_{I-j}^{j} . \tag{16}$$

The generalization to more than one shell is straightforward. For example [6], if $\overline{K}$ and K refer to the K-shells of the projectile and target,

$$Q^{\overline{K}}{}_{K} \equiv 2Q^{\overline{K}}{}_{1s\uparrow} = 2(\rho^{\overline{1s\uparrow}}_{1s\uparrow} + \rho^{\overline{1s\downarrow}}_{1s\uparrow}) \tag{17}$$

$$= P^{\overline{K},K}_{\overline{K},K} + 2(P^{\overline{K}^2,K}{}_{K} + P^{\overline{K}}_{\overline{K},K^2}) + 4\, P^{\overline{K}^2}{}_{K^2} , \tag{18}$$

where the arrows in eq. (17) represent projections of the intrinsic spin.

Cross sections for charge transfer in coincidence with a target K vacancy have been measured for H^+ + Ar [10] and for (H^+, He^{2+}, and Li^{3+}) + (C and Ne) [11]. In our present notation and with $\overline{C}$ standing for the set of bound states of the projectile (charge transfer states) the measured cross section is denoted by $\sigma^{\overline{C}^1,\,K}_{\;\;\;\;\;K}$. We first attempted [12] to describe these data in terms of the IFPM cross section $\sigma^{\overline{C}}{}_{K}$, taken to be 1.2 $\sigma^{\overline{K}}{}_{K}$, where the factor 1.2 involves an estimate of capture into higher shells ($\propto n^{-3}$). In Eq. (17)

$$\rho_{1s\uparrow}^{\overline{1s}\downarrow} = \rho^{\overline{1s}}\,\rho_{1s} \tag{19a}$$

just as in the SPM, but

$$\rho_{1s\uparrow}^{\overline{1s}\uparrow} = \rho^{\overline{1s}}\,\rho_{1s} + |a^{(2)}_{\overline{1s},2s}|^2 \ . \tag{19b}$$

The PET is

$$|a^{(2)}_{\overline{1s},1s}|^2 = |\sum_{h=1}^{F} a^{*}_{\overline{1s},h}\,a_{1s,h}|^2 = |a_{\overline{1s},1s}|^2\,|a_{1s,1s}|^2 + \sum_{h\neq 1s}^{F}{}' |a_{\overline{1s},h}|^2\,|a_{1s,h}|^2 + \ldots \tag{20}$$

We refer [1] to $|a_{\overline{1s},1s}|^2$ as the single-electron-transition (SET) contribution, which we denoted by SP in [12]. Thus, we have in three different levels of approximation

$$Q^{\overline{K}}(K) = 2|a_{\overline{1s},1s}|^2 \qquad \text{(SET)} \tag{21a}$$

$$Q^{\overline{K}}_{K} = \begin{cases} 2\rho^{\overline{1s}}\cdot 2\rho_{1s} & \text{(SPM)} \quad (21b) \\ 2\rho^{\overline{1s}}\cdot 2\rho_{1s} + 2|a^{(2)}_{\overline{1s},1s}|^2 & \text{(IFPM)} \quad (21c) \end{cases}$$

Similar equations apply when the vacancy is in the L shell. We note the vacancy weighting factor v (see eq. (16) with n=1) in

$$\sigma^{\overline{K}}_{\overline{K},L} = \sum_{v=1}^{8} v\,\sigma^{\overline{K},L^{I-v}}_{\overline{K},L^{v}} \ . \tag{22}$$

More recently [6] we have calculated the NEHI cross sections. In the newer calculations, we have used our one-and-a-half-center-expansion (OHCE) method [13] for coupled-channels theory instead of the single-center-expansion (SCE) method used in the earlier calculations [12]. We compare the various levels of approximation for a specific collision system in Table 1. One notices that the SET contribution is rather close to the IFPM single-charge-transfer cross section both for K and for L vacancies. The SPM gives only 32% and 78% of the IFPM values for K and L vacancies, respectively.

The IFPM outer-shell vacancy distributions (in coincidence with charge transfer) deviate from the binomial distribution by nearly lacking v=0 for single-transfer [1] and by nearly lacking v=0 and 1 for double charge-transfer, as shown in Table 2. These very small values would be zero except for transfer from the K-shell. It is easy to see how the PET's in the IFPM reduce the v=0 probability nearly to zero. In neon (I=8) one has

$$P^{\overline{K},L^8}_{\overline{K},L^0} = Q^{\overline{K},L^8} - 2Q^{\overline{K^2},L^8} = 2R^{\overline{1s},L^4}\left[R^{L^4} - R^{\overline{1s},L^4}\right] \qquad (23)$$

where the R's are hyperinclusive expected values, like the Q's but in which all the spin-orbitals have the same projection of the intrinsic spin [4]. The factor $R^{\overline{1s},L^4}$ can be written

$$R^{\overline{1s},L^4} = \rho^{\overline{1s}}\, R^{L^4} + C \qquad (24)$$

where the first term is close to the SPM value and C is a sum of PET's. For the case calculated in Tables 1 and 2, at B≈0 $\rho^{\overline{1s}}R^{L^4} \approx 0.9942 \times 10^{-2}$, but $C \approx -0.9936 \times 10^{-2}$ so $R^{\overline{1s},L^4} \approx 0.6 \times 10^{-5}$, smaller than the SPM value by a factor $\sim 10^{-3}$. The elimination of the L-shell v=0 component does not occur in argon, because the one or two electrons transferred to the projectile come primarily from the M shell. For argon, it is the M-shell $v=0$ component which is greatly reduced from its SPM value.

4. Nearly binomial distribution for K^nL^v vacancies in the IFPM

4.1. Random phases

In contrast to the case of L-shell vacancies in coincidence with one or two charge transfers, the case of K_α satellites shows only slight deviations of the IFPM distribution from the SPM (nearly binomial) one. The contrast is illustrated in Table 3 in which the IFPM hyperexclusive expected values R, see eqs. (23) and (24), in both the occupancy and vacancy formalisms, are compared with the corresponding SPM values. The only striking deviation is for $R^{\overline{1s},L^4}$, discussed in sect. 3. We have previously expounded [14,7] how the IFPM K^nL^v distributions nearly reduce to the SPM ones because of a nearly random distribution of phases of the transition amplitudes. One common feature is that the second moment (variance) of the IFPM distribution is somewhat smaller than that of the binomial. See Table 4 for an example.

4.2. Negligible effect of undetected charge transfer to the $\overline{K}$ shell

Our OHCE method [13] in coupled-channels theory includes charge transfer and therefore gives different amplitudes for vacancy production than a similar calculation without charge transfer. We have performed OHCE calculations [6] of F^{9+} + Ne at 1.5 MeV/amu. Table 4 gives inclusive K- and L-shell vacancy cross sections and $\overline{p}_L$ for K_α satellites and hypersatellites. The K-vacancy cross section is increased by 67%, but the L-shell vacancy cross section and $\overline{p}_L$ are hardly changed at this high energy

(v/v_L = 6.7). Moreover, the K^nL^v distributions are altered only slightly. It remains to be seen what effect transfer to the L shell of the projectile might have.

A coincidence experiment could measure the KL^v distribution for collisions in which there is a charge transfer to the $\overline{K}$ shell. Rødbro et al. [11] have, in fact, done this for the no-L-shell-vacancy case, v=0, by resolving the K_α diagram line in neon under He^{2+} impact. The theory would involve the NEHI probabilities $P^{\overline{K},K,L^{I-v}}_{\overline{K},K,L^v}$.

5. Shakeoff

An orbital ϕ_h which is bound in the initial Hartree-Fock field has a non-zero projection onto unbound eigenstates ϕ_k^f of the final Hartree-Fock field corresponding to a configuration with inner-shell holes. This fact results in a "shakeoff" contribution to multiple vacancy production following collisional inner-shell hole production. The shaking process has been almost completely neglected for ion impact, although used widely for photon and electron impact ionization of the K shell, for which the small $\overline{p}_L$ is produced almost exclusively by shaking. In a conventional treatment, one gets final vacancy probabilities $\overline{P}$ from collisional ones, P, and shakeoff probabilities, P^{Sh}, by

$$\overline{P}^{K^{2-n},\ L^{I-v}}_{K^n,\ L^v}(Z_p,E,B) = \sum_{v'} P_n^{Sh}(v,v')\, P^{K^{2-n},\ L^{8-v'}}_{K^n,\ L^{v'}}(Z_p,E,B). \qquad (25)$$

Noticing that the shakeoff probability for hypersatellites should be roughly twice that for satellites, we thought [15] that a comparison of

$\overline{p}_L$'s for hypersatellites and satellites might yield information on shaking. Because ion-impact and shaking contributions to L-shell hole production lead to the same final states, a quantal treatment should deal with interfering amplitudes. We developed a unified theory [15,7] of collisional and shaking contributions to hole production in the sudden approximation. It gives the unified transition amplitudes in two formulations,

$$s_{k,h}(Z_p,E,B) = \sum_{k'} \langle\phi_k^f|\phi_{k'}\rangle\, a_{k',h}(Z_p,E,B), \tag{26a}$$

analogous to eq. (25), and

$$s_{k,h} = \sum_{k'} a^f_{k,k'}\, \langle\phi^f_{k'}|\phi_h\rangle\ . \tag{30b}$$

Calculations of $\overline{p}_L$ for He^{2+} + Ne [15] and for C^{6+} + Ne [7] have been compared with the scarce satellite and hypersatellite data at high energies. The situation is inconclusive, but it appears that the $\overline{p}_L$'s calculated before including shakeoff are too large. Many more data are needed.

6. Systematics of $\overline{p}_L(Z_p,v)$

Because both the experimental and IFPM theoretical K^nL^v distributions are so nearly binomial, the main interest lies in the function $\overline{p}_L(Z_p,v,Z_T,B,\ldots)$. Our coupled-channels [2,7] and first Magnus [7] values of $\overline{p}_L$ for H^+, He^{2+}, C^{6+}, F^{9+}, and Si^{14+} on Ar were the first to exhibit the "saturation" of $\overline{p}_L$ as a function of Z_p, i.e. the gradual approach of $\overline{p}_L$ to unity in a unitary theory as Z_p is increased, rather than continuation of the initial Z_p^2 dependence predicted by first-order approximations.

More recently two relatively simple, analytically solvable, unitary approximations to $\overline{p}_L$ for B=0 have been developed [16,17]. We have reviewed them briefly in [1]. They have the merit of providing a scaling in the variable Z_p/v. An empirical scaling in the inverse variable, v/Z_p, had been discussed in several experimental papers in the last few years (see [18]). Our results [2] together with those of the geometrical-encounter-probability model of Sulik, Hock, and Berényi [16] are shown in Fig. 1. Now that "saturation" has been obtained, it remains to understand why the calculated values of $\overline{p}_L$ are still systematically somewhat larger than the experimental values. We have discussed the weakness of the IFPM for large Z_p/v as resulting from the "non-additivity of first ionization potentials" in multiple vacancy production [14,7]. The persistence of the discrepancy when $\overline{p}_L$ is small is not yet understood.

References

[1] R. L. Becker, A. L. Ford and J. F. Reading, in Proc. Second Workshop on High-Energy Ion-Atom Collision Processes, Debrecen, 1984 (Akadémiai Kiadó, 1985), to be published.

[2] R. L. Becker, A. L. Ford and J. F. Reading, Nucl. Instr. and Meth. B3 (1984) 43.

[3] R. L. Becker, J. F. Reading and A. L. Ford, IEEE Trans. Nucl. Sci. NS-28 (1981) 1092.

[4] R. L. Becker, A. L. Ford and J. F. Reading, Phys. Rev. A29 (1984) 3111.

[5] T. Åberg and O. Goscinski, in X-Ray and Atomic Inner-Shell Physics - 1982, edited by B. Crasemann (American Institute of Physics, New York, 1982), p. 121.

[6] R. L. Becker, unpublished.

[7] R. L. Becker, A. L. Ford and J. F. Reading, Nucl. Instr. and Meth. B4 (1984) 271.

[8] J. M. Hansteen and O. P. Mosebekk, Phys. Rev. Lett. 29 (1972) 136; later papers cited in Ref. [4].

[9] J. F. Reading, Phys. Rev. A8 (1973) 3262; J. F. Reading and A. L. Ford, Phys. Rev. A21 (1980) 124.

[10] J. R. Macdonald, C. L. Cocke and W. W. Eidson, Phys. Rev. Lett. 32 (1974) 648; E. Horsdaal-Pedersen, C. L. Cocke, J. L. Rasmussen, S. L. Varghese and W. Waggoner, J. Phys. B16 (1983) 1799.

[11] M. Rødbro, E. Horsdaal-Pedersen, C. L. Cocke and J. R. Macdonald, Phys. Rev. A19 (1979) 1936.

[12] For argon, R. L. Becker, A. L. Ford and J. F. Reading, J. Phys. B13 (1980) 4059; for neon and carbon, A. L. Ford, J. F. Reading and R. L. Becker, Phys. Rev. A23 (1981) 510.

[13] J. F. Reading, A. L. Ford and R. L. Becker, J. Phys. B14 (1981) 1995.

[14] R. L. Becker, A. L. Ford and J. F. Reading, Nucl. Instr. and Meth. 214 (1983) 49.

[15] R. L. Becker, A. L. Ford and J. F. Reading, IEEE Trans. Nucl. Sci. NS-30 (1983) 1076.

[16] B. Sulik, G. Hock and D. Berényi, J. Phys. B17 (1984) 3239, and in the proceedings cited in [1].

[17] L. Végh, 1984 preprint and in the proceedings cited in [1].

[18] R. L. Watson, O. Benka, K. Parthasaradhi, R. J. Maurer and J. M. Sanders, J. Phys. B16 (1983) 835.

Table 1. Cross sections for vacancy production in coincidence with charge transfer calculated [6,1] for He^{2+} + Ne at impact energy 0.1 MeV/amu in the unitary version of the OHCE method [13]. The units are 10^{-24} $(10^{-20})m^2$ for K(L) vacancies.

	$\sigma^{\bar{K}}(K)$	$\sigma^{\bar{K}}_{K}$	$\sigma^{\bar{K}}_{\bar{K},K}$	$\sigma^{\bar{K}^2}_{\bar{K}^0,K}$	$\sigma^{\bar{K}}(L)$	$\sigma^{\bar{K}}_{L}$	$\sigma^{\bar{K}}_{\bar{K},L}$	$\sigma^{\bar{K}^2}_{\bar{K}^0,L}$
SET	1.06				2.71			
SPM		0.53	0.37	0.16		3.71	2.30	0.70
IFPM		1.54	1.16	0.19		5.27	2.96(a)	1.16

(a) The contribution from v=1 is only 1.01.

Table 2. Non-binomial distributions, $P^{\bar{K}^n, L^{8-v}}_{\bar{K}^{2-n}, L^v}$, of Ne L-shell vacancies in coincidence with one or two charge-transfers to He^{2+} at impact energy 0.1 MeV/amu, as calculated [6] with the unitary OHCE method. The symbol a^{-b} means a x 10^{-b}.

v	n=1	n=2
0	0.38^{-4}	0.18^{-9}
1	0.56	0.60^{-5}
2	0.30	0.54
3	0.10	0.34
4	0.30^{-1}	0.95^{-1}
$\bar{P}_L$	0.204	0.324

Table 3. Ratios which represent deviations of IFPM expected values from SPM ones, calculated [6] for He^{2+} + Ne at 0.1 MeV/amu and B=0.

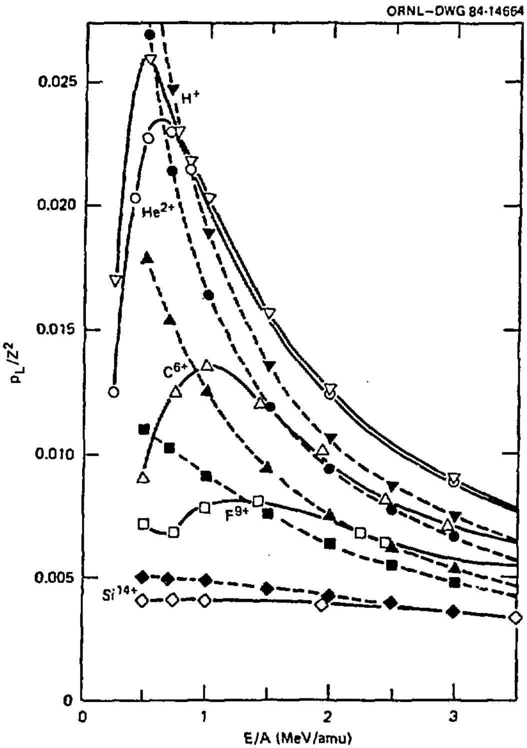
m	$\frac{R^{1s,L^m}}{\rho^{1s}R^{L^m}}$	$\frac{R^{\overline{1s},L^m}}{\rho^{\overline{1s}}R^{L^m}}$	$\frac{R_{1s,L^m}}{\rho_{1s}R_{L^m}}$	$\frac{R_{\overline{1s},L^m}}{\rho_{\overline{1s}}R_{L^m}}$
1	.99991	.81	.95	.95
2	.99983	.62	.89	.90
3	.99965	.38	.83	.82
4	.99951	$.67^{-3}$	.74	.68

Table 4. Comparison of coupled-channels calculations of vacancy production with and without inclusion of charge transfer (C.T.) to the projectile K shell for F^{9+} + Ne at 1.5 MeV/amu. Inclusive vacancy-production cross sections, σ_i, in 10^{-20} m^2. K_α satellite (j=1) and hypersatellite (j=2) mean L-shell vacancy probability per electron, $\overline{p}_L^{(j)}$, and ratio, $R^{(j)}$, of IFPM to binomial variance (both from distributions with the IFPM value of $\overline{p}_L^{(j)}$).

	Without C.T.	With C.T.
σ_K	0.086	0.144
σ_L	24.245	24.465
$\overline{p}_L^{(1)}$	0.759	0.754
$p_L^{(2)}$	0.781	0.799
$R^{(1)}$	0.976	0.939
$R^{(2)}$	0.832	0.863

Figure Caption

Fig. 1. Theoretical scaled K_{α}-satellite mean L-shell vacancy probability per electron in argon for bare projectiles with $Z_p = 1,2,6,9$, and 14. Full curves, coupled-channels calculations [2]; dashed curves, model of Ref. [16].


ORNL-DWG 84-14664
0.025
0.020
0.015
0.010
0.005
0
P_L/Z^2
H+
He2+
C6+
F9+
Si14+
0
1
2
3
E/A (MeV/amu)

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