NONSTATISTICAL THEORY OF MULTIPLE VACANCY PRODUCTION IN ATOMIC COLLISIONS

MASTER

Richard L. Becker*

Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37830

and

J. F. Reading† and A. L. Ford†

Department of Physics, Texas A & M University, College Station, TX 77843

By acceptance of this article, the publisher or recipient acknowledges the U.S. Government's right to retain a nonexclusive, royalty-free license in and to any copyright covering the article.

Summary

Till now interpretation of x-ray satellite data has been limited to the use of models in which the emissions of electrons are treated as statistically independent. This assumption leads to a product of binomial distributions, one for each shell. However, even in the independent Fermi particle model of the target atom, collision theory predicts that the holes are correlated. At a given impact parameter the independent-Fermi-particle probability for producing several holes in a given shell can be written as a term containing only probabilities for the individual vacancies which reduces for "average holes" to the binomial distribution, plus a correlation term which involves interference among amplitudes for the single-electron transitions. Expressions for the general case are given. To evaluate such expressions, one needs calculations in which the single-electron amplitudes are obtained with consistent relative phases. These have now begun by employing coupled-channels theory.

Introduction

In the last decade the detailed investigation of multiple inner-shell vacancy states of atoms has been made possible by the copious production of K- and L-shell x-ray satellites and Auger line spectra by heavy-ion bombardment and their measurement with high resolution spectrometers.^{1,2} The various K_{α} ($2p \rightarrow 1s$) and K_{β} ($3p \rightarrow 1s$) satellites in high energy collisions are interpreted in terms of corresponding numbers of L-shell holes in addition to a single K-shell hole, or two K-shell holes (hypersatellites). Burch and Swanson³ were the first to point out that the K_{α} satellite intensity ratios in the earliest experiments roughly followed a binomial distribution for the probability of producing m holes in the L-shell in terms of a mean probability, $\langle p_L \rangle$, for producing precisely one average L-hole. In a classical or semiclassical calculation of the collision, each cross section is written as an integral over the impact parameter, b . Because

$$1 = [p + (1-p)]^n = \sum_{m=0}^n \binom{n}{m} p^m (1-p)^{n-m},$$

the cross section for precisely one K-hole and m statistically independent average L-holes is

$$\sigma_{KL}^{8-m} = 2\pi \int_0^{\infty} db \cdot b \cdot 2\bar{p}_K(b) [1 - \bar{p}_K(b)] \binom{8}{m} [\bar{p}_L(b)]^m \times [1 - \bar{p}_L(b)]^{8-m}. \quad (1)$$

Since the K-shell probability is concentrated well within the L-shell radius, and the L-shell probability is slowly varying for small radii, $\langle \bar{p}_L \rangle \approx \bar{p}_L(0)$.

The statistical formulation has been generalized to distinguish between L-subshells⁴ and to allow for changes in single electron binding energy if the holes are produced sequentially.⁵ The single-electron probability $\bar{p}_L(0)$ has been used widely as a parameter in fitting spectral distributions.^{3,2} However, cases of striking deviation from a binomial distribution have been reported,⁶ and the assumption of statistical independence neglects the interference of amplitudes which may be expected in a quantum mechanical formulation.

Time Dependent Independent Fermi Particle Model (IFP)

In the IFP we deal with a time dependent single-particle (s.p.) Hamiltonian,

$$H = \sum_{i=1}^F H_i^{(1)}(t),$$

such as that of coupled-channels theory⁷ or time dependent Hartree Fock theory. With single particle wave functions satisfying

$$[H^{(1)}(t) - i\frac{\partial}{\partial t}] \psi_{\alpha}^{(+)}(t) = 0 \text{ and } \psi_{\alpha}^{(+)}(t) \xrightarrow{t \rightarrow \infty} \phi_{\alpha}^{+}(t),$$

the s.p. reaction amplitudes are $a_{\alpha\beta} = \lim_{t \rightarrow \infty} (\phi_{\alpha}^{(-)} | \psi_{\beta}^{(+)})$.

The entire system of F electrons is described by Slater determinants $\psi_{\alpha_1, \dots, \alpha_F}^{(+)}$ which approach the unperturbed determinants $\phi_{\alpha_1, \dots, \alpha_F}^{(+)}$ as $t \rightarrow \infty$. The amplitude for the exclusive reaction leading from the initial state $(h_1, \dots, h_F)$ to an arbitrary final state is

$$A_{\alpha_1, \dots, \alpha_F} \equiv \lim_{t \rightarrow \infty} (\phi_{\alpha_1, \dots, \alpha_F}^{(-)} | \psi_{h_1, \dots, h_F}^{(+)}) = \sum_P (-1)^P \prod_{i=1}^F a_{\alpha_i, \phi_{h_i}} \quad (2)$$

where P represents a permutation. The probability of the inclusive reaction in which the s.p. state k is

*Research sponsored by the U.S. Department of Energy, Division of Basic Energy Science under Contract No. W-7405-eng-26 with Union Carbide Corporation.

†Research supported by the National Science Foundation and the Center for Energy and Mineral Resources, Texas A and M University.

occupied, P^k , or not occupied, P_k , is a sum of s.p. probabilities:⁶

$$P^k \equiv \sum_{\alpha_1 < \dots < \alpha_{F-1}} |A_{\alpha_1, \dots, \alpha_{F-1}, k}|^2 = \sum_h^{\text{occ}} |a_{k,h}|^2 \quad (3a)$$

$$P_k \equiv \sum_{\alpha_1 < \dots < \alpha_F} |A_{\alpha_1, \dots, \alpha_F}|^2 = 1 - P^k \quad (3b)$$

($\neq k$)

However, for more than one specified final s.p. state the inclusive probability depends on interferences of amplitudes through

$$a_{kk'}^{(2)} \equiv \sum_h^{\text{occ}} a_{kh}^* a_{kh'} = a_{kk}^{(2)*}; \quad (4)$$

for example,⁸

$$P^{k_1, \dots, k_n} \text{ or } P_{k_1, \dots, k_n} = \begin{vmatrix} (P^{k_1} \text{ or } P_{k_1}) & a_{k_1 k_2} & \dots & a_{k_1 k_n}^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ a_{k_n k_1}^{(2)} & \dots & a_{k_n k_{n-1}}^{(2)} & (P^{k_n} \text{ or } P_{k_n}) \end{vmatrix} \quad (5)$$

The states k_i may belong to different shells. A subscript can be raised or a superscript lowered by using

$$P_{k_1 k_2}^{k'_1 k'_2} \dots + P_{k_1 k_2}^{k''_1 k''_2} \dots = P_{k_1 k_2}^{k'_1 k'_2} \dots \quad (6)$$

For cases with both occupancies and non-occupancies specified, the inclusive probability is not simply a determinant.

Hyperinclusive Probabilities

We use the prefix "hyper" in referring to the specification only of the numbers of holes and/or occupancies in various shells. The simplest examples are the hyperinclusive probabilities for the K shell:

$$P_K = P_K^K + P_{K^2}, \quad P^K = P_K^K + P^{K^2}$$

with

$$P_K^K = P_{1s^+}^{1s^+} + P_{1s^+}^{1s^+}, \quad P_{K^2} = P_{1s^+, 1s^+}, \quad P^{K^2} = P_{1s^+, 1s^+}.$$

In terms of the simple expressions (sums of determinants)

$$Q_K = P_{1s^+} + P_{1s^+} = P_K^K + 2P_{K^2}$$

$$Q_{K^2} = P_{1s^+, 1s^+} = P_{K^2}$$

$$Q^K = P_{1s^+}^{1s^+} + P_{1s^+}^{1s^+} = P_K^K + 2P^{K^2}$$

$$Q^{K^2} = P_{1s^+, 1s^+} = P^{K^2}$$

we have

$$P^{K^2} = Q^{K^2}, \quad P_K^K = Q_K - 2Q_{K^2} = Q^K - 2Q_{K^2}, \quad P_{K^2} = Q_{K^2}. \quad (7)$$

In general for any set S_N of N s.p. states we introduce the auxiliary sums of determinants

$$Q_m \text{ or } Q^m \equiv \sum_{\lambda_1 < \dots < \lambda_m} (P_{\lambda_1, \dots, \lambda_m} \text{ or } P^{\lambda_1, \dots, \lambda_m}) \quad (8)$$

where each λ_i belongs to S_N . Then the general result of some combinatorial algebra is that the hyperinclusive probability for precisely n holes in S_N is given by

$$P_n^{N-n} = Q_n - \binom{n+1}{1} Q_{n+1} + \binom{n+2}{2} Q_{n+2} - \dots + (-)^{N-n} \times \binom{N}{N-n} Q_N \quad (9)$$

$$= Q^{N-n} - \binom{N-n+1}{1} Q^{N-n+1} + \dots + (-)^n \binom{N}{n} Q^N. \quad (10)$$

Equation (10) is the simpler to evaluate when $n < N/2$ and (9) when $n > N/2$. If the single hole production probability is very small, $P_n^{N-n} \approx Q_n$. The probability P_n^{N-n} for one shell is inclusive with respect to all other shells, i.e. it includes a sum over all numbers of holes in the other shells.

The neglect of all $a^{(2)}$'s in Eq. (5) is equivalent to the assumption of statistically independent vacancy or occupancy production because it leads to

$$P_{k_1, \dots, k_n} \text{ or } P^{k_1, \dots, k_n} \rightarrow \prod_{i=1}^n (P_{k_i} \text{ or } P^{k_i}).$$

If in addition we make the average hole assumption that each $P_k = \bar{p}$, and hence $P^k = 1 - \bar{p}$, then

$$Q_m \text{ or } Q^m \rightarrow \binom{N}{m} [\bar{p}^m \text{ or } (1 - \bar{p})^m]$$

and

$$P_n^{N-n} \rightarrow \binom{N}{n} \bar{p}^n (1 - \bar{p})^{N-n}, \quad (11)$$

the binomial distribution.

The correlations contained in $a_{k_1 k_2}^{(2)}$ have been found to be significant for the hyperinclusive probability P_K^C , where C stands for charge transfer to the projectile⁷, when the projectile charge becomes large. Similar, more elaborate coupled-channels calculations of multiple hole production by the authors are in progress.

DISCLAIMER

This work was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

References

1. J. D. Garcia, R. J. Fortner, and T. M. Kavanagh, *Revs. Mod. Phys.* 45, 111 (1973).
2. P. Richard, Chap. 2, *Atomic Inner-Shell Processes*, Vol. I, edited by B. Crasemann (Academic Press, New York, 1975); D. H. Madison and E. Merzbacher, loc. cit., Chap. 1.
3. D. Burch and H. Swanson, in *Proceedings of International Conference on Inner Shell Ionization Phenomena and Future Applications*, April 1972, edited by R. W. Fink, S. T. Manson, J. M. Palms, and P. Venugopala Rao (U.S. Atomic Energy Commission, Tech. Information Center, Oak Ridge, TN, CONF-720404) Vol. 2, p. 1464.
4. J. M. Hansteen and O. P. Mosebekk, *Phys. Rev. Letters* 29, 1361 (1972).
5. R. L. Watson, B. I. Sonobe, J. A. Demarest, and A. Langenberg, *Phys. Rev.* A19, 1529 (1979).
6. R. L. Watson, F. E. Jenson, and T. Chiao, *Phys. Rev.* A10, 1230 (1974); D. L. Mathews, R. J. Fortner, D. Schneider, and C. F. Moore, *Phys. Rev.* A14, 1561 (1976).
7. R. L. Becker, A. L. Ford, and J. F. Reading, *J. Phys. B: Atomic and Molecular Physics* (in press).
8. J. F. Reading and A. L. Ford, *Phys. Rev.* A21, 124 (1980).