Cross Section for a K-Shell Vacancy Produced by Heavy Projectile in an Independent-Particle-Model Atom*

J. F. Reading
Cyclotron Institute and Department of Physics, Texas A&M University, College Station, Texas 77843
(Received 30 July 1973)

In the Born approximation as the interaction occurs with only one electron, the total cross section for producing a K-shell vacancy with a heavy projectile is obtained by requiring the electron to be excited above the Fermi sea. We demonstrate that for an independent-particle model of the atom this result is true to all orders of the Born series. This means the codes currently developed for proton-hydrogen scattering are immediately applicable to K-shell ionization.

In the Born approximation one calculates the cross section for producing a K-shell vacancy with a heavy projectile by requiring that the electron be excited above the Fermi sea.[1] In a higher-order calculation it is not obvious *ab initio* that this is the correct thing to calculate.

A K-shell hole created by the projectile might subsequently be filled after collision with another electron. Further it may not be necessary to excite the electron above the Fermi sea as holes may have already been produced by passage of the projectile through the atom allowing an energetically easier creation of a K-shell vacancy by promoting the K-shell electron to one of these holes. In this comment it is pointed out that if one is prepared to approximate the atom by an independent-particle model, i.e., ignore correlations, rearrangement energies, and so on, then all these processes cancel and the simple requirement that the K-shell electron be excited above the Fermi sea gives the exact prescription for calculating the total cross section.

The importance of this result is that computer codes developed over the years for the proton-hydrogen problem[2] are now immediately applicable to K-shell vacancy production. One can ignore the presence of the other electrons.

A heavy projectile moving through the atom at constant impact parameter $\vec{B}$ and constant velocity $\vec{v}$ provides a time-dependent perturbation of the atom described by

$$i\hbar \frac{\partial}{\partial t} \psi_s(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; \vec{B}, vt)$$
$$= i\hbar v \frac{\partial}{\partial Z} \psi_s(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; \vec{B}, Z)$$
$$= \left(H(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) - \sum_i Z_p e^2 \Big/ |\vec{R} - \vec{r}_i| \right) \psi_s .$$

In the interaction picture we may write this equation as

$$i\hbar v \frac{\partial}{\partial Z} \psi = e^{iHZ/\hbar v} \times \left(-\sum_i Z_p e^2 \Big/ |\vec{R} - \vec{r}_i| \right) e^{-iHZ/\hbar v} \psi ,$$

where

$$\psi = e^{-iHZ/\hbar v} \psi_s .$$

The amplitude for producing an excited state of the atom $\chi^{(m)}$ is given by[3]

$$f_m(Q) = (2m_p Z_p e^2 / 4\pi\hbar^2) \int \chi^{(m)*} e^{-i\vec{Q}\cdot\vec{B} + iHZ/\hbar v} \left(\sum_i 1 \Big/ |\vec{R} - \vec{r}_i| \right) \psi_s \prod_i d^3 r_i \, d^3 R$$
$$= (m_p v / 2\pi i \hbar) \int e^{-i\vec{Q}\cdot\vec{B}} \langle \chi^{(m)} | \psi(\vec{r}, \vec{r}_2, \ldots, \vec{r}_N; \vec{B}, \infty) \rangle \, d^2 B .$$

The total cross section for producing this state σ_m is given by

$$\sigma_m = \int d^2 B \, | \langle \chi^{(m)}, \psi(\vec{B}, \infty) \rangle |^2 . \quad (1)$$

In an independent-particle model of the atom, $\chi^{(m)}$ and ψ may be written as products of single-particle wave functions $\chi_n(r)$, $\psi_i(r; B, Z)$ suitably antisymmetrized. Here

$$H_{sp} \chi_n(\vec{r}) = \epsilon_n \chi_n(\vec{r}) \quad (2)$$

and

$$i\hbar v \frac{\partial}{\partial Z} \psi_i(\vec{r}, \vec{B}, Z) = -e^{iH_{sp}Z/\hbar v} Zpe^2/|\vec{R}-\vec{r}| \times e^{-iH_{sp}Z/\hbar v}\psi_i(\vec{r};\vec{B}, Z). \quad (3)$$

In Eq. (3) H_{sp} is the single-particle Hamiltonian and ϵ_n the single-particle energy. The wave function $\psi_i(\vec{r}; B, Z)$ is labeled according to the boundary condition it satisfies at $Z \approx -\infty$, i.e.,

$$\lim_{Z\to-\infty}\psi_i(\vec{r};\vec{B}, Z) = \chi_i(\vec{r})\, e^{in\ln(R-Z)},$$

where $n = -Zpe^2/\hbar v$ and the label i runs over states initially occupied. We note from the Hermiticity property of H_{sp} that

$$\int d^3r\, \psi_i^*(\vec{r};\vec{B}, Z)\psi_j(\vec{r};\vec{B}, Z) \equiv (\psi_i, \psi_j) = \delta_{ij}. \quad (4)$$

In Eq. (1) we now consider that

$$\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N; \vec{R}) = (\sqrt{N!})^{-1} \det[\psi_1, \psi_2, \ldots, \psi_N]$$

and that

$$\chi^{(m)}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \chi_n(\vec{r}_1)\chi_m(\vec{r}_2), \ldots, \chi_q(\vec{r}_N).$$

If we require a K-shell hole none of the states $\chi_n, \chi_m, \ldots, \chi_q$ can be equal to χ_0 the ground state of the K-shell orbit, otherwise there is no restriction. Summing on all n, m, ... q, etc. we therefore can write the total cross section for producing a K-shell vacancy as

$$\sigma_K = (2/N!)\int d^2B \int \prod_i d^3r_i \prod_i d^3r_i' \det[\psi_1^*(\vec{r}_1'; \vec{B}, \infty), \ldots, \psi_N^*(\vec{r}_N'; B, \infty)] \times \det[\psi_1(\vec{r}_1; \vec{B}, \infty), \ldots, \psi_N(\vec{r}_N; \vec{B}, \infty)] \prod_i [\delta(\vec{r}_i - \vec{r}_i') - \chi_0(\vec{r}_i)\chi_0^*(\vec{r}_i')]. \quad (5)$$

The factor of 2 in Eq. (5) is due to spin. Noting that an integral involving a product of

$$\chi_0(\vec{r}_i)\chi_0(\vec{r}_j)\det[\psi_1(\vec{r}_1; B, \infty), \ldots, \psi_N(\vec{r}_{N_i}\vec{B}\infty)]$$

is zero, Eq. (5) reduces to

$$\sigma_K = 2\int d^2B \left(1 - \sum_i |(\chi_0, \psi_i)|^2\right). \quad (6)$$

In Eq. (6) the sum is taken over all occupied states. However by time reversal symmetry

$$\int d^2B\,|(\chi_0, \psi_i)|^2 = \int d^2B\,|(\chi_i, \psi_0)|^2.$$

Hence,

$$\sigma_K = 2\int d^2B \left(1 - \sum_i |\langle \chi_i, \psi_0\rangle|^2\right). \quad (7)$$

This is just twice the result we would have obtained if we had calculated the cross section for a single electron in the K-shell being excited above the Fermi sea.

*Work supported by the Air Force Office of Scientific Research under Grant No. AFSOR-73-2484.

[1]E. Merzbacher and M. W. Lewis, in *Encyclopedia of Physics*, edited by S. Flügge (Springer, Berlin, 1957), Vol. 34, p. 166.

[2]L. Wilets and D. F. Gallaher, Phys. Rev. 147, 13 (1966); D. F. Gallaher and L. Wilets, Phys. Rev. 169, 139 (1968).

[3]J. F. Reading, Phys. Rev. A 1, 1642 (1970).