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VAINSHTEIN METHOD APPLIED TO ELECTRON IMPACT EXCITATION AND IONIZATION OF ATOMS

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In most calculations on inelastic collision of electrons with atoms there has been a general lack of agreement with observation mainly due to the treatment of the interelectronic interaction as a perturbation. In a recent calculation by Vainshtein et al.,[1-3] full account is given to this interaction by treating the problem as a binary collision between the incident and atomic electrons with the motion of their center of mass in the Coulomb field of the nucleus, and marked improvement in comparison of theory and observation has resulted. Three approximations are applied in this calculation which will be described briefly.

For the case of electron-hydrogen system, let $\vec{r}_1, \vec{r}_2$ represent the position vectors of the atomic and incident electrons, and $\psi(\vec{r}_1, \vec{r}_2)$ the total wave function of the system. By writing

$$\psi(\vec{r}_1, \vec{r}_2) = \varphi_1(\vec{r}_1) g(r_1, r_2), \tag{1}$$

where $\varphi_1(\vec{r}_1)$ is the initial eigenfunction of the atomic electron, and introducing $\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$ and $\vec{\rho} = \frac{1}{2}(\vec{r}_1 - \vec{r}_2)$, the Schroedinger equation reduces to an equation for g with variables $\vec{R}$ and $\vec{\rho}$. The first approximation is to neglect certain terms in this equation (cf. Ref. 1) in which case the solution to g will be the produce of two Coulomb functions:

$$g(\vec{r}_1, \vec{r}_2) = \pi\nu(\sinh\pi\nu)^{-1} \exp[i\vec{k}_1\cdot(\vec{R}+\vec{\rho})] F(i\nu, 1, ik_1R - i\vec{k}_1\cdot\vec{R}) F(-i\nu, 1, ik_1R - i\vec{k}_1\cdot\vec{\rho}), \tag{2}$$

with $\vec{k}_1$ the momentum of the incident electron and $\nu = \zeta/k_1$. The parameter ζ, called the effective charge, is introduced to minimize the effect of the neglected terms and is given by

$$\zeta = k_1/(k_1 + \epsilon_0^{1/2}), \tag{3}$$

with ϵ_0 the ionization energy of the atom.

Neglecting the exchange the transition amplitude is given by

$$T(1,2) = \langle \varphi_2(\vec{r}_1) e^{i\vec{k}_2\cdot\vec{r}_2} \left| |\vec{r}_2 - \vec{r}_1|^{-1} - r_2^{-1} \right| \psi(\vec{r}_1, \vec{r}_2) \rangle, \tag{4}$$

where 1 and 2 refer to the initial and final states, $\varphi_2(\vec{r}_1)$ to the final eigenfunction of atomic electron, and $\vec{k}_2$ to the momentum of the scattered electron. With g given by (2), a "peaking approximation" is applied to (4). In this approximation the value of a slowly varying function is assumed constant when it is multiplied by a rapidly varying function, and a value is assigned to the argument of the slowly varying function at which the rapidly oscillating function becomes infinite. In this way it is found that

$$T(1, 2) = (4\pi/q^2) A \langle 2 | e^{i\vec{q}\cdot\vec{r}} | 1 \rangle, \tag{5}$$

with $q = \vec{k}_1 - \vec{k}_2$, and

$$A = \frac{Nq^2}{\pi}\int d\vec{r}\,\frac{e^{2i\vec{q}\cdot\vec{r}}}{r}F(i\nu, 1, ik_1 r - i\vec{k}_1\cdot\vec{r}) \times F(-i\nu, 1, ik_1 r - i\vec{k}_1\cdot\vec{r}), \quad (6)$$

with $N = \pi\nu(\sinh\pi\nu)^{-1}$. The third approximation consists in replacing $2i\vec{q}\cdot\vec{r}$ in the above integral by $-2i\vec{q}\cdot\vec{r}$, apparently to facilitate the integration in (6).

It is the purpose of the present note to evaluate this integral exactly, revealing new structure in the theory and obtaining over-all improvement in comparison of theory and observation. Choosing the z axis along $\vec{k}_1$ and introducing the spherical coordinates q, θ_1, φ_1 for $\vec{q}$, and parabolic coordinate ξ, η, φ for $\vec{r}$, with $\xi = r - z$, and $\eta = r + z$, it follows that[4]

$$A = N\left(\frac{iq}{\cos\theta_1}\right)\int_0^\infty \exp\left[\frac{-iq\xi}{\cos\theta_1}\right]F(i\nu, 1, ik_1\xi) \times F(-i\nu, 1, ik_1\xi)d\xi$$

$$= NF(i\nu, -i\nu, 1, x), \quad x = \left(\frac{k_1^2 - k_2^2 + q^2}{k_1^2 - k_2^2 - q^2}\right)^2. \quad (7)$$

The analytic continuation of this is given as

$$A = (\pi\nu\coth\pi\nu)^{1/2}\,\mathrm{Re}[e^{i(\varphi - \nu\ln 4x)} \times F(i\nu, i\nu, 2i\nu + 1, 1/x)], \quad (8)$$

where

$$\varphi = \arg\Gamma(1 + i\nu) - \arg\Gamma(\tfrac{1}{2} + i\nu). \quad (9)$$

With $T(1, 2)$ determined, the cross section in units of πa_0^2 is given by

$$Q(1, 2) = \frac{1}{2\pi a_0^2 k_1^2}\int_{k_1 - k_2}^{k_1 + k_2} |T(1, 2)|^2 q\,dq. \quad (10)$$

At the threshold of excitation we obtain

$$Q(1s, 2lm) = f\epsilon^{1/2}(1 - \tfrac{2}{3}\delta_{l0})\delta_{m0}, \quad (11)$$

where

$$f = \frac{2^9}{3^5\sqrt{3}}(\pi\nu\coth\pi\nu)\left[1 + \mathrm{Re}\frac{e^{2i\nu\ln 3\epsilon}}{1 + 4i\nu}\right], \quad (12)$$

ϵ being the excess energy above threshold. For ionization we find similarly

$$Q(1s, c) = \frac{1}{2}\left(\frac{16}{3e}\right)^2(\pi\nu\coth\pi\nu) \times \left[1 + 3\mathrm{Re}\frac{e^{2i\nu\ln 4\epsilon}}{(1 + 4i\nu)(3 + 4i\nu)}\right]\epsilon^{3/2}. \quad (13)$$

With $\nu = \frac{1}{2}$ at threshold, this reduces to

$$Q(1s, c) = 0.857Q_B[1 + 0.372\cos(\ln\epsilon - 0.310)], \quad (14)$$

where $Q_B = 3.85\epsilon^{3/2}$ is the Born cross section.

In Fig. 1, $Q(1s\text{-}2s)$ and $Q_\perp(1s\text{-}2p) = 0.918Q(1s, 2p) + 0.246Q(1s, 2pm = 0)$ are plotted as functions of the incident energy. In both $1s\text{-}2s$ and $1s\text{-}2p$ excitations a narrow maximum appears at 0.03 Ry above threshold before the broad maximum. These maxima have also been found in $1s\text{-}2s\text{-}2p$ coupling,[5,6] and observed for $1s\text{-}2p$ excitation.[7] Recent measurement of Hils,

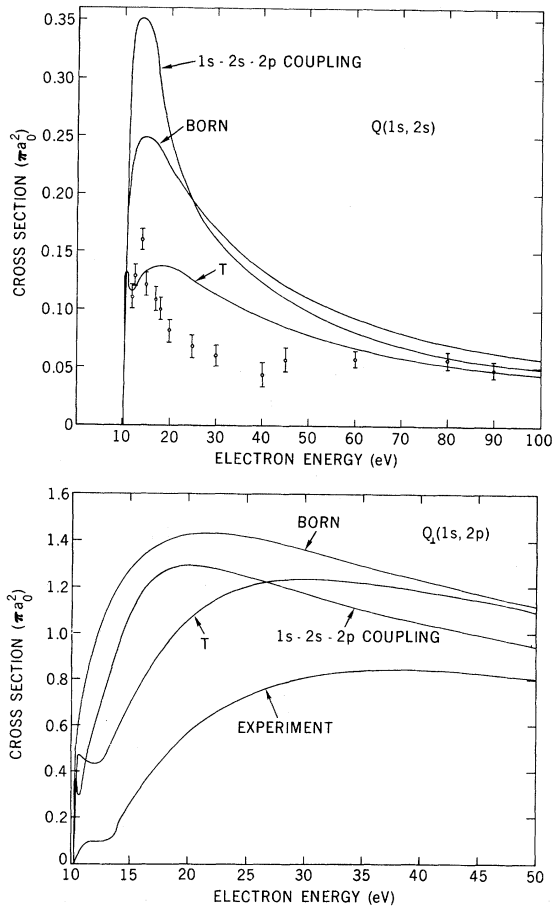

FIG. 1. $Q(1s, 2s)$: The present theory (T), the Born, and the $1s\text{-}2s\text{-}2p$ close coupling [P. G. Burke and K. Smith, Rev. Mod. Phys. 34, 458 (1962); M. Gailitis and R. Damburg, Proc. Phys. Soc. (London) 82, 192 (1963); K. Omidvar, Phys. Rev. 113, A970 (1964)] calculations are compared with measurement [R. F. Stebbings, W. L. Fite, D. G. Hommer, and R. T. Brackmann, Phys. Rev. 119, 1939 (1960)] (circles with error bars). $Q(1s, 2p)$: The present theory (T), the Born, and the $1s\text{-}2s\text{-}2p$ close coupling are compared with measurement [W. L. Fite and R. T. Brackmann, Phys. Rev. 112, 1151 (1958)].

Kleinpoppen, and Koschmieder[8] gives $(0.11 + 0.025)\pi a_0^2$ for the broad maximum of $Q(1s\text{-}2s)$ in better agreement with the present calculation.

In Fig. 2 the ionization cross section is plotted versus the incident energy. Away from threshold the agreement of the present calculation with measurements is better than any other previously reported calculation. At the threshold the T curve is a plot of Eq. (14). This curve crosses the Born curve at intervals at which the excess energy increases by a factor of $e^{\pi} \cong 23$. However, in the figure the crossing is seen only at 0.008 Ry. From about this point to 0.025 Ry, the curve is hardly distinguishable from a straight line, and below 0.002 Ry it coincides with the Born approximation. The measurement of Fite and Brackman[9] indicates a linear dependence of the cross section on excess energy up to 4 eV, but the measurement does not extend to the very vicinity of the threshold. Recent measurement of McGowan et al.[10] indicates a departure from this linear dependence very close to the threshold. With reference to Fig. 2, the implication of the present theory is that although the measured cross section in the approximate range of the threshold gives the appearance of a linear dependence on excess energy, the actual dependence may be a complicated function of this energy.

Introduction of the effective charge and neglect of exchange are the two main approximations used in the derivation of Eqs. (11)-(13). From the formalism of the problem it is evident that as long as the approximation of "effective charge" is valid, the functional form of the ionization cross section at threshold will not change by assigning better values to the effective charge. Similarly, incompleted studies on exchange amplitude show similarity in form to the direct amplitude. Nevertheless, whether the improvement of the theory will improve or worsen the agreement with experiment is left to the future studies.

The energy dependence of the cross sections given by Eqs. (11), (12), and (14) is different from this dependence in the Born approximation despite the fact that in the present and the Born calculations the wave functions have the same asymptotic forms. Since the energy dependence of the cross section depends on the nature of the long-range forces,[11] it may be argued that long-range forces, in particular, $1/r^2$ potential, are implicit in the present calculation.[12]

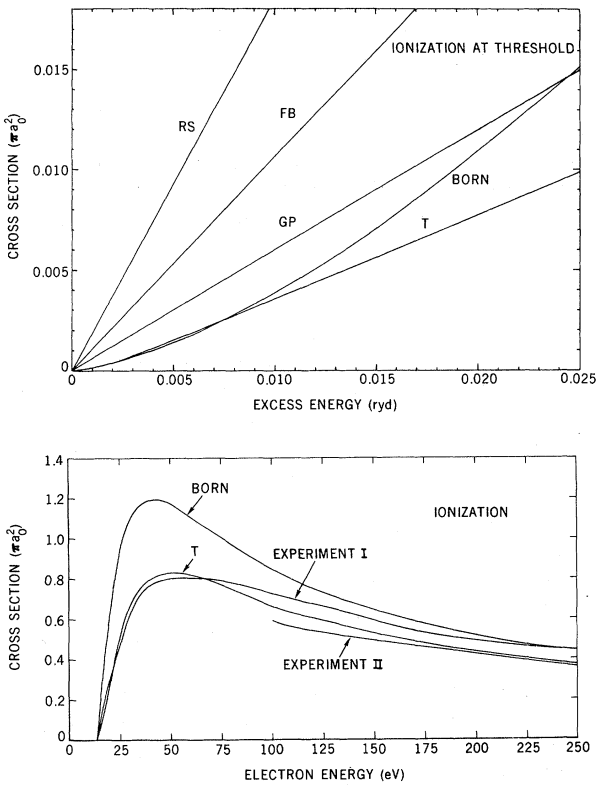

FIG. 2. Ionization: The present theory (T) and the Born calculations are compared with experiment I [W. L. Fite and R. T. Brackmann, Phys. Rev. 112, 1141 (1958)] and experiment II [E. W. Rothe, L. L. Marino, R. H. Neynaber, and S. M. Trujillo, Phys. Rev. 125, 582 (1962). An independent measurement has also been given by A. Boksenburg, thesis, University College, London, 1960 (to be published)]. Ionization at threshold: T is present theory, GP and RS are calculations of S. Geltman [Phys. Rev. 102, 171 (1956)] and R. K. Peterkop [Izvest. Akad. Nauk Latv. S.S.R. 9, 79 (1960); 24, 947 (1960)] and of M. R. Rudge and M. J. Seaton [Proc. Roy. Soc. (London) A283, 262 (1965)]. FB is the measurement of Fite and Brackmann (loc. cit.).

More fundamental studies on ionization threshold have been made by Wannier,[13] Rudge and Seaton,[14] and Temkin.[15] The linear threshold law predicted by Rudge and Seaton has been questioned by Temkin, who has indicated that the asymptotic form of the total wave function derived by Peterkop,[16] and Rudge and Seaton, and used in the derivation of the threshold law, becomes singular at $\vec{r}_1 = \vec{r}_2$ due to the nature of the long-range forces.

A more detailed calculation with inclusion of the electron nucleus interaction and the ex-

change effects, as well as a discussion of the validity of the effective charge approximation [cf. Eq. (3)], will be presented in the future.

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VANISHING KNIGHT SHIFT IN SUPERCONDUCTING ALUMINUM

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We report here a new measurement of the Knight shift in superconducting aluminum which differs from a previous result[1] in that now the Knight shift extrapolates to a value at $T=0°K$ which is essentially zero, as predicted by the BCS theory of superconductivity,[2] according to which the ground state consists of a coherent superposition of Cooper pairs in singlet spin states.

Previous measurements of the Knight shift in superconductors have all shown that the spin susceptibility at $T=0$ remains finite, contrary to the prediction of the BCS theory. In the elements tin,[3] mercury,[4] and vanadium[5] these results have been explained either on the basis of spin-orbit scattering or on the basis of contributions to the Knight shift that are unaffected by the transition to the superconducting state.[6,7] Aluminum, however, was expected to be one example where these effects might not play a significant role: (1) Spin-orbit coupling (both to displaced surface atoms and to the crystalline field) should be small because aluminum is the superconducting metal with the smallest atomic weight, and (2) aluminum has no d electrons so that one can assume that the paramagnetic susceptibility is entirely due to conduction electrons. The result[1] of a measurement made on one sample of aluminum films a number of years ago was that the Knight shift at $T=0°K$ was about 75%. In considering this unexpected result, Appel[7] concluded that all of the possible contributions to the Knight shift in superconducting aluminum should nearly