

for Kr, and for very low energies E (in eV), we have

$$\tan\delta(l=2) = (\pi/105)(16.6)(E/13.6) + O(E^2),$$

leading to values of $\delta(l=2)$ much larger than those obtained from Fig. 3 of Ref. 1.]

The basic argument, presupposing the existence of a bound state and considering only that δ for the given l and j , is a very specialized one and is not conclusive. It proves only that regions of strong interaction need not lead to significant R effects, not that they cannot. It would be difficult to give a conclusive argument without getting closer to first principles in discussing the equivalent one-body potential to be used. Cowardice inhibits us from making quick simple estimates of the R effects, while sloth and the absence of more compelling reasons for believing R effects to be really significant keep us from making a serious theoretical analysis. The results of Rotenberg and those presented here, combined with the feeling that $v_\lambda - V_\lambda$ will be large only in that

region, near the origin, where the valence electron or the incident particle spend little time because of the Pauli principle and (for $l \neq 0$) the centrifugal barrier, suggest that it is highly unlikely that the S and D equations, properly used, can really lead to results differing by a factor of 10. In fact, one suspects that R effects are probably much smaller, in general, than present uncertainties in NR calculations.

*Work sponsored by the U. S. Office of Naval Research, the Advanced Research Projects Agency under Contract No. Nonr-285 (49), NRO12-109, and the National Aeronautics and Space Administration under Contract No. NSG699.

¹H. N. Rotenberg and E. Bauer, Phys. Rev. Letters **16**, 495 (1966).

²M. Rotenberg, Phys. Rev. Letters **16**, 969 (1966).

³L. Spruch, T. F. O'Malley, and L. Rosenberg, Phys. Rev. Letters **5**, 375 (1960); T. F. O'Malley, L. Spruch, and L. Rosenberg, J. Math. Phys. **2**, 491 (1961).

IMPORTANCE OF CORRELATION EFFECTS IN THE IONIZATION OF HELIUM BY ELECTRON IMPACT*

F. W. Byron, Jr.,[†] and C. J. Joachain

Department of Physics, University of California, Berkeley, California

(Received 16 May 1966)

The phenomena of single and double ionization of helium by electron impact have received much recent interest both from the theoretical¹ and experimental²⁻⁵ points of view.

Perhaps a fruitful way of looking at the double-ionization process is to say that it proceeds via final- (initial-) state interactions between the atomic electrons, following (preceding) a single interaction with the projectile electron. If we use exact initial- and final-state helium wave functions in the Born approximation to first order in the interaction between the projectile and the atom, we are essentially including initial- and final-state interactions between the two atomic electrons to all orders. Figure 1(a) shows a typical perturbation-theory diagram which is important for double ionization while Fig. 1(b) shows a diagram which, being of second order in the interaction with the projectile electron, is unimportant at high incident energies.

We consider the case where the incoming electron, although nonrelativistic, has sufficiently high energy so that we may neglect exchange between the incident and bound electrons. Then, applying the first Born approximation, we get

$$\frac{d\sigma_{n+}}{d\Omega} = \frac{m^2 e^4}{4\pi^2 \hbar^4} \sum_f \frac{k_f}{k_i} |\langle \exp(i\vec{k}_f \cdot \vec{r}_0) \Psi_f(\vec{r}_1, \vec{r}_2) | \times V | \exp(i\vec{k}_i \cdot \vec{r}_0) \Psi_i(\vec{r}_1, \vec{r}_2) \rangle|^2 \quad (n=1, 2), \quad (1)$$

where \vec{k}_i and \vec{k}_f are the initial and final propagation vectors of the projectile electron and

$$V = -\frac{2}{r_0} + \frac{1}{r_{01}} + \frac{1}{r_{02}} \quad (2)$$

is the interaction potential. The coordinates \vec{r}_0 , \vec{r}_1 , and \vec{r}_2 denote the incoming and the two atomic electrons, respectively. The function $\Psi_i(\vec{r}_1, \vec{r}_2)$ is the exact ground-state helium wave

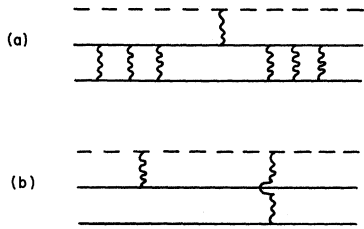


FIG. 1. Typical perturbation-theory diagrams for ionization processes. Solid lines refer to electron propagation in a central Coulomb field. Dashed lines denote free-electron propagation. Wavy lines refer to interelectronic interactions.

function while $\Psi_f(\vec{r}_1, \vec{r}_2)$ describes the final state of the atomic system including in principle the interaction between the two atomic electrons.

If we neglect completely the correlation⁶ between the atomic electrons in both initial and final states (i.e., both Ψ_i and Ψ_f are products of hydrogenic functions with $Z = 2$), then by orthogonality and Eqs. (1) and (2) we have exactly $\sigma_{++} = 0$, showing that the double-ionization process in first Born approximation is purely a correlation effect. This is clearly not the case for single ionization.

After integration over the \vec{r}_0 coordinate it is easily shown from Eq. (1) that the total cross sections are given by

$$\sigma_{n+} = \frac{4\pi m e^4}{\hbar^2 E_i} \sum_f \int_{k_i - k_f}^{k_i + k_f} \frac{1}{\Delta^3} \times |\langle \Psi_f(\vec{r}_1, \vec{r}_2) [\exp(i\vec{\Delta} \cdot \vec{r}_1) + \exp(i\vec{\Delta} \cdot \vec{r}_2)] | \Psi_i(\vec{r}_1, \vec{r}_2) \rangle|^2 d\Delta, \quad (3)$$

where E_i is the incident projectile energy and we have used the change of variable implied by

$$\vec{\Delta} = \vec{k}_i - \vec{k}_f. \quad (4)$$

It is apparent from looking at Eq. (3) that the dominant contribution to both single and double ionization comes from electrons which are ejected with low velocities (i.e., $k_i - k_f$ is small) and from the term linear in Δ in the expansion of $\exp(i\vec{\Delta} \cdot \vec{r})$ for small Δ .

Keeping this in mind we now calculate the single-ionization process. Since the double-ionization cross section is very small, the cross

section for single ionization is nearly equal to the total ionization cross section. In addition, because we assume that the incident electron energy is large, we may neglect kinematical restrictions in summing over final states. We can therefore evaluate the single-ionization cross section by making use of the closure theorem. This yields

$$\sigma_+ = \sigma_0 \left[\langle \Psi_i | (r_1 \cos \theta_1 + r_2 \cos \theta_2)^2 | \Psi_i \rangle - \sum_{n \text{ bound}} |\langle \Psi_i | r_1 \cos \theta_1 + r_2 \cos \theta_2 | \Psi_n \rangle|^2 \right], \quad (5)$$

where

$$\sigma_0 = (4\pi a_0^2 \ln E_i) / E_i, \quad (6)$$

E_i being measured in Rydbergs. Using a Hartree-Fock wave function for the ground state and simple Eckart-type wave functions⁷ for the relevant excited states, we get

$$\sigma_+ = 0.516 \sigma_0. \quad (7)$$

Using a more elaborate variational wave function for the helium ground state given by Eqs. (10) and (11) below, we find

$$\sigma_+ = 0.485 \sigma_0. \quad (8)$$

This shows that the single-ionization cross section at high energies is relatively insensitive to correlation effects. The experimental result⁴ is $\sigma_+ = 0.489 \sigma_0$.

Next, we turn to the calculation of the double-ionization process. In this case

$$\sigma_{++} = \sigma_0 \sum_f |\langle \Psi_i(\vec{r}_1, \vec{r}_2) | (r_1 \cos \theta_1 + r_2 \cos \theta_2) | \Psi_f(\vec{r}_1, \vec{r}_2) \rangle|^2, \quad (9)$$

where $\Psi_f(\vec{r}_1, \vec{r}_2)$ is a state of angular momentum $L = 1$, $M_L = 0$, with both electrons in the continuum. We have included increasing amounts of correlation in the initial state by making the following choices for the form of the ground-state wave function Ψ_i : (1) a one-parameter Hylleraas wave function with effective charge $Z^* = 27/16$; (2) a Hartree-Fock wave function;

(3) a wave function of the form

$$\Psi_i(\vec{r}_1, \vec{r}_2) = (1/4\pi)[f_1(r_1, r_2) + f_2(r_1, r_2) \cos\theta_{12}], \quad (10)$$

where

$$f_i(r_1, r_2) = \sum_{m \geq n}^{m+n \leq 3} A_{mn}^{(i)} (r_1^m r_2^n + r_1^n r_2^m) \exp[-\frac{1}{2}a(r_1 + r_2)] \quad (i=1, 2), \quad (11)$$

and where the parameters a and $A_{mn}^{(i)}$ are determined variationally. One finds $a = 3.70$. The values of the 12 coefficients $A_{mn}^{(i)}$ are given in Table I. These wave functions give, respectively, for the ground-state energy of helium the values $E_0 = -2.847$ a.u., $E_0 = -2.862$ a.u., and $E_0 = -2.898$ a.u. Henceforth, the wave function given by Eq. (10) will be referred to as the "exact" wave function.

For the final state we use product wave functions of the form

$$\Psi_f(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \sum_{m_1 m_2} (l_1 m_1 l_2 m_2 | 10) [\varphi_{k_1 l_1}^{Z_1}(r_1) \varphi_{k_2 l_2}^{Z_2}(r_2) Y_{l_1 m_1}(\Omega_1) Y_{l_2 m_2}(\Omega_2) + (\vec{r}_1 \leftrightarrow \vec{r}_2)], \quad (12)$$

in which Z_1 and Z_2 are the effective charges seen by the outgoing atomic electrons and \vec{k}_1 and \vec{k}_2 are their propagation vectors. Using this final-state wave function along with our three approximations for the initial state, we have evaluated σ_{++} by using the closure theorem on the single-particle states. This enables us to reduce the integration over the double continuum of final states to a discrete sum which was readily evaluated numerically.

Figure 2 displays the quantity σ_{++}/σ_0 (in the case $Z_1 = Z_2 = \bar{Z}$) as a function of \bar{Z} . The three curves correspond to the three choices of initial states discussed above. It can be seen that the inclusion of increasing amounts of correlation in the initial state significantly modifies σ_{++}/σ_0 in the region of relevant \bar{Z} , which lies between $\bar{Z} = 1.5$ and $\bar{Z} = 2.0$. This latter choice corresponds to no correlation in the final state, whereas $\bar{Z} = 1.5$ corresponds to a model in which each outgoing electron shields the other one half of the time. We feel that the actual physical situation is closer to the

Table I. The coefficients $A_{mn}^{(i)}$ of the "exact" wave function.

(m, n)	$A_{mn}^{(1)}$	$A_{mn}^{(2)}$
(0, 0)	8.77412	0.10706
(0, 1)	2.87912	-1.96291
(0, 2)	4.27527	2.17677
(0, 3)	-0.22646	-0.45481
(1, 1)	-3.78099	-2.39768
(1, 2)	0.44706	0.60797

latter case than it is to the former. Experimental results^{4,5} suggest a value of $\sigma_{++}/\sigma_0 \cong 2.5 \times 10^{-3}$, i.e., $\sigma_{++}/\sigma_{++} \cong 200$, which is obtained from the "exact" initial-state wave function with a reasonable choice of $\bar{Z} \cong 1.55$ for the final state. The striking difference in Fig. 2 between the Hartree-Fock and "exact" cases is due primarily to the inclusion of angular

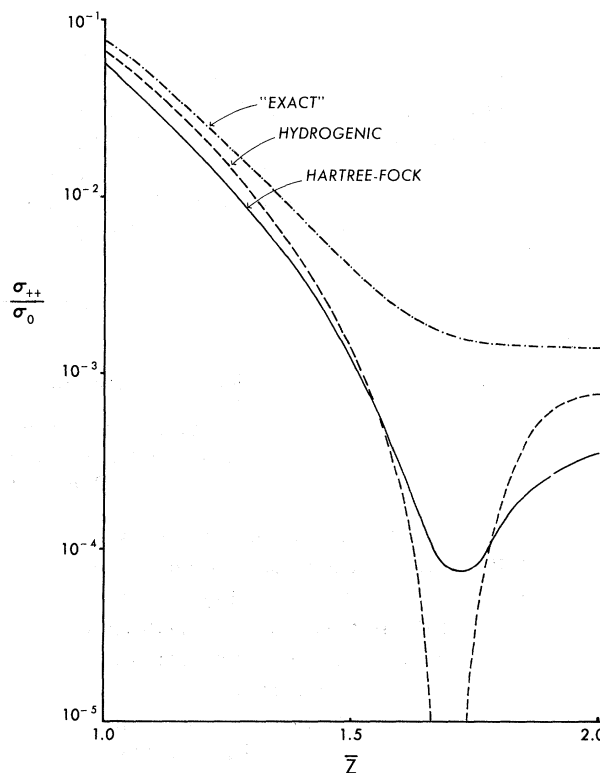


FIG. 2. The ratio σ_{++}/σ_0 vs \bar{Z} .

correlations through the relative p -wave term in Eq. (10). Although this term is smaller in magnitude than the relative s -wave term, its effect is greatly magnified because of suppression (due to small overlap with the final state) of the relative s wave in the region of interesting \bar{Z} .

Under the less realistic assumption $Z_1 = 1$ and $Z_2 = 2$ and using a Hartree-Fock wave function for the initial state (it can be shown that these assumptions are essentially equivalent to those made in Ref. 1), one obtains after some manipulation the ratio $\sigma_+/\sigma_{++} = 210$ which is very close to the value computed in Ref. 1 using the sudden approximation. However, if we include angular correlation by using the wave function given in Eq. (10), we find that the agreement with experiment is considerably worsened: $\sigma_+/\sigma_{++} = 275$.

It should be noted that the experimental ratio $\sigma_+/\sigma_{++} \approx 200$ which we used above is inferred from the work of Kistemaker *et al.*⁴ below an incident electron energy of 1 keV. Beyond this energy, a serious departure of σ_{++} from a $(\log E_i)/E_i$ dependence seems to appear.^{3,4} This cannot be explained by the approach discussed above. In fact, it is possible that higher terms of the Born series, whose size will not be reduced because of small overlaps (which was the case above for the first Born contribution to σ_{++}) could contribute significantly to σ_{++} up to rather large energies. Also to be considered are terms proportional to $1/E_i$ coming from the first Born approximation. Thus, although we conclude that the asymptotic behavior of σ_{++} at sufficiently high energy must be of

the form $(\log E_i)/E_i$, it is difficult to ascertain precisely how large this energy should be. In view of the implications of these results for the understanding of ionization phenomena and multiparticle scattering theory, it is important that further experimental studies at high energies be carried out.

We would like to thank Professor C. Schwartz for helpful comments.

*Research supported in part by the U. S. Air Force Office of Scientific Research Grant No. AF-AFOSR-130-63.

†Alfred P. Sloan Foundation Fellow.

¹M. H. Mittleman, Phys. Rev. Letters **16**, 498 (1966). See also W. E. Lamb, Jr., and Miriam Skinner, Phys. Rev. **78**, 539 (1950).

²B. L. Schram, F. J. de Heer, M. J. van der Wiel, and J. Kistemaker, Physica **31**, 94 (1965).

³F. Fiquet-Fayard, F. Muller, and J. P. Ziesel, in Abstracts of Papers of the Fourth International Conference on the Physics of Electronic and Atomic Collisions (Science Bookcrafters, Inc., Hastings-on-Hudson, New York, 1965), p. 413.

⁴B. L. Schram, F. J. de Heer, M. J. van der Wiel, A. J. H. Boerboom, H. R. Moustafa, J. Schutten, and J. Kistemaker, *ibid.*, p. 434.

⁵D. D. Briglia and D. Rapp, Bull. Am. Phys. Soc. **11**, 69 (1966).

⁶In this note "correlation" refers to effects due to the interaction between the two atomic electrons. Thus, the completely uncorrelated helium ground-state wave function is $(8/\pi) \exp[-2(r_1 + r_2)]$, i.e., the product of two hydrogenic ground-state wave functions with $Z = 2$.

⁷H. A. Bethe and E. E. Salpeter, Quantum Mechanics of One- and Two-Electron Atoms (Academic Press, Inc., New York, 1957), p. 158.

NUCLEAR RELAXATION STUDIES OF IMPURITY MOMENTS IN FERROMAGNETIC METALS

N. Kaplan, V. Jaccarino, and J. H. Wernick
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received 13 May 1966)

The Mn^{55} nmr of dilute impurities of Mn in Fe exhibits a temperature dependence to the frequency for resonance ν_T below T_C which is distinctly different from the corresponding behavior of the iron-host magnetization σ_T .¹ This dependence has been interpreted^{2,3} as direct evidence for the existence of a localized moment on the Mn ion of fixed magnitude S . The behavior of the thermal average $\langle S_T \rangle$, to

which ν_T is proportional, relative to σ_T indicates that the Mn-Fe exchange coupling is substantially weaker than the Fe-Fe interaction. Neutron scattering experiments⁴ appear to contradict these results, suggesting instead that a negligible spin magnetization, either "local" or not, resides on the Mn site. The interpretation and results of recent Mössbauer studies⁵ of the Fe near neighbors to a given Mn seem