

# PHYSICAL REVIEW LETTERS

VOLUME 17

15 AUGUST 1966

NUMBER 7

## ELECTRON-IMPACT EXCITATION OF $n=2$ STATES IN He

P. G. Burke\*

United Kingdom Atomic Energy Authority, Harwell, England

and

J. W. Cooper

National Bureau of Standards, Washington, D. C.

and

S. Ormonde†‡

Lockheed Research Laboratories, Palo Alto, California

(Received 14 March 1966; revised manuscript received 17 June 1966)

In this Letter we present the results of calculations of the excitation of the  $n=2$  states of He by electron impact which agree substantially with recent experiments.<sup>1-4</sup> We show that the structure in these cross sections is due to two previously unreported resonances<sup>5</sup> in the  $^2P$  and  $^2D$  states in addition to the now well-known 19.3-eV  $^2S$  resonance.<sup>6-8</sup> The calculation is carried out in the close-coupling approximation including the ground state and all the  $n=2$  excited states of He. Our calculation differs substantially from previous work<sup>9</sup> in the inclusion of the  $2^3,^1P$  states, which allows implicitly for the polarizability of the  $2^3,^1S$  states, and which, we feel, enables the first qualitatively accurate calculations to be made. Other results obtained<sup>10</sup> include a value in agreement with experiment<sup>11</sup> for the  $2^1S$ - $2^3S$  "super-elastic" cross section at thermal energies, and the absence of any low-energy structure in the elastic cross section.<sup>12</sup> One failure in the calculation was our inability to obtain a completely satisfactory  $S$ -wave result although we did obtain a  $^2S$  resonance at 19.33 eV (but with too large a width). Fortunately, it will be seen

that the  $S$  wave plays only a minor role in the excitation cross sections.

The basic approach of close coupling to this problem is the same as for the two-electron system.<sup>13</sup> The total wave function is expanded in terms of an antisymmetrized sum of products of helium bound-state wave functions  $\varphi_{nls}$  and functions representing the scattered electron. For the bound states we use numerical solutions of the Hartree-Fock equations obtained with the additional restriction that one of the electron orbitals in each state is given by a hydrogenic  $1s$  function with  $Z=2$ . This is an improvement over the helium wave functions used previously,<sup>9</sup> and also ensures that our  $1^1S$  and  $2^1S$  wave functions are orthogonal. Our Hartree-Fock (H-F) total energies  $E_{nls}$  for the five states are compared with experimental values<sup>14</sup> in Table I. Before solving the close-coupling equations, we have simplified the exchange terms by using the relation

$$\left( \nabla_i^2 + \nabla_j^2 + \frac{4}{r_i} + \frac{4}{r_j} - \frac{2}{r_{ij}} + E_{nls} \right) \varphi_{nls}(i,j) = 0, \quad (1)$$

care being taken in the use of Eq. (1) to preserve

Table I. Total energies for the first five levels in He.

State	$E_{nls}$ (Hartree-Fock) (Ry)	$E_{nls}$ (Expt.) (Ry)
$1s^2\ ^1S$	5.7450	5.8074
$1s2s\ ^3S$	4.3485	4.3507
$1s2s\ ^1S$	4.2869	4.2922
$1s2p\ ^3P$	4.2626	4.2665
$1s2p\ ^1P$	4.2449	4.2475

the symmetry of the exchange interaction. This relation is not exactly satisfied but we expect the error to be small except perhaps for the  $S$  wave. The open-channel scattering matrix and cross-section matrix were obtained below, between, and above all the  $n=2$  thresholds from the asymptotic form of the noniterative<sup>15</sup> numerical solution of the close-coupling equations.

Because we are interested in excitation cross sections close to threshold, we have considered only the  $^2S$ ,  $^2P$ , and  $^2D$  states. In order to make the calculation consistent with Eq. (1), it was decided to use the H-F energies given in Table I in our coupled equations. This procedure gave results for  $P$  and  $D$  waves which appeared reasonable. However, the corresponding  $S$ -wave calculations, which are much more sensitive to details of the short-range interactions, were found to be inconsistent with experiment. We do not regard our  $S$ -wave results as more than an order-of-magnitude estimate of the true result. In the results quoted below we have, therefore, taken all  $S$ -wave excitation amplitudes scaled down by a factor of about three to agree with the experimental width of the 19.3-eV  $^2S$  resonance.<sup>16</sup> This procedure is suggested on the basis of effective-range theory.<sup>17</sup> We find on these grounds that the  $S$  wave makes a small contribution to the total excitation cross section for all  $n=2$  channels. Its relative importance is greater, however, at larger scattering angles.

An analysis of the eigenphases and scattering amplitudes<sup>10</sup> shows that the  $P$  wave resonates at 20.2 eV with a total width of 0.52 eV, and the  $D$  wave resonates at 21.0 eV with a total width of 0.4 eV. About 1% of the width of each resonance represents decay into the ground-state channel and, further, the nonresonant contribution of these partial waves to the excitation cross sections is much smaller than

the resonant contribution. Figure 1 shows our results for the  $n=2$  total excitation cross sections together with experimental results from Refs. 1 and 4. The  $2^3S$  cross section shows two peaks corresponding to the  $^2P$  and  $^2D$  resonances. The  $P$ -wave contribution to the  $2^1S$  cross section is large very close to threshold and rises slowly thereafter, and the  $D$ -wave contribution peaks at approximately the same energy as for the  $2^3S$ . For the  $2^3P$  and  $2^1P$  excitation cross sections, the dominant contributions arise from the  $P$  and  $D$  wave as close to threshold as we have calculated. Adding the full  $S$ -wave component instead of scaling it down would increase the absolute value of the  $2^3S$  and  $2^1S$  cross sections by approximately a factor of 2 and leave the  $2^3P$  and  $2^1P$  cross sections unchanged. The spectral profiles would not be appreciably affected.

In Fig. 2 we compare the  $2^3S$  excitation spectra calculated at 0 and 72° with the experiments of Refs. 2 and 3. Figure 2(a) shows that at 0° the amount of  $S$ -wave contribution we include does not appreciably affect the shape of the spectrum. However, to reproduce the bump observed at threshold<sup>18</sup> would require a larger  $S$  wave than we include. Figure 2(b) shows that the larger dip in the experimental results at 72° than at 0° is consistent with our calculation but that we overestimate the size of the second peak. Adding the  $S$ -wave component gives an

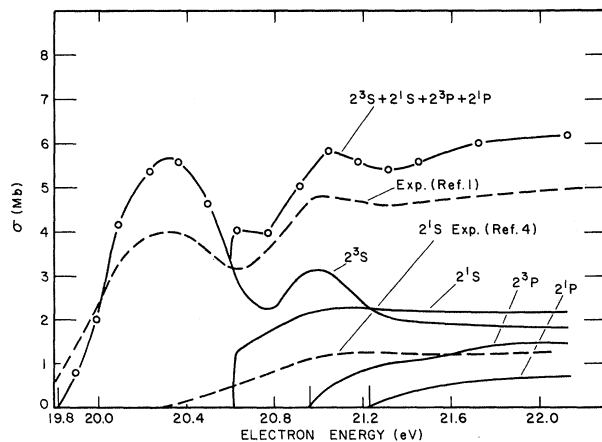


FIG. 1. Total metastable cross sections for electron impact on He and the individual  $2^3S$ ,  $2^1S$ ,  $2^3P$ , and  $2^1P$  contributions. Dashed curves are obtained from the experiments of Refs. 1 and 4. Calculated curves for all cross sections are based on computations at the points shown in the total metastable cross-section curve. The normalization of Ref. 4 was taken to agree with Ref. 1 which is an absolute measurement.

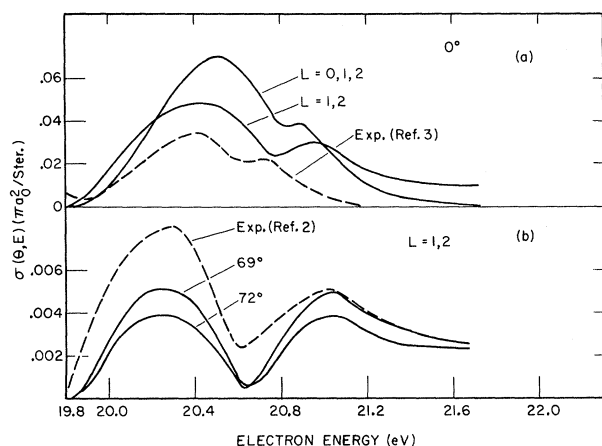


FIG. 2. Spectra for  $2^3S$  excitation at 0 and  $72^\circ$  relative to the incident-electron beam direction, compared with experimental results from Refs. 2 and 3. The experimental normalization in these curves is arbitrary and has been adjusted for clarity of presentation.

even larger second peak. At  $72^\circ$  the observed spectrum is more difficult to estimate for two reasons. First, the  $S$ -wave component has a larger relative effect on this spectrum than at  $0^\circ$ . Second, the experiment was performed by collecting electrons over an angular range of  $\sim 6^\circ$  and the spectrum is changing with angle at  $72^\circ$  much more rapidly than at  $0^\circ$ . This effect is indicated by the calculation at  $69^\circ$  and  $72^\circ$  shown in Fig. 2(b). Better agreement with experiment will require a better estimate of the  $S$ -wave contribution and probably some estimate of the contribution of higher partial waves.

In conclusion, we have seen that taking account of all of the  $n=2$  channels introduces a multi-resonance structure into the  $e$ -He scattering problem. The large polarizability of the  $2^3S$  and  $2^1S$  states due to the neighboring  $2^3P$  and  $2^1P$  states is the essential feature of this resonance structure.<sup>19</sup> We expect that polarizability is also the dominant feature of resonances that have been observed at the higher thresholds.<sup>3</sup>

We would like to thank Dr. U. Fano and Dr. J. H. Macek for many helpful discussions during the course of this work. We also gratefully acknowledge the aid of the U. S. Air Force Weapons Laboratory, Albuquerque, New Mexico, where most of the calculations were carried out and, in particular, the help of Mr. W. Huebner of that Laboratory in carrying out the computations.

\*Work performed in part at National Bureau of Standards, Washington, D. C., while a guest worker under NATO sponsorship.

†Work supported by the U. S. Air Force Special Weapons Center under Contract No. AF 29(601)-6801.

‡Present address: United Kingdom Atomic Energy Authority, Harwell, England, and Department of Mathematics, Royal Holloway College, Englefield Green, Surrey, England.

<sup>1</sup>G. J. Schulz and R. E. Fox, *Phys. Rev.* **106**, 1179 (1957).

<sup>2</sup>G. J. Schulz and J. W. Philbrick, *Phys. Rev. Letters* **13**, 477 (1964).

<sup>3</sup>G. E. Chamberlain and H. G. M. Heideman, *Phys. Rev. Letters* **15**, 337 (1965).

<sup>4</sup>H. K. Holt and R. Krotkov, *Phys. Rev.* **144**, 82 (1966).

<sup>5</sup>Resonant structure in these processes has been discussed previously in terms of a  $2^3S$  compound-ion model. E. Baranger and E. Gerjuoy, *Proc. Phys. Soc. (London)* **A72**, 326 (1958).

<sup>6</sup>G. J. Schulz, *Phys. Rev. Letters* **10**, 104 (1963).

<sup>7</sup>J. A. Simpson and U. Fano, *Phys. Rev. Letters* **11**, 158 (1963).

<sup>8</sup>R. J. Fleming and G. S. Higginson, *Proc. Phys. Soc. (London)* **81**, 974 (1963).

<sup>9</sup>H. S. W. Massey and B. L. Moiseiwitsch, *Proc. Roy. Soc. (London)* **A227**, 38 (1954); R. Marriott, *Atomic Collision Processes*, edited by M. R. C. McDowell (North-Holland Publishing Company, Amsterdam, 1964), p. 114; *Proc. Phys. Soc. (London)* **87**, 407 (1966).

<sup>10</sup>A detailed description and further results will be published elsewhere.

<sup>11</sup>A. V. Phelps, *Phys. Rev.* **99**, 1307 (1955). The experimental value is  $340\pi a_0^2$ . Our calculation yields  $360\pi a_0^2$  due almost entirely to  $P$  wave.

<sup>12</sup>C. Ramsauer and R. Kollath, *Ann. Phys. (N.Y.)* **3**, 536 (1929); G. J. Schulz, in *Proceedings of the Fourth International Conference on the Physics of Electronic and Atomic Collisions, Quebec, Canada, August, 1965* (Science Bookcrafters, Inc., Hastings-on-Hudson, New York, 1965), p. 117. These experiments indicated structure in elastic  $e^-$ -He scattering below 2 eV. However, other experimental work has not shown these effects (D. E. Golden and H. W. Bandel, private communication).

<sup>13</sup>I. C. Percival and M. J. Seaton, *Proc. Cambridge Phil. Soc.* **53**, 654 (1957).

<sup>14</sup>C. E. Moore, *Atomic Energy Levels*, National Bureau of Standards Circular No. 467 (U. S. Government Printing Office, Washington, D. C., 1948).

<sup>15</sup>R. Marriott, *Proc. Phys. Soc. (London)* **A72**, 121 (1958); K. Omidvar, New York University Report No. CX-37, 1959 (unpublished).

<sup>16</sup>We estimate the width of the  $2^3S$  resonance at 19.31 eV to be 0.004 eV taking account of Doppler broadening and of the resolution of the experimental measurements.<sup>6,7</sup> Our calculated  $2^3S$  resonance is at 19.33 eV and its width is 0.039 eV.

<sup>17</sup>P. G. Burke, *Advan. Phys.* **14**, 521 (1965). By means of effective-range extrapolation, the  $S$ -wave component of the  $2^3S$  excitation cross section can be

estimated close to threshold from the position, width, and nonresonant phase obtained from the  $2^1S$  resonance at 19.31 eV.<sup>7</sup> After the initial  $E^{1/2}$  rise, the cross section is essentially flat over the energy range considered in this paper and its magnitude is proportional to the resonance width. Our calculated  $S$ -wave  $2^3S$  and  $2^1S$  excitation cross sections have the same spectral behavior as those obtained by this extrapolation. This suggests our scaling procedure, although there may be a phase shift in the amplitude which we do not include.

<sup>18</sup>It is interesting to note, however, that the signs of our  $S$ - and  $P$ -wave amplitudes are such as to give the interference effect required by the bump.

<sup>19</sup>The importance of the polarizability of the  $2^3S$  state may be seen as follows. In the absence of coupling to other channels the effective range formula of T. F. O'Malley, L. Spruch, and L. Rosenberg [J. Math. Phys. **2**, 491 (1961)] predicts a linear rise of the  $P$  phase with energy close to threshold. We find that the linear rise in the  $2^3S$  phase continues all the way up to the  $2^1S$  threshold where the phase has reached more than  $\pi$  rad. Substitution of the  $2^3S$  polarizability ( $313a_0^3$ ) in the effective-range formula of O'Malley *et al.* yields a width of  $\Gamma=0.42$  eV, in good agreement with the result obtained here by direct calculation. Similar arguments can be applied to higher thresholds.

### INTERFERENCE BEATS IN PULSE-STIMULATED CYCLOTRON RADIATION\*

J. M. Wachtel and J. L. Hirshfield  
Yale University, New Haven, Connecticut  
(Received 16 May 1966)

About a year ago, Hill and Kaplan<sup>1</sup> discovered experimentally that a weakly ionized gas in a dc magnetic field gave a transient response to two or more cyclotron-resonant rf pulses, which was reminiscent of Hahn echoes from precessing spins.<sup>2,3</sup> The purpose of this Letter is to point out that certain free-electron systems can also exhibit a related transient effect whose nuclear resonance analog is the interference beating ascribed to the chemical Larmor shift, which was first observed by Hahn with  $F^{19}$  nuclei in certain organic compounds.<sup>2</sup> For the free-electron system, the beating phenomenon can arise from the spread in cyclotron frequencies which is imposed on a cloud of initially monoenergetic weakly relativistic electrons in a uniform dc magnetic field, using one or more cyclotron resonant pulses. We report here the experimental observation of such a beat envelope, following single-pulse excitation, and offer a brief theory for comparison with experiment.

The apparatus employed to study this effect is shown schematically in Fig. 1. It was designed so as to impose the cyclotron-resonant impulse on electrons at cavity No. 1 as they drifted from left to right along a dc magnetic field. As the electrons drifted through cavity No. 2, one could measure whatever coherent cyclotron radiation was emitted. Stainless-steel construction of the experimental tube, using copper or gold sealing gaskets and ceramic feed-throughs and rf windows, afforded

base pressures of  $\sim 10^{-9}$  Torr after extended bake-out at 400°C. The system was continuously pumped. Electrons were accelerated through potentials of from 1 to 5 keV in a region immersed in a longitudinal magnetic field of approximately 150 G, over which a weak (<15 G), twisted transverse magnetic field generated

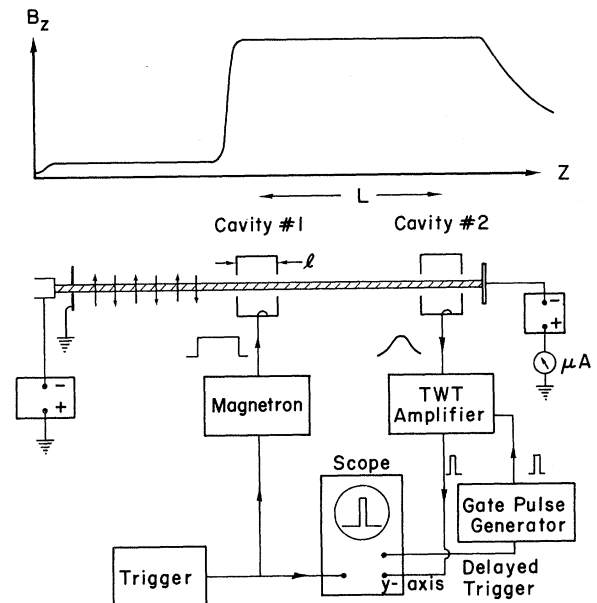


FIG. 1. Diagram of experimental apparatus. Upper plot shows axial magnetic field along apparatus. The impulse length is determined by the drift velocity and cavity dimension  $l$ , while the delay time is determined by the drift velocity and the cavity spacing  $L$ .