[1]D. Burch and P. Richard, Phys. Rev. Lett. 25, 983 (1970); P. Richard, I. L. Morgan, T. Furuta, and D. Burch, Phys. Rev. Lett. 23, 1009 (1969).

[2]The notation $K\alpha$ with no subscript on α is herein used to designate *any* $1s \rightarrow 2p$ transition independent of the number or orbitals of the other electrons. This is to be distinguished from, for example, $K\alpha_1$ which implies a distinct energy and an initial- and final-state configuration.

[3]R. L. Blake, thesis, University of Colorado, 1968 (unpublished).

[4]J. A. Bearden, Rev. Mod. Phys. 39, 78 (1967).

[5]F. Herman and S. Skillman, *Atomic Structure Calculations* (Prentice-Hall, Englewood Cliffs, N.J., 1963).

[6]F. P. Larkins, private communication.

[7]E. J. McGuire, Phys. Rev. A 3, 587 (1971).

[8]J. C. Slater, Phys. Rev. 36, 57 (1930).

[9]E. J. McGuire, Phys. Rev. 185, 1 (1969); F. P. Larkins, to be published.

[10]J. H. Scofield, Phys. Rev. 179, 9 (1969).

[11]M. H. Chen, B. Crasemann, and V. O. Kostroun, to be published.

[12]J. S. Hansen, H. U. Freund, and R. W. Fink, Nucl. Phys. A142, 604 (1970).

[13]D. Burch and P. Richard, Bull. Amer. Phys. Soc. 16, 74 (1971).

[14]L. G. Parratt, Phys. Rev. 50, 1 (1936); D. J. Candlin, Proc. Phys. Soc., London, Sect. A 68, 323 (1955).

[15]D. Burch and P. Richard, to be published.

[16]L. C. Northcliffe and R. F. Shilling, Nucl. Data, Sect. A 7, 233 (1970).

[17]R. L. Blake and L. L. House, to be published.

[18]T. H. Lie and R. C. Elton, Phys. Rev. A 3, 865 (1971).

Photoionization Cross Section of the Neutral Iron Atom*

Hugh Kelly and Akiva Ron†

Department of Physics, University of Virginia, Charlottesville, Virginia 22901

(Received 31 March 1971)

The photoionization cross section of the neutral iron atom is calculated from threshold at 7.90 eV to 36 eV. Results are presented for the Hartree-Fock approximation and correlations are included by many-body perturbation theory.

We have calculated the photoionization cross section $\sigma(\omega)$ of the neutral iron atom by means of the many-body perturbation theory of Brueckner[1] and Goldstone[2] and by our methods[3,4] for evaluating the diagrams for atoms. This calculation was stimulated by its relevance for astrophysics[5] and by the fact that there does not seem to be any measurement of $\sigma(\omega)$ for Fe.[6] In these calculations we use the relation[7]

$$\sigma(\omega) = (4\pi/c)\omega \operatorname{Im}\alpha(\omega), \tag{1}$$

where $\alpha(\omega)$ is the frequency-dependent polarizability.[8,9] Atomic units are used throughout this paper unless otherwise indicated.

In calculating the perturbation-theory diagrams[9] for $\alpha(\omega)$, we treat energy denominators according to the usual prescription $\mathrm{P}-i\pi\delta$, where P represents a principal-value integration. Then $\operatorname{Im}\alpha(\omega)$ consists of all diagrams in which we have an odd number of contributions from $-i\pi\delta$. The lowest-order diagram contributing to $\alpha(\omega)$ is shown in Fig. 1(a). The horizontal line represents use of $-i\pi\delta$. This notation has also been used by Wendin who has discussed calculation of resonances in $\sigma(\omega)$ by many-body theory.[10] In Fig. 1, the heavy dot represents matrix elements of z. [In calculating $\alpha(\omega)$ we take the perturbing electric field in the $\hat{z}$ direction and average over M_L.] The dashed lines with no heavy dot represent Coulomb correlations. In the next order of perturbation theory there are diagrams as shown in Figs. 1(b) and 1(c). These diagrams also occur inverted and there are corresponding exchange diagrams. When there is no horizontal

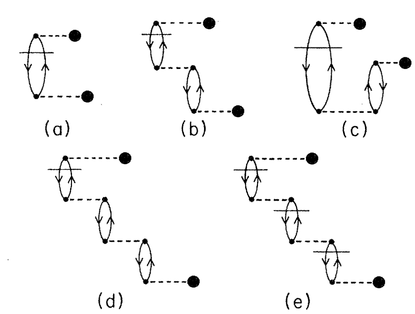

FIG. 1. Lowest-order diagrams contributing to the photoionization cross section or $\operatorname{Im}\alpha(\omega)$. The horizontal line indicates a denominator contribution $-i\pi\delta$. The heavy dot indicates a matrix element of z. (a) Lowest-order diagram. (b), (c) Diagrams with one Coulomb interaction. These diagrams also occur inverted. The corresponding exchange diagrams should also be included. (d), (e) Higher-order diagrams.

line, denominators are treated by principal-value integration.

In calculating $\sigma(\omega)$ for the $(3d)^6(4s)^2\,{}^5D$ ground state of Fe, we have used our complete set of single-particle states from a calculation of the hyperfine contact interaction in Fe. We carried out the calculations with $M_S=+2$ and averaged over M_L. Our cross section of course is independent of M_S. There are higher-order diagrams[9] which shift the single-particle energies $\epsilon(n)$ so as to give correct ionization energies $\epsilon'(n)$. We calculated the shifted energies $\epsilon(4s^\pm)$, and $\epsilon(4s^-)$ agreed well with the experimental ionization energy.[11] We used spectroscopic data[11] to determine $\epsilon(3d^-)$, and we obtained an average $\epsilon(3d^+)$ by calculating the difference from $\epsilon(3d^-)$. Our shifted energies for $\epsilon(4s^-)$ and $\epsilon(4s^+)$ are -0.2903 and -0.3104 a.u., respectively. For $\epsilon(3d^-)$ and $\epsilon(3d^+)$ we obtained -0.3965 and -0.5811 a.u., respectively. The difference between $\epsilon(4s^-)$ and $\epsilon(4s^+)$ is due to the fact that (for $M_S=+2$) the $4s^+$ electron has exchange interactions with the five $3d^+$ electrons whereas the $4s^-$ electron has an exchange interaction with the single $3d^-$ electron.

Results for $\sigma(\omega)$ are shown in Fig. 2. The dashed line represents the Hartree-Fock result obtained from the diagram of Fig. 1(a). The solid line is the result including correlations. We included diagrams like Figs. 1(b) and 1(c), their inverses, and also the corresponding exchange diagrams. We also included some higher-order diagrams like Figs. 1(b) and 1(c) in which the part of the diagram above the horizontal line is identical to that below. Diagrams like Fig. 1(d) were approximately included. Diagrams like Fig. 1(e) were also included. The maximum contribution from Fig. 1(e) came near threshold and reduced $\sigma(\omega)$ by approximately 8 %. Our results in Fig. 2 have only included correlations among $4s$ and $3d$ electrons and correlations of $3d$ with $3p$ electrons. The $3d$-$3p$ correlations were found to be small, and it was estimated that the omitted correlations affect $\sigma(\omega)$ very little.

The large increase over the Hartree-Fock result is due mostly to the diagram of Fig. 1(b) when the bottom matrix element is $\langle 4p|z|4s\rangle$. This matrix element is so much larger than $\langle kp|z|4s\rangle$ that it more than compensates for the reduction due to the Coulomb matrix element. This diagram corresponds to configuration mixing in the many-particle final state between $4skp$ and $4p4s$. We expect that this effect will be found in all atoms with an outer $(ns)^2$ subshell with $n \geq 2$. In such atoms, Hartree-Fock results may be expected to differ significantly from experiment. In diagrams like Fig. 1(d), when all but the top excited states are $4p^\pm$ and the hole lines are $4s^\pm$, we may sum the diagrams geometrically.[4]

We note that the important configuration mixing in the final state between $4skp$ and $4p4s$ is an example of intrachannel interaction described by

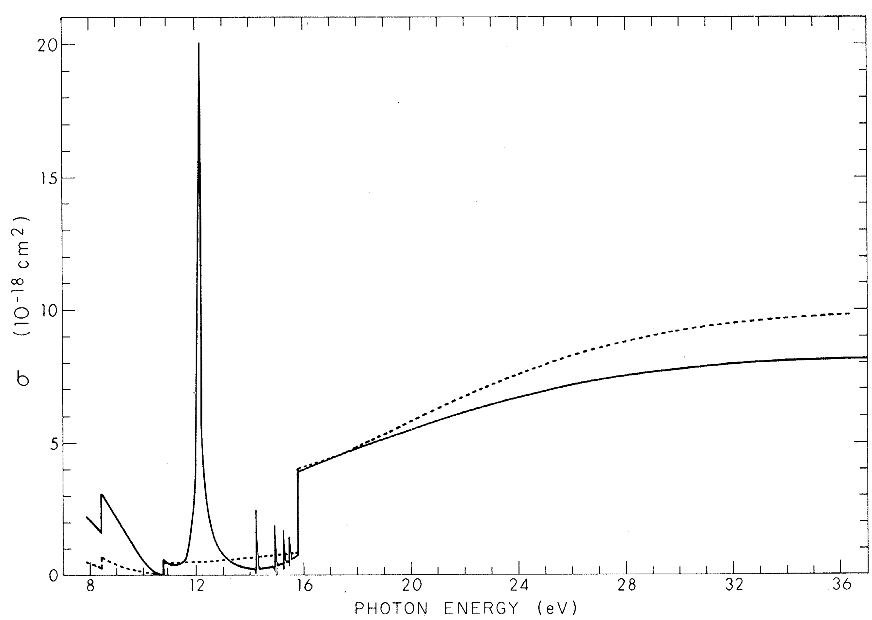

FIG. 2. Photoionization cross section $\sigma(\omega)$ for Fe. Dashed line, lowest-order or Hartree-Fock result. Solid line, correlations included.

Fano and Cooper.[7] Recent calculations by Starace[12] on argon and xenon have included the intrachannel effect by the reaction matrix method.[7,13] Intrachannel effects are also included in Altick's calculation[14] of the photoionization cross section of Be by means of configuration interaction. For Be they also cause a large increase of the cross section near threshold over the Hartree-Fock results.

In Fig. 2 we note the strong resonance at 12.13 eV and lesser resonances from 14.26 to 15.81 eV. The resonance at 12.13 eV is due to $3d^+ \to 4p^+$ excitations which are degenerate in energy with $4s^\pm \to kp^\pm$ and $3d^- \to kf^-, kp^-$ excitations. These resonances occur in diagrams like Fig. 1(b) in which the bottom excitation is $3d^+ \to np^+$. We have not made an accurate determination of the height and shape of the resonances, which would involve including many higher-order diagrams. There are also narrow resonances (not shown in Fig. 2) from $3d^+ \to nf^+$ excitations and from $4s^+ np^+$ for high n. Many other resonances also occur in higher-order diagrams. We expect that the most important of these involve $(4s)^2 \to mpns$ or $(4s)^2 \to mpnd$ excitations. We plan to investigate these effects in a future paper.

At higher energies than shown in Fig. 2, there are contributions to $\sigma(\omega)$ from the inner subshells and these will be described in a more complete account of this work. At present we are also calculating contributions to $\sigma(\omega)$ in which two or more electrons are ejected, and processes in which one electron is ejected and the atom is left in an excited state. We also plan to extend our results to higher orders in perturbation theory. There is a definite need for continued experimental and calculational effort on atoms such as Fe.

We wish to thank Professor O. Gingerich for his comments which stimulated this work. We also thank Professor J. W. Beams for his encouragement, and Dr. R. L. Chase for the use of two computer programs.

---

*Research supported by the Aerospace Research Laboratories, U. S. Air Force Office of Aerospace Research, under Contract No. F 33615-69-C-1048.

†Permanent address: Department of Theoretical Physics, The Hebrew University, Jerusalem, Isreal.

[1]K. A. Brueckner, Phys. Rev. 97, 1353 (1955), and in *The Many-Body Problem*, edited by C. DeWitt (Wiley, New York, 1959).

[2]J. Goldstone, Proc. Roy. Soc., Ser. A 239, 267 (1957).

[3]H. P. Kelly, Phys. Rev. 131, 684 (1963).

[4]H. P. Kelly, Phys. Rev. 136, B896 (1964).

[5]O. Gingerich, private communication.

[6]G. V. Marr, *Photoionization Processes in Gases* (Academic, New York, 1967).

[7]U. Fano and J. W. Cooper, Rev. Mod. Phys. 40, 441 (1968).

[8]A. Dalgarno, in *Perturbation Theory and Its Applications in Quantum Mechanics*, edited by C. H. Wilcox (Wiley, New York, 1966), p. 145.

[9]H. P. Kelly, Phys. Rev. 182, 84 (1969).

[10]G. Wendin, J. Phys. B: Proc. Phys. Soc., London 3, 446, 455 (1970).

[11]C. E. Moore, *Atomic Energy Levels as Derived from Analyses of Optical Spectra*, National Bureau of Standards Circular No. 467 (U.S.G.P.O., Washington, D. C., 1949), Vol. I.

[12]A. F. Starace, Phys. Rev. A 2, 118 (1970).

[13]P. L. Altick and E. N. Moore, Phys. Rev. 147, 59 (1966).

[14]P. L. Altick, Phys. Rev. 169, 21 (1968).