ability agrees extremely well with the 52-term calculation for ω less than 2.2 a.u. A detailed calculation shows that the transition energy ω for the 80-parameter wave function is 2.2884 a.u. corresponding to 199.157 Å. The accurate calculation of Pekeris[9] and his collaborators gives -7.27991 a.u. for the ground state of Li^+ and -4.99335 a.u.[14] for the $2\,^1p$ state of Li^+. Thus the accurate transition energy should be 2.28656 a.u. corresponding to 199.317 Å in wavelength. The error in the present calculation is less than 0.1%. The results for the Li^+ calculation are shown in Table III and Fig. 2. In Fig. 2 only one curve is shown because the 28-, 52-, and 80-term calculations essentially fall on each other. The refractive index of Li^+ is given in Table IV.

To summarize this work, we have calculated the dynamic polarizabilities of H^- and Li^+ with convergent results. It is our conjecture that the resulting dynamic polarizabilities are accurate to at least three or possibly four significant figures for ω slightly displaced from the transition energy. This implies that the first-order frequency-dependent wave functions are accurately calculated and can be used to investigate other processes.

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Electron Correlation Energies in the Neutral Iron Atom*

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The many-body perturbation theory of Brueckner and Goldstone is used to calculate the electron correlation energy among the $n=3$ and $n=4$ electrons of Fe I. The result is -0.7155 a.u. Combined with a semiempirical estimate of correlations from the $(1s)^2(2s)^2(2p)^6$ core, the total correlation energy of Fe I is -1.165 a.u.

The perturbation theory of Brueckner[1,2] and Goldstone[3] has been useful in calculating atomic properties for many atoms.[4–8] One such property is the atomic correlation energy, and detailed calculations using the Brueckner-Goldstone (BG) perturbation theory have been carried out for the correlation energies of lithium,[8] beryllium,[4] carbon,[9] and oxygen.[5] The results of these calculations are summarized in Table I. Other methods have also been used to calculate correlation energies of the first-row atoms.[10–15] In this paper, we report results of a correlation-energy calculation for the neutral iron atom. These calculations used our methods[4,5] for applying the BG perturbation theory to atoms. The correlation energy of Fe among the $(3s)^2(3p)^6(3d)^6(4s)^2$ outer electrons, which are of most interest, was explicitly calculated. Correlations of $n=3$ and $n=4$ electrons with the inner $(1s)^2(2s)^2(2p)^6$ core electrons and also correlations among the core electrons were estimated from the semiempirical values of Clementi.[16]

Our calculations include excited states with $l=0, 1, 2, 3, 4$. Bound and continuum states were calculated numerically. All $l=0$ states were calculated with the Hartree-Fock (HF) $4s$ equation, and so the $4s$ is an HF orbital, but $1s$, $2s$, and $3s$ states are not exactly HF states. However, they differ from the corresponding HF states by at most 0.001 a.u.

TABLE I. Electron correlation energies in a.u. for ground states.[a]

	Li[b]	Be[c]	C[d]	O[e]
Single excitations	0.000	0.000	−0.002	−0.003
Pair correlations	−0.046	−0.093	−0.158	−0.271
Three-body terms	0.0002	0.001	0.004	0.011[f]
Total[g]	−0.046	−0.092	−0.156	−0.260
Experiment	−0.0453	−0.094	−0.157	−0.258

[a] Calculations prior to the present one which were carried out using the methods of Ref. 4 for applying many-body perturbation theory to atoms.

[b] Reference 8.

[c] Reference 4.

[d] Reference 9.

[e] Reference 5.

[f] Based on calculation among $(2p)^4$ and estimate of $2s$ and $1s$ contributions.

[g] Calculated results are estimated to be accurate to ±5%.

in the radial wave function. As in the oxygen case,[5] single-particle energies ϵ_α for $\alpha = 1s, 2s$, and $3s$ differed appreciably from the HF values. However, because of insertions on hole lines,[5] we should shift ϵ_α by

$$\Delta(\alpha)=\sum_{n=1}^{N}\left(\langle \alpha n \mid v \mid \alpha n\rangle-\langle \alpha n \mid v \mid n\alpha\rangle\right)-\langle\alpha\mid V\mid \alpha\rangle, \quad (1)$$

where v is the Coulomb interaction, and V is the potential used to calculate ϵ_α. The largest shift, 0.354 75 a.u., occurs for ϵ_{3s}, which is −4.524 58 a.u. before the shift and −4.169 83 after the shift as compared with the HF value −4.169 72 a.u. Including the shift, both ϵ_{1s} and ϵ_{2s} became almost exactly equal to the HF values. Because of the expected importance of $4s \rightarrow 4p$ excitations, we calculated all $l = 1$ states in the field of neutral Fe with one $4s$ electron missing. Although the $2p$ and $3p$ states are now not exactly HF states, they differ from the HF states[16] by at most 0.004 a.u. in the radial function. Including $\Delta(\alpha)$, ϵ_{2p} and ϵ_{3p} are almost exactly equal to the HF values. The $l = 2$ states were calculated with the HF $3d$ equation, and $l = 3$ and $l = 4$ states were also calculated in the field of Fe with one $3d$ electron missing. To check the completeness of our radial states, we evaluated the sum rule

$$\sum_k \langle\alpha \mid r \mid k\rangle\langle k \mid r^{-1} \mid \beta\rangle = \delta_{\alpha\beta},$$

which was satisfied to one digit in the third decimal place for α, β occupied states.

To obtain the correlation energy, we first calculated the second-order diagrams shown in Figs. 1(a)–1(f). In addition to Figs. 1(a)–1(c), there are also diagrams in which the top interaction is an exchange interaction or interaction with $-V$, as indicated by the crossed line. In Fig. 1(d), we show an insertion on a hole line which contributes to $\Delta(\alpha)$. Our "second-order" results include these shifts. Contributions from Figs. 1(a)–1(f) are in the top of Table II and contribute −0.0071 a.u. We expect the second-order correlation diagrams of Figs. 1(e) and 1(f) to give the total pair-correlation energies to an accuracy of at least 10% because of our choice for V.[4,5] Results for Figs. 1(e) and 1(f) are given in Table II.

The largest contribution to the $3d$-$3d$ correlation energy was from excitations into two $l = 2$ continuum states. In this case, Fig. 1(e) contributed −0.099 42 a.u. and Fig. 1(f) contributed +0.017 54 a.u. The next largest $3d$-$3d$ contribution came from excitations into two $l = 3$ states: −0.069 52 a.u. from Fig. 1(e) and +0.007 46 from Fig. 1(f). Diagrams involving excitations of the occupied $3d^-$ electron into the unoccupied $3d^-$ states were small.

For $3d-3p$ correlations, the largest contribution came from $3d \rightarrow kd$, $3p \rightarrow kp$ excitations which contributed −0.118 62 a.u. to Fig. 1(e) and +0.027 88 a.u. to Fig. 1(f). The $3p \rightarrow 3d^-$, $3d \rightarrow kf$ excitations contributed −0.093 89 a.u. to Fig. 1(e). We note from the results of Table II that the pair correlations decrease as the spatial separation increases.

The lowest-order three-body diagrams are the third-order ring diagrams, as shown in Fig. 1(g), and the corresponding exchange diagrams, two of which are shown in Figs. 1(h) and 1(i). A complete listing of the exchange diagrams is given in Ref. 9. We first calculated the ring diagram of Fig. 1(g) for three $3d$ electrons with excitations into $l = 2$ states and obtained 0.036 18 a.u. For excitations into $l = 3$ states, we obtained 0.006 25 au. Exchange diagrams for three $3d$ electrons were esti-

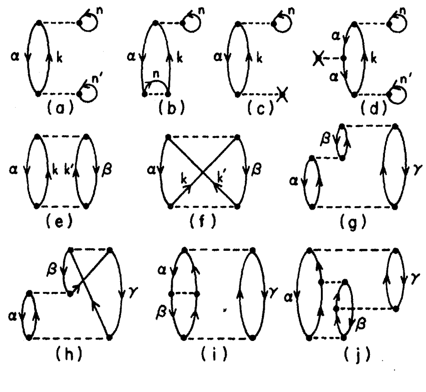

FIG. 1. Correlation-energy diagrams: (a)–(c) second-order diagrams with single excitations; (d) insertion on hole line; (e) direct pair-correlation diagram; (f) pair exchange; (g) ring diagram; (h) and (i) are typical exchange diagrams corresponding to (g); (j) typical fourth-order three-body diagram.

TABLE II. Contributions to the correlation energy in a.u.

Diagram	Energy in a.u.
Single excitations [Figs. 1(a)–1(c)]	
$4s$	−0.001 56
$3d$	−0.003 79
$3p$	−0.001 47
$3s$	−0.000 16
Subtotal	−0.006 98

Second-order pair correlations

	Fig. 1(e)	Fig. 1(f)	Fig. 1(e) + Fig. 1(f)
$4s-4s$	−0.050 16	0.000 00	−0.050 16
$4s-3d$	−0.060 33	0.010 23	−0.050 10
$4s-3p$	−0.019 89	0.001 75	−0.018 14
$4s-3s$	−0.002 05	0.000 55	−0.001 51
$3d-3d$	−0.211 19	0.038 42	−0.172 77
$3d-3p$	−0.348 85	0.072 10	−0.276 75
$3d-3s$	−0.067 44	0.018 44	−0.049 00
$3p-3p$	−0.132 47	0.023 71	−0.108 76
$3p-3s$	−0.081 72	0.033 51	−0.048 21
$3s-3s$	−0.006 62	0.000 00	−0.006 62
Subtotal	−0.980 72	0.198 71	−0.782 01

mated to be small. Since $l=2$ and $l=3$ excited states contributed most of the $3d$-$3d$ pair-correlation energy, we estimate contributions from the other excitations as small. Our total three-body contribution among $3d$ electrons then reduces the $3d$-$3d$ pair results by approximately 25%. We also calculated the diagram of Fig. 1(g) for one $3p$ electron and two $3d$ electrons including only $3d \rightarrow kd$ and $3p \rightarrow kp$ excitations. The result is 0.054 40 a.u. For one $3d$ hole and two $3p$ holes with $3p \rightarrow kp$ and $3d \rightarrow kd$, we obtained 0.024 66 a.u. For three $3p$ electrons, including only $l=1$ excited states, we obtained 0.003 25 a.u. Our final result for the three-body ring diagrams which we calculated among $3d$ and $3p$ electrons is then 0.1247 a.u. Our results for three-body diagrams with $3p$ hole states are probably less accurate than our $3d$-$3d$-$3d$ result since we have not included $3p \rightarrow kd$ excitations in Fig. 1(g). However, in these cases we expect considerable cancellation from exchange diagrams of the types shown in Figs. 1(h) and 1(i). We also expect smaller contributions from three-body diagrams involving $4s$ or $3s$ electrons. Fourth- and higher-order diagrams involving a triple of electrons are estimated to be small since they involve interactions with particle lines or hole lines as shown in the middle two particle-line interactions of Fig. 1(j). For each particle-line interaction, there is a corresponding hole-line interaction of opposite sign and of approximately the same magnitude.[6, 17] Four-body and higher effects are estimated to be −0.015 a.u.

Our total calculated result for correlations among the $n=3$ and $n=4$ electrons of Fe is then −0.6721 a.u. From the semiempirical data of Clementi,[16] we estimate the correlation energy from interactions of $n=3$ and $n=4$ electrons with the $(1s)^2(2s)^2(2p)^6$ core as approximately −0.100 a.u. Estimating the correlation energy among the $(1s)^2(2s)^2(2p)^6$ core as that for Ne, −0.393 a.u., we obtain a total E_{corr} for Fe equal to −1.165 a.u.

In calculating the correlation energy among a fixed pair pq, many higher-order rearrangement terms are included by shifting the denominators of second-order terms by $E_{\text{corr}}(p,q)$, the pair-correlation energy. In configuration-interaction (CI) calculations which include only single and double excitations, one has a Brillouin-Wigner situation[2] corresponding to denominator shifts in perturbation theory by E_{corr}, the total correlation energy.[18] The correct shift is given by[18]

$$\sum_{\alpha} E_{\text{corr}}(p,\alpha)+\sum_{\beta\neq\alpha} E_{\text{corr}}(q,\beta). \tag{2}$$

Recalculating $E_{\text{corr}}(4s,4s)$ with the shift of Eq. (2), we obtained −0.037 10 a.u. We obtained −0.043 24 a.u. with the shift $E_{\text{corr}}(4s,4s)$, and −0.012 13 a.u. with the shift E_{corr}. These shifts should make less difference for the other pairs since the denominators are larger. However, these results indicate the importance of including fourfold excitations in certain CI calculations.

Future calculations will include a more detailed study of three-body effects and will also explicitly include the correlations with the $(1s)^2(2s)^2(2p)^6$ electrons.

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Lamb Shift in Singly Ionized Helium[†]

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The energy separation $\mathcal{S}$ between the $2\,^2S_{1/2}$ and $2\,^2P_{1/2}$ states of singly ionized helium was measured using a microwave method. Helium atoms in the space between the plates of a spherical-mirror Fabry-Perot resonator are bombarded continuously by electrons of 200-eV energy to produce helium ions in the $2\,^2S_{1/2}$ metastable state. The applied modulated rf power induces transitions in the metastable ions to the short-lived $2\,^2P_{1/2}$ state. The 40.8-eV photons emitted by the decay of the $2\,^2P_{1/2}$ ions to the ionic ground state $1\,^2S_{1/2}$ are quantum converted to visible photons by a scintillator and are then guided to a photomultiplier. The output of the photomultiplier is detected and amplified synchronously with the rf power. The experiment made use of the Zeeman effect of the fine structure and is performed in an applied homogeneous magnetic field. Three different operating values for the helium pressure are used and the result is extrapolated to a zero-pressure value. A thorough search was made for all possible systematic errors in the experiment. The value for $\mathcal{S}$ thus obtained is 14 046.2 ± 2.0 MHz. The quoted uncertainty consists of three standard deviations for the statistical error plus estimates of systematic errors. This result agrees with the previous experimental values for $\mathcal{S}$ (within three standard deviations), and with the latest theoretical value of 14 044.5 ± 5.2 MHz.

I. INTRODUCTION

The fine structure of the $n=2$ level of hydrogen and deuterium has been studied by Lamb and his collaborators,[1] using an atomic-beam rf power method. Their experiments established the existence of a small energy separation between the $2\,^2S_{1/2}$ and $2\,^2P_{1/2}$ levels of these atoms, which are degenerate according to the Dirac theory, and also gave precise values for these separations. This separation, the Lamb shift, is a result of the interaction of the atomic electron with its own (virtual) radiation field; thus, purely of radiative origin, it provided a test for the validity of the theory of quantum electrodynamics. Measurements of the Lamb shift in hydrogen by Robiscoe[2] and deuterium by Cosens[3] have been made using a level-crossing technique with results of precision equal to those of Lamb.

The Lamb shift in the $n=2$ level of singly ionized helium has been measured by Lamb and Skinner[4]; Yergin[5]; Novick, Lipworth, and Yergin[6]; and Lipworth and Novick.[7] The values they measured for $\mathcal{S}$ are 14 020 ± 100, 14 021 ± 60, 14 043 ± 13, and 14 040.2 ± 4.5 MHz, respectively.

The work reported here is directed towards precision remeasurement of the Lamb shift $\mathcal{S}$ in the $n=2$ level of singly ionized helium. Radio frequency power was used to induce the Lamb-shift transition. A phase-sensitive detection scheme was used for the signal measurements. Considerable effort was made to keep the apparatus stable during the period of an experimental run, and a procedure that provides a check on the stability of the system in each run was employed to obtain precision resonance data. Much of the data was collected under different operating characteristics of the apparatus, and a thorough search was made for possible systematic corrections to the final result.

Section II describes the experimental method, Sec. III discusses the details of the apparatus, and Sec. IV includes the operating characteristics of