High-precision spectroscopic study of heliumlike iron

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The x-ray spectrum emitted by high-velocity heliumlike iron ions has been studied with a crystal spectrometer. The absolute energies of the $n=2\rightarrow n=1$ lines have been measured with a precision of 40 ppm. A very good agreement has been found between our experimental values and a very accurate multiconfiguration Dirac-Fock calculation. The precision of the measurement and the calculation of the energies are such that for the first time the magnetic correlation energy (spin-spin) as well as the screening of quantum-electrodynamic effects can now be appreciated. The contamination of the considered lines by the so-called dielectronic recombination satellites has been studied in great detail by varying the nature and the thickness of the targets.

INTRODUCTION

The relativistic corrections to the electron-electron repulsion in atoms (Breit term) constitute, for the heaviest atomic systems, a very substantial part of the energy of the levels. Unfortunately, these effects cannot be specifically studied in neutral heavy atoms owing to the large number of electrons present. Heliumlike heavy ions then constitute the most elementary systems to study specifically all these effects. The excited states of the helium atom are presently known with a precision of ~ 1 ppm, i.e., of the same order of magnitude as that of the fine-structure constant.[1,2] As was pointed out further in Refs. 3 and 4, however, this precision is insufficient to study some corrections which are only of importance for the heavy ions such as the second-order relativistic effects, the screening and many-body effects in QED corrections, the magnetic correlation effects, and so on.

Up to now heavy heliumlike systems have only been produced and observed in very hot plasma sources like fusion and solar-corona plasmas. Heliumlike iron ions, which constitute the most abundant and the heaviest ionic species in both kinds of plasmas, have recently been studied carefully.[5] These ions are observed in media in which internal or external fields as well as hot electron gas can dramatically change the energy of the lines (namely, the contamination of the rays by the so-called dielectronic recombination satellites). We have studied, for the first time, with a crystal spectrometer of high resolution and high precision, the x rays emitted in flight by heliumlike ions in a beam foil experiment in a vacuum and outside any electric and magnetic field. The precision we obtained (40 ppm) is now such that most of the considered relativistic and QED effects can be appreciated when compared to our calculations whose precision is of the same order.

EXPERIMENTAL

The ions studied were produced by stripping the 480 MeV Fe^{18+} beam delivered by the SuperHILAC (super heavy-ion linear accelerator) of Berkeley through a 300 $\mu g\,cm^{-2}$ carbon foil. The typical charge-state distribution obtained under these conditions is presented in Table I. Downstream from the stripping foil the ions were excited or dressed by a second very thin (50 $\mu g\,cm^{-2}$) carbon foil. The fast radiative decay of the ions which takes place just after the foil ($\bar{x} < 1$ μm) (see Table II) was observed at 90° with respect to the heavy-ion beam by an x-ray spectrometer specially designed for this purpose (Fig. 1) and described in more detail in Refs. 3 and 4. The x-ray spectrometer was made of a Si220 flat crystal mounted on a precision goniometer (3×10^{-4} deg) and located 3.6 m away from the slit fixed just in the vicinity of the second target.

The reflected x rays were analyzed with a position-sensitive detector of the backgammon type mounted on a

TABLE I. Charge-state distribution of a iron beam of 480 MeV through a 300 $\mu g\,cm^{-2}$ carbon foil.

Charge state	26+	25+	24+	23+	22+
Intensity	5%	32%	46%	16%	1.3%

TABLE II. Lifetimes and mean ranges of ($n=2$) excited heliumlike iron ions (the x rays were detected through a 0.15-mm slit).

Transition	Nature	τ (s)	$\bar{x}$ (mm)
$1s^2$-$1s2p$ $1\,^1S_0$-$2\,^1P_1$	$E1$	theor: 2×10^{-15} (Ref. 6)	8×10^{-5}
$1s^2$-$1s2p$ $1\,^1S_0$-$2\,^3P_1$	$E1^*$	theor: $\sim2.3\times10^{-14}$ (Ref. 6)	8×10^{-4}
$1s^2$-$1s2p$ $1\,^1S_0$-$2\,^3P_2$	$M2$	expt: 1.5×10^{-10} (Ref. 7)	4.5
$1s^2$-$1s2s$ $1\,^1S_0$-$2\,^3S_1$	$M1$	expt: 4.8×10^{-9} (Ref. 7)	144

circular track of 21 cm of radium around the axis of the crystal goniometer. Its partial resolution was about 100 μm. The position of the localization chamber (Bragg angle 2θ) was controlled by a translator whose linear accuracy was of 1 μm. The whole system was mounted under a vacuum except for the localization chamber. The housing of the goniometer was closed by a curved beryllium foil of 250 μm allowing a detection of the reflected x rays over a large angular range. A schematic of the experimental setup is presented in Fig. 1.

The principle of the measurement was to observe, at the correct Bragg angle, the Lyman α lines emitted by the excited hydrogenlike fraction of the beam and then to make a given θ—2θ rotation of the spectrometer such that heliumlike characteristic lines can be detected at the same place in the position-sensitive detector as the reference line. The energy of the line being studied with respect to that of the Lyman α could then be directly obtained by measuring the rotation angles. This procedure avoided all the possible errors due to (i) the relativistic aberrations (the heliumlike rays were detected when emitted at the same angle with regard to the heavy ion beam), (ii) the crystal imperfections and the possible detector nonlinearity (reflection on the same part of the crystal), and (iii) the measurement of the exact energy of the heavy ions. The error in the measurement was then mainly fixed by the error of the angle measured by the goniometer and the statistical error in the determination of the peaks. The absolute overall error at 7 keV was found to be less than 0.25 eV.

HELIUMLIKE SPECTRUM

We present in Figs. 2 and 3 the decay scheme of a heliumlike ion and the observed iron heliumlike spectrum when using a 200 $\mu g\,cm^{-2}$ stripper and a 100 $\mu g\,cm^{-2}$ carbon dresser. Among the four possible transitions in the $n=2\rightarrow n=1$ decay of a heliumlike iron ion, only three of them can be observed through the 150-μm slit located behind the dressing foil: the two $E1$ transitions that fully decay in front of the slit (the $^1P_1\rightarrow{}^1S_0$ and the $^3P_1\rightarrow{}^1S_0$ intercombination line) and the $M2$ transition which only partly decays in front of the slit owing to its long lifetime (Table II). The $M1$ transition which has a very long lifetime has not been observed in this experiment. The major problem to be solved when considering the decay of ions after passing through a foil is to make sure that there is no extra outermost-shell spectator electron present in the ion at the time of the decay which may slightly change the energy of the lines under study. This is the situation in hot plasmas where extra electrons may be added to outermost shells of heliumlike ions and where the main diagram lines are so strongly contaminated that it is not possible to perform precise energy measurements.

When using a beam foil excitation it is possible, however, to control the capture of extra electrons by varying the nature and the thickness of the foils; this is the way we used to get rid of the contamination of the considered lines by the dielectronic satellites.

The energy of the satellite lines when an extra electron is present during the decay of the heliumlike ion strongly depends on the shell into which the spectator electron has been captured. If the electron is captured in the $n=2$ shell ($1s^22l$-$1s2l^2$ transitions), the energy difference between the satellite line and the diagram line (pure heliumlike ion) is usually larger than the experimental linewidth and can easily be observed with a crystal spectrometer of even a poor resolution (this is what we shall name "far satellites"). If the electron is captured in an $n>2$ shell, the energy difference between the satellites and the diagram lines are much smaller and usually of the same order as the experimental linewidth. The observed lines will then

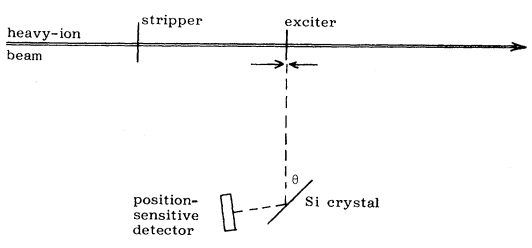

FIG. 1. Design of the experiment.

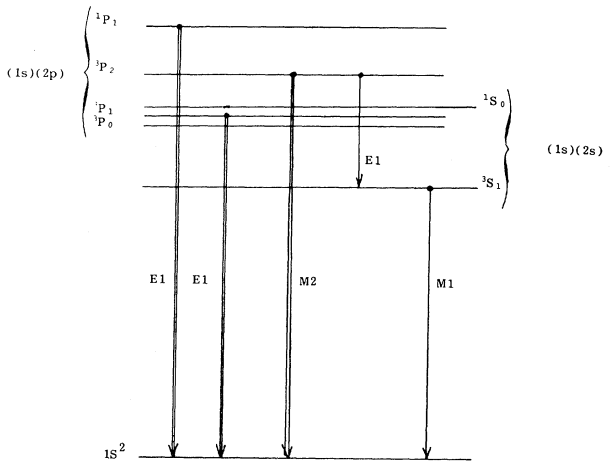

FIG. 2. Radiative decay scheme of heliumlike ions.

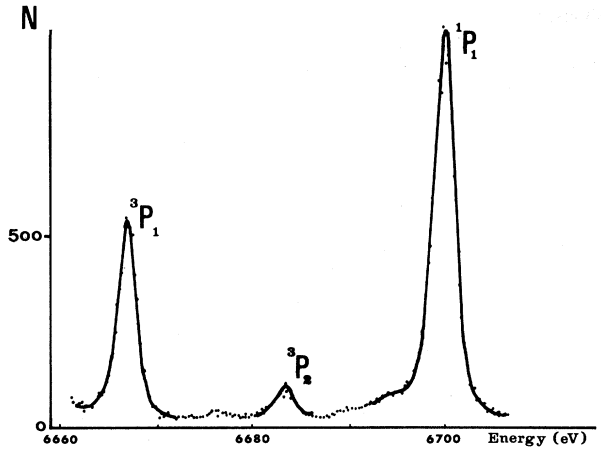

FIG. 3. Iron heliumlike spectrum observed with a C 100 $\mu g\,cm^{-2}$ target.

correspond to some complex unresolved multiplets whose mean energy values may be slightly different from that of the diagram lines (contamination satellites). The energies of these satellite lines have been calculated by Bely-Dubau *et al.*[8] up to $n=15$ but it appears that the energy shift of the satellite lines can only appreciably change the energy of the observed lines for $n<5$. We have calculated, using the radiative and nonradiative transition probabilities of Bely-Dubau,[8,9] the relative probability of the multiplet components for each of the $3s$, $3p$, $3d$, and $4l$ extra electron of the $^1P_1$ transition and made a simulation of each of these resultant lines with the present experimental resolution. This simulation is presented in Fig. 4 where it appears that the contamination of the lines by an unknown amount of satellites may change the energies of the observed lines by a quantity that can be sometimes much greater than 1 eV. In Fig. 5 we present the experimental profile of the $^1P_1$ line observed with a 100 $\mu g\,cm^{-2}$ Al foil in which the probability of capturing an extra outermost-shell electron is very probable. It can be seen in the figure that the capture of an $n=3$ electron does not happen appreciably in the $3d$ subshell. A more detailed analysis shows that the capture mainly occurs in the $3p$ subshell.

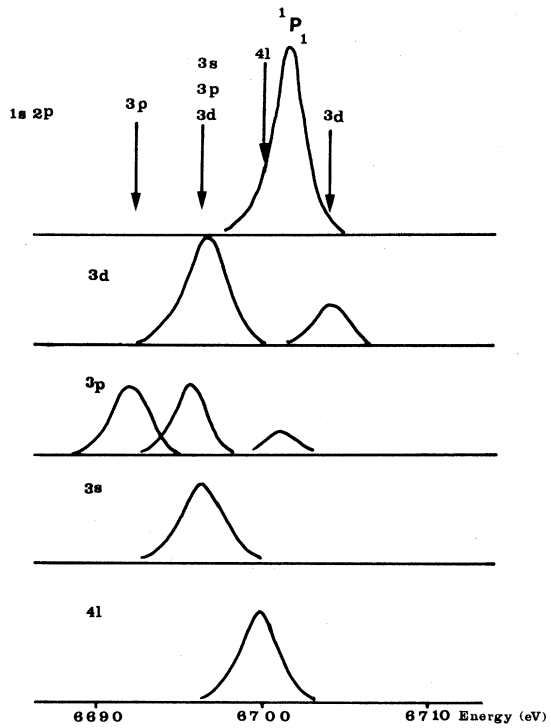

FIG. 4. Relative positions and intensities of the $n=3$ and $n=4$ "dielectronic recombination" satellites. (A statistical distribution of the terms of each configuration has been assumed.)

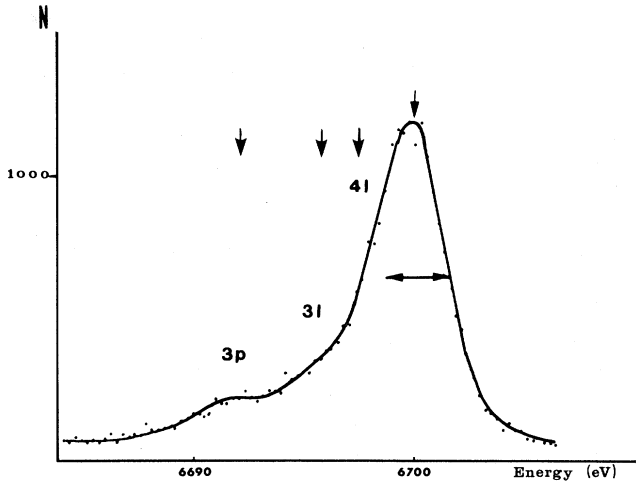

FIG. 5. Experimental profile of the $^1P_1$ line observed with a 100 $\mu g\,cm^{-2}$ aluminium target.

The contamination of the $^1P_1$ and $^3P_1$ lines by the $n=3$ satellites is, however, very different for iron ions owing to the very different lifetimes of the $^1P_1$ and $^3P_1$ heliumlike core. In Table III, we present the radiative transition probabilities of the $2p$, $3s$, $3p$, and $3d$ excited states in a hydrogenlike ion and those of the $1s2p$ states of a heliumlike ion. It appears that the presence of an additional electron in the $n=1$ shell of a hydrogenlike ion can dramatically hinder the decay of the $2p$ excited electron. This comes from the fact that iron ions are still in the region where intermediate coupling prevails and that the coupling of the two electrons in the triplet state to the singlet ground state is still appreciably forbidden (by a factor of 10 compared to the $^1P_1$ decay rate).

If we now add to a heliumlike excited core an extra electron in the $n=3$ shell, there will be a competition between the $n=2$ and $n=3$ electron to fill the K hole. It can be seen from Table III that (i) if the excited core is in

TABLE III. Comparison of lifetimes in hydrogenlike iron ions (approximate values using the Z^4 scaling law) and heliumlike ions (Ref. 6).

	Hydrogenlike				
Transition	$2p\rightarrow 1s$	$3s\rightarrow 2p$	$3p\rightarrow 1s$	$3p\rightarrow 2s$	$3d\rightarrow 2p$
Decay rate ($10^{13}\,s^{-1}$)	3	0.3	7	1	3
	Heliumlike				
$1s2p\,^1P_1\rightarrow 1s^2\,^1S_0$	$\lambda=46$ ($10^{13}\,s^{-1}$)				
$1s2p\,^3P_1\rightarrow 1s^2\,^1S_0$	$\lambda=4.2$ ($10^{13}\,s^{-1}$)				

the $^1P_1$ state, the $2p$ electron always decays prior to the $3l$ one. The decay takes place in the presence of the spectator electron, and we will observe some satellite lines; (ii) if the excited core is in the $^3P_1$ state whose decay rate is much smaller than in the previous case, the $3l$ electron has a much greater probability of filling the K hole than the $2p$ one. The $n=2\rightarrow n=1$ x-ray line will not then be observed and the characteristic lines will mainly be observed only in cases where no extra electron has been captured. The observed $^3P_1$ characteristic line will not then be appreciably contaminated by the satellites.

This is what we observed when we used thick targets of quite large atomic number where the probability of multiple capture is very great and where we noticed a large broadening and deformation of the $^1P_1$ lines as compared to the characteristic $^3P_1$ line (Fig. 6). The way to get rid of the satellite contamination or to take it into consideration is then obvious. We have performed several experiments making use of various targets of different thicknesses, i.e., in experimental situations in which the multiple capture in the target can be controlled until we reach a spectrum where the two $^1P_1$ and $^3P_1$ lines (i) have similar linewidths, (ii) do not exhibit any shape alteration, and (iii) do not contain any far satellite (the ratio between capture in $n=2,3,4,\ldots$ shell does not change appreciably with the nature and the thickness of the target), and the presence of these far satellites is obviously a test of the presence of contamination satellites in the line (Fig. 6). The energy of the lines which are presented in Table IV were obtained by using the spectrum shown in Fig. 3. The precision of the energy measurement of the $M2$ line, which is less than the one for the two other lines, comes from the fact that the $M2$ line decays on an extended range much larger than the spectrometer slit and then appears with a slightly larger linewidth. As was mentioned above, the energy of the lines, whose precision is only that of the angle measurement and therefore very good (0.25 eV), is given relatively to that of *the theoretical Lyman α_1 line of hydrogenlike ions in the same experimental conditions.*[3,4] Although there are some previous observations of these lines by various authors in hot plasma sources (solar-corona plasmas,[10,11] laboratory plasmas,[12,13] or tokamak plasmas,[5] it does not seem possible owing to the previous considerations to compare all those (mainly relative) measurements.

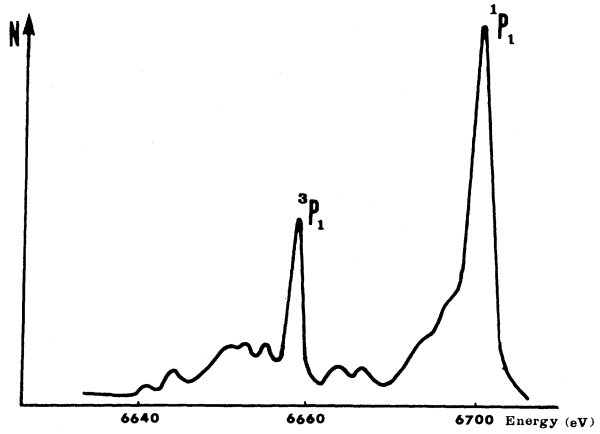

FIG. 6. Comparison of the $^1P_1$ and $^3P_1$ line shapes observed with a 100 μg cm^{-2} aluminium target.

TABLE IV. Experimental energy values of the $n=2\rightarrow n=1$ transitions in heliumlike iron.

$1s^2\,{}^1S_0$-$1s2p\,{}^1P_1$	$1s^2\,{}^1S_0$-$1s2p\,{}^3P_1$	$1s^2\,{}^1S_0$-$1s2p\,{}^3P_2$
6700.9 eV	6667.5 eV	6682.7 eV

COMPARISON WITH THEORY

Two-electron ions have been the subject of many theoretical investigations since it is possible to carry out most sophisticated calculations for these systems. Although the transition energies considered here have already been calculated by various authors,[14–18] none of the methods used so far are completely satisfactory. Either nonrelativistic many-body effects have been considered very carefully but relativistic corrections were added with unscreened hydrogenic approximation, or relativistic effects were included in a nonperturbative way but the influence of the nonrelativistic correlation was not fully taken into account. For example, it is well known that in the random-phase approximation only the so-called bubble diagrams are considered. Under these circumstances it seems worthwhile to look for another approach to include the relativistic and correlation effects together. For this purpose we use the multiconfiguration Dirac-Fock (MCDF) method. This method not only included all leading relativistic effects (i.e., the ones arising from the Dirac Hamiltonian) to all orders in perturbation theory and the intermediate coupling scheme in a completely *ab initio* manner, but also allows for a systematic investigation of relativistic and correction contributions as explained below.

The MCDF method[19] is by now well known and we outline here only its main features. Then we compare our theoretical values with previous ones and the present experimental results. In its commonly used form, the MCDF method starts from the following zero-order Hamiltonian:

$$H=\sum_1 H_D(i)+\sum_{\substack{i,j\\ i<j}} 1/r_{ij}\ , \tag{1}$$

i.e., a sum of one-electron Dirac operators H_D plus the Coulomb repulsion between the electrons. Parenthetically, we note that there is no fundamental reason to make such a restriction for the electron-electron interaction as long as one restricts the variational space to electronlike solutions only.[20,21] On the other hand, it is well established that for medium Z values, including the Breit operator in the self-consistent-field (SCF) procedure or treating it as a first-order perturbation, essentially produces the same numerical results. The total wave function for a given state is then expressed as a linear combination of configuration-state functions (CSF) ϕ:

$$\Psi=\sum_\nu w_\nu\phi_\nu(J,M,\Pi)\ , \tag{2}$$

where each of the ϕ's is a simultaneous eigenfunction of the total angular momentum J, its projection M, and the parity Π (the only good quantum numbers in the relativistic case). Also, in Fig. 2 ν stands for all the other quantities (occupation numbers, coupling scheme, seniority, etc.) necessary to unambiguously define a given CSF, which are Slater determinants of four component Dirac spinors. Then, using the variational principle, both the mixing coefficients w and the radial components (large and small) of the Dirac spinors are optimized in a self-consistent process. After self-consistency has been achieved, it is necessary, as already said, to correct the total energy for higher relativistic effects. For spin-spin, spin-other-orbit, and retardation in the Coulomb interaction, first-order perturbation theory is used by calculating the exact expectation value of the low-frequency limit of the Breit operator

$$B(i,j)=-[\vec{\alpha}_i\cdot\vec{\alpha}_j+(\vec{\alpha}_i\cdot R)(\vec{\alpha}_j\cdot R)/R^2]/R\ , \tag{3}$$

where $R=|\vec{r}_i-\vec{r}_j|$ is the interelectronic distance and the $\vec{\alpha}$'s are the usual Dirac matrices. Radiative corrections are accounted for by calculating the expectation value of the Uehling potential[22] which is known[23] to give the dominant contribution to the vacuum polarization, while the self-energy correction is deduced from the hydrogenic results of Mohr[24] for $1s$, $2s$, $2p_{1/2}$, and $2p_{3/2}$ electrons. Screening corrections obtained from the comparison of the mean radius of the Dirac-Fock orbitals and that of their hydrogenic counterparts have been used. Although this prescription for introducing the screening due to the other electron cannot be rigorously justified, it appears to give reasonable agreement with more elaborate calculations for K electrons.[25]

For two-electron systems it can be shown[26] that the expansion of the MCDF wave function is given by

$$|\,1s^2,\ ^1S_0\rangle=\sum_{n,l} w_{n,l}\phi_{n,l}(nl^2,\ ^1S_0) \tag{4}$$

for the ground state, while for the $1s2p$ excited states one has

$$\begin{aligned}|\,1s2p,\ ^{1,3}P_J\rangle=&\sum_n w_n\phi_n[ns,(n+1)p,\ ^{1,3}P_J]\\&+\sum_{n'} w_{n'}\phi_{n'}[n'p',(n'+1)d,\ ^{1,3}P_J]\\&+\sum_{n''} w_{n''}\phi_{n''}[n''d',(n''+1)f,\ ^{1,3}P_J]\\&+\cdots\ .\end{aligned} \tag{5}$$

For simplicity we have used nonrelativistic labels for the orbitals, but it should be understood that we have included all the jj subconfigurations arising from a single LS one when necessary (e.g., $1s2p$ stands for both $1s2p_{1/2}$ and $1s2p_{3/2}$ if $J=1$). The primes indicate that, in principle, the second set of $p,d,\ldots$ radial functions is different from the first one. The underlying reason is explained in Ref. 26 and has to do with the fact that the reduced MCDF expansion as given in Eq. (5) results from a series of orthogonal transformations, each of which is acting on a different l,l' subspace. The reduced form of the MCDF expansion is very convenient since the various CSF's differ by two electrons, and consequently a relatively small number of Slater integrals appears in the energy expression. Furthermore, a systematic extension of the basis (in terms of n and l orbitals) allows us to check the convergence of the radial and angular contributions to the correlation energy. As the present version of the MCDF program does not allow more than one orbital with the same set of quantum numbers, we used the approximation $np'=np$, $nd'=nd$. The effect of this approximation can be estimated in simple cases by using the unreduced form of the MCDF expansion, i.e., by including, besides the double excitations which appear in Eq. (5), single excitations of the type $1s2p\ 1s3p$ or $1s2p\ 2s2p$, which greatly increase the computer time. In all the cases we had tested, we found that the effect of the above approximation was always less than a few hundredths of an eV.

The present calculations were performed with $1s$, $2s$, $2p$, $3s$, $3p$, and $3d$ basis orbitals for the ground states, while for the excited ones we added the $4p$ orbital. This basis appears to be flexible enough to obtain good convergence for both the radial and angular contributions to the correlation energy as can be seen from the decrease in the value of the weights (w_ν^2) listed in Table V. This is also confirmed by the comparison with the results of the Z-expansion method. For the $1s^2$ ground state, the nonrelativistic correlation energy up to the $1/Z$ term is given in atomic units by[27]

$$E_{\text{correl}}^{\text{NR}}=0.046\,66-0.009\,76/Z \tag{6}$$

which gives 1.26 eV for $Z=26$. The MCDF value of 1.16 eV given in Table V shows that it is quite reasonable to assume an accuracy of roughly 0.1 eV in our estimate of the correlation energy. In the third column of Table V we list the contribution of the Breit interaction. Besides its significant value, it is interesting to observe the variation of this contribution when extra configurations (essentially $2p^2$) are added. The Breit term changes by 0.2 eV due to correlation and consequently increases the pure Coulomb part by 15%. Although the importance of the Breit term in accurately reproducing fine-structure splittings has been recognized for some time, there are only a few examples of its prime importance in the calculation of precise correlation energies so clearly demonstrated.

In Table VI we list various contributions to the transition energies and compare the resultant transition energies

TABLE V. Multiconfiguration Dirac-Fock results for Fe^{24+} $1s^2\,^1S_0$ (in eV).

Configuration	Total energy[a]	ΔE[b]	Breit term	Weights[c]
$1s^2$	18 118.48	0	−6.20	0.999 96
$+2s^2$	18 118.85	0.37	−6.15	0.136(−4)
$+3s^2$	18 118.88	0.40	−6.14	0.291(−6)
$+2p^2$	18 119.50	1.02	−6.02	0.223(−4)
$+3p^2$	18 119.57	1.09	−6.00	0.742(−6)
$+3d^2$	18 119.64	1.16	−5.98	0.111(−5)

[a]Without Breit and radiative corrections.
[b]Contribution of the correlation energy.
[c]Coefficients w_ν^2 of Eq. (1). Numbers in parentheses are powers of ten.

TABLE VI. Various contributions to the transition energy (in eV).

	$^1P_1 \rightarrow {}^1S_0$	$^3P_1 \rightarrow {}^1S_0$	$^3P_2 \rightarrow {}^1S_0$
Hartree-Fock	6638.81	6616.77	6616.77
Dirac correction	70.22	59.00	74.06
Breit interaction	−6.10	−5.70	−6.08
Radiative corrections	−3.52	−3.58	−3.55
Correlation	1.29	1.30	1.28
Total	6700.70	6667.79	6682.48
Experiment	6700.9	6667.5	6682.7

TABLE VII. Comparison of theoretical transition energies (in eV).

	$^1P_1 \rightarrow {}^1S_0$	$^3P_1 \rightarrow {}^1S_0$	$^3P_2 \rightarrow {}^1S_0$
Safronova[a]	6700.24	6667.88	6682.40
Johnson and Lin[b]	6700.92	6667.67	6682.09
Present	6700.70	6667.79	6682.48

[a]Reference 18.
[b]Reference 16 corrected with the present radiative contributions.

with the present experimental results. It may be more important than the agreement, which is quite satisfactory in all cases, to evaluate the accuracy to which various contributions have been obtained in order not to be misled by fortuitous cancellations between the estimates of individual terms. We have already stated that the correlation contribution (which is the least important one but by no means negligible) is certainly correct within 0.1 eV. The Breit interaction has been obtained as a first-order perturbation and at the low-frequency limit. We have checked that, for single configurations, the inclusion of the dominant part of the Breit term, i.e., the spin-spin interaction, in the self-consistent process does not change our results by more than a few hundredths of an eV. Work is in progress to include the Breit term in the multiconfiguration self-consistent field process. The low-frequency-limit approximation is justified for this medium Z ion and an upper limit of the transverse (high frequency) contribution can be estimated from the 3.4 eV contribution found by Beatham *et al.*[28] for the $K\alpha$ x ray of mercury. Assuming a $Z^{3.6}$ dependence for the total Breit term,[29] we obtain 0.07 eV for iron in quite good agreement with the difference between the Breit interaction and the full transverse interaction as given by Mann and Johnson.[29] The accuracy of the radiative corrections is more difficult to assess due to the lack of accurate QED calculations for many electron systems. Nevertheless, it is known[30] that the lowest-order QED correction in two-electron atoms is essentially of hydrogenic form modified by the screened densities at the nucleus. These screening effects have been introduced in an approximate way as explained above. If we take the difference between pure hydrogenic self-energies and screened ones as the order of magnitude of the missing contributions, we can guess a relative uncertainty of about $(Z-\sigma/Z)^4$. With a screening coefficient σ of typically 0.3, this gives 5% of the calculated radiative corrections which amounts to 0.15 eV in the present case. In conclusion, the accuracy of the calculated transition energies is quite similar to the experimental uncertainty.

We turn now to the comparison with previous theoretical values. Those reported by Bely-Dubau *et al.*[17] have been adjusted by a few eV in order to reproduce the known experimental values of the resonant transition energies and cannot be compared with our present completely *ab initio* results. Among others, we consider the results of Johnson and Lin[15] obtained in the framework of the relativistic random-phase-approximation (RPA) method and those of Safronova[18] calculated through the double Z^{-1} and αZ series expansion. Parenthetically we notice that the results of Drake[16] are, in this Z region, comparable to the relativistic RPA ones, while, as was pointed out by Safronova,[18] the good agreement between her results and those by Ermolaev[14] for Fe XXV is due to fortuitous cancellations between omitted terms in the calculation of Ermolaev. The comparison in Table VII shows a reasonable agreement between the various theoretical values. It should be pointed out that this agreement is in some sense misleading since Safronova used unscreened, self-energy corrections while the screening effects amount to 0.4 eV. Clearly the 0.4 eV difference is compensated by the way she introduced other corrections and very likely by the Breit interaction treated in the Pauli approximation. On the other hand, the small differences with the relativistic RPA results (to which we added our estimate of the radiative corrections) may well be attributed to the different way of including correlation effects.

[1]A. Kponou, V. W. Hughes, C. E. Johnson, S. A. Lewis, and F. M. Pichanick, Phys. Rev. A 24, 264 (1981).
[2]W. Frieze, E. A. Hinds, V. W. Hughes, and F. M. Pichanick, Phys. Rev. A 24, 279 (1981).
[3]J. P. Briand, M. Tavernier, P. Indelicato, R. Marrus, and H. Gould, Phys. Rev. Lett. 50, 832 (1983).
[4]J. P. Briand, *Proceedings of the International Conference on X-ray and Atomic Inner-shell Physics, Eugene, Oregon, 1982* (in press).
[5]M. Bitter, K. W. Hill, N. R. Sauthoff, P. C. Efthimion, E. Meservey, W. Roney, S. Van Goeler, R. Horton, M. Goldman, and W. Stodiek, Phys. Rev. Lett. 43, 129 (1979).
[6]C. D. Lin, W. R. Johnson, and A. Dalgarno, Phys. Rev. A 15, 154 (1977).
[7]H. Gould, R. Marrus, and P. Mohr, Phys. Rev. Lett. 33, 676 (1974).
[8]F. Bely-Dubau, A. H. Gabriel, and S. Volonté, Mon. Not. R. Astron. Soc. 189, 801 (1979).
[9]F. Bely-Dubau, A. H. Gabriel, and S. Volonté, Mon. Not. R. Astron. Soc. 186, 405 (1979).

[10]W. Neupert, Sol. Phys. 18, 474 (1971).
[11]Y. U. Grineva, V. I. Karev, V. V. Korneev, V. V. Krutov, S. L. Mandelstam, L. A. Vainstein, B. N. Vasilyev, and I. A. Zhitnik, Sol. Phys. 29, 441 (1973).
[12]T. N. Lie and R. C. Elton, Phys. Rev. A 3, 865 (1971).
[13]E. Ya Kononov, K. N. Koshelev, and Yu V. Sidel'nikov, Sov. J. Plasma Phys. 3(3), 375 (1977) [Fiz. Plazmy 3, 663 (1977)].
[14]A. M. Ermolaev, M. Jones, and K. F. H. Phillips, Astron. Lett. 12, 53 (1972).
[15]A. M. Ermolaev, Phys. Rev. A 8, 1651 (1973).
[16]W. R. Johnson and C. D. Lin, Phys. Rev. A 14, 565 (1976).
[17]G. W. F. Drake, Phys. Rev. A 19, 1387 (1979).
[18]U. I. Safronova, Phys. Scr. 23, 241 (1981).
[19]J. P. Desclaux, Comput. Phys. Commun. 9, 31 (1975).
[20]J. Sucher, Phys. Rev. A 22, 348 (1980).
[21]I. P. Grant, in *Relativistic Effects in Atoms, Molecules and Solids,* edited by G. L. Malli (Plenum, New York, in press).
[22]E. A. Uehling, Phys. Rev. 48, 55 (1935).
[23]E. H. Wichmann and N. M. Kroll, Phys. Rev. 101, 843 (1956).
[24]P. J. Mohr, Ann. Phys. (N.Y.) 88, 52 (1974); Phys. Rev. Lett. 34, 1050 (1975) and unpublished.
[25]A. M. Desiderio and W. R. Johnson, Phys. Rev. A 3, 1267 (1971).
[26]C. F. Fischer, *The Hartree-Fock Method for Atoms: A Numerical Approach* (Wiley-Interscience, New York, 1977).
[27]U. I. Safronova, J. Phys. B 10, 1591 (1975); see, also, Ref. 18.
[28]N. Beatham, I. P. Grant, B. J. McKenzie, and S. J. Rose, Phys. Scr. 21, 423 (1980).
[29]J. B. Mann and W. R. Johnson, Phys. Rev. A 4, 41 (1971).
[30]P. K. Kabir and E. E. Salpeter, Phys. Rev. 108, 1256 (1957).