Relativistic effects, correlation, and QED corrections on $K\alpha$ transitions in medium to very heavy atoms

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(Received 19 December 1991)

$K\alpha$ ($1s^{-1}$–$2p^{-1}$) transition energies for atoms in the range $31 \leq Z \leq 100$ have been calculated using the Dirac-Fock model with self-consistent magnetic interaction and full relaxation. Complete retardation, hydrogenic radiative corrections (with finite nucleus effects), as well as screening corrections are included. Electrostatic and Breit correlation energies have been computed with relativistic many-body perturbation theory. Auger shifts and core-core contributions have also been added. Comparison of these theoretical results with a large body of experimental results shows that the agreement is well within theoretical and experimental uncertainties up to $Z = 83$, but experiments for larger Z show a very large scatter, which remains to be explained.

PACS number(s): 31.10.+z, 31.20.Di, 31.30.Jv

I. INTRODUCTION

Estimates for energies of inner-shell transitions in heavy atoms require a many-body relativistic theory of bound states in very high fields. In response to this evident complexity, recent theoretical and experimental work has focused on high-Z ions with few electrons for which complete *ab initio* calculations are more manageable. While precise experimental data are available for one, two, and three electron ions up to $Z = 54$ (and even 92 for the $2p$-$1s$ transition in heliumlike uranium [1], and for the $2p$-$2s$ transition in lithiumlike uranium [2]), with generally satisfactory concordance with theory, experimental tests involving $1s$ electrons for Z around 92, and with a precision better than 10 ppm are still years away.

By contrast rather precise experimental data on $K\alpha$ transition energies are available up to $Z = 94$, and some less precise data for Z up to 100. While theoretical progress has been made over the past few years, the problem was evidently considered sufficiently difficult that "complete" calculations would be inappropriate. In addition, several key features needed for 10 ppm estimates were missing. Very recently, however, a very complete comparison between experimental and theoretical K and L transitions in xenon has shown that such a goal is now reachable [3]. This work reports an attempt to estimate a wide range of medium- to very-heavy-atom inner-shell transition energies taking into account all the progress made in the few-electron systems in recent years. Among the progress that has been instrumental in reaching high accuracy, we can point to the ability to compute correlation energies in a relativistic framework, using many-body perturbation theory, as developed by Johnson and collaborators [4–12] and by Lindgren's group [3, 13–18]. The latter method was used in this work. For very high Z it was also very important to realize that due to the deformation of atomic nuclei, extrapolations of nuclear radii made from lighter elements (as done, for example, in Ref. [19]) are unusable. They provide systematic deviations of 0.11 fm, which lead to systematic discrepancies between theoretical and experimental energies. This problem was identified and solved in earlier stages of the present work [20]. Finally recent progress in the calculation of screening corrections to the self-energy [21, 22] have made it possible, if not yet to base directly all calculations to a sound QED calculation, at least to get reliable estimates of the error associated with the semiclassical estimates developed in earlier stages [23].

II. CALCULATION

The calculation consists of a fully relaxed Dirac-Fock (DF) calculation, described below, and corrections from correlation and other many-body effects as described in Secs. II A and II B, respectively, as well as from QED effects as described in Sec. II C. The Breit interaction is treated on the same footing as the Coulomb interaction all through the calculation. Retardation of the electromagnetic field beyond what is included in the Breit interaction was added on the Dirac-Fock level.

In previous studies [24, 25] of fermium the Dirac-Fock method was used to test the validity of the conventional QED against nonlinear QED predictions. In this work a more precise Dirac-Fock calculation has been performed, with full exchange and relaxation, using most recent values for fundamental constants [26]. A Fermi model is used for the nucleus and the grid used to tabulate electronic wave functions has at least 64 points inside the

nucleus, in order to get very precise wave functions in the region where they will contribute most to radiative corrections. This number of points was obtained by increasing the number of grid points inside the nucleus from 30 (its original value) until the vacuum polarization value obtained for the $1s$ orbital of a hydrogenic uranium ion matched closely (better than 0.1 eV) the value in Ref. [19]. In fact, we also had to improve slightly the integration scheme (close to the origin) for the vacuum polarization, to get a complete agreement.

The parameters for the Fermi distribution are calculated using spherical mean radii from Ref. [19] up to Z=70. From Z=70 to Z=83 we used nuclear sizes from a more recent compilation [27]. For Z higher than 90, one has to take into account nuclear deformation. We used more recent experimental data when available, which have been obtained from muonic x rays [28–30]. Following earlier work [10], we computed an averaged mean-square nuclear radius from the parameters deduced from muonic x rays. Whenever no experimental nuclear radius was available, we fitted the difference between mean-square radii obtained from the formula proposed in Ref. [19] and the averaged mean-square radii. This difference is roughly constant and equal to 0.11 fm. The nuclear radii used for $Z \geq 90$ are displayed in Table I. For high Z the theoretical results are very sensitive to the nuclear mean radius and above Z=90 an uncertainty of 0.1 fm leads to an uncertainty in the transition energy of several eV as discussed in Sec. III. We performed a separate calculation for each isotope for which an experiment has been done.

The magnetic interaction is included in the self-consistent-field process. While this gives a relatively small change in the Dirac-Fock energy of the atom [31], it does change the wave function at the origin to the extent that the vacuum polarization contribution is affected. Complete retardation in the Coulomb gauge has been evaluated as a first-order perturbation. The use of the Coulomb gauge, in such a nonlocal method as the Dirac-Fock one, is very important to avoid spurious contributions as has been shown theoretically [32–34] and by comparing high precision two-electron multiconfiguration Dirac-Fock (MCDF) results with experiment [35].

A. Correlation

Relativistic many-body perturbation theory is the method of choice for computing correlation energy on K and L electrons in heavy atoms. In earlier attempts by Chen *et al.* [36] the nonrelativistic correlation contribution to the K and L shell was calculated for zinc. This number was then used for all elements heavier than zinc, as a rough estimate of the Coulomb correlation energy. In a relativistic calculation the correlation contribution can be separated into two parts, one due to the pure

TABLE I. Mean-square radii and Fermi distribution t parameter (fm). Comparison between extrapolated values and values deduced from muonic atom x-ray measurements (underlined values). Nonunderlined values are deduced from extrapolated values corrected with the average of the last column.

Z	A	Extrapolated (Ref. [19])	Muonic atoms	Expt. prec.	t	Muonic minus extrapolated values
90	232	5.7070	<u>5.8045</u>	0.0043	2.2456	0.0975
91	231	5.6995	5.8114		2.2939	
92	233	5.7143	<u>5.8158</u>	0.0066		0.1015
	234	5.7216	<u>5.8289</u>	0.0031		0.1073
	235	5.7290	<u>5.8343</u>	0.0028		0.1053
	238	5.7510	<u>5.8625</u>	0.0023	2.2174	0.1115
93	237	5.7440	5.8559		2.2939	
94	239	5.7581	<u>5.8765</u>	0.0022	2.1906	0.1184
	240	5.7653	<u>5.8867</u>	0.0030	2.2214	0.1214
	242	5.7797	<u>5.8973</u>	0.0025	2.1920	0.1176
	244	5.7940	5.9059		2.2939	
95	241	5.7725	5.8928		2.2939	0.1203
	243	5.7869	5.9047		2.2939	0.1179
96	245	5.8011	5.9130		2.2939	
	247	5.8160	5.9279		2.2939	
	248	5.8224	5.9343		2.2939	
97	247	5.8160	5.9279		2.2939	
	249	5.8294	5.9413		2.2939	
	250	5.8365	5.9483		2.2939	
98	249	5.8294	5.9413		2.2939	
	250	5.8365	5.9483		2.2939	
	251	5.8435	5.9554		2.2939	
99	251	5.8435	5.9554		2.2939	
	252	5.8505	5.9624		2.2939	
100	253	5.8575	5.9693		2.2939	
	254	5.8644	5.9763		2.2939	

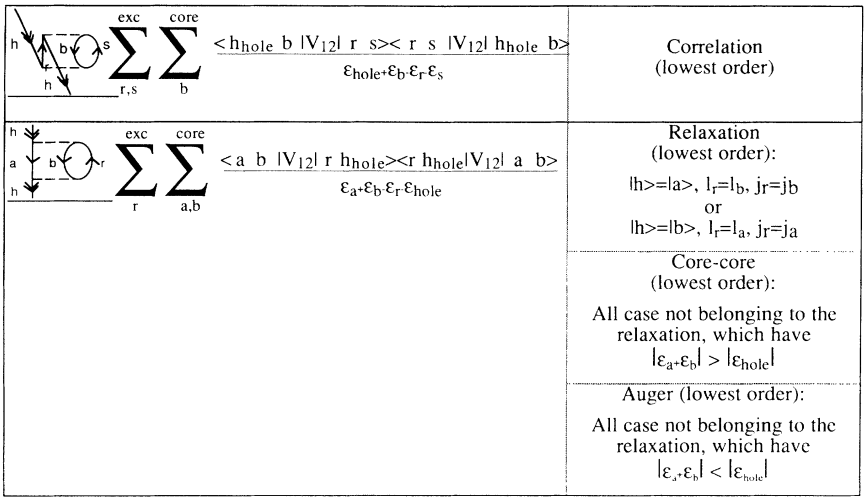

FIG. 1. Diagrams and expressions for correlation, Auger-shift, and core-core contributions.

Coulomb interaction between the electrons, and one due to the Breit part of the electron-electron interaction. The Breit interaction consists of the magnetic interaction and the first term in the expansion of the retardation of the electromagnetic field. Correlation corrections due to the magnetic interaction have been shown to equal Coulomb correlation at $Z = 54$ and to be four times larger at $Z = 92$ for the ground state of two-electron systems [37]. For hole states the Breit correlation was computed for the first time, to our knowledge, in Ref. [3] for xenon, together with the relativistic Coulomb correlation. A discretized Dirac-Fock-Breit basis set, as described in Refs. [13, 14], was used to calculate the lowest-order correlation as illustrated in Fig. 1. The sum over excited states, $|r\rangle$ and $|s\rangle$, includes angular momenta up to $l = 10$ for Coulomb correlation as well as for the Breit interaction for the K shell. For the L-shell Breit correlation, which is considerably less important, angular momenta up to $l = 6$ were included. The contributions from the highest angular momenta included can be used to estimate the uncertainty caused by the truncation of the l sum. That is, for the L shell in xenon the contributions from $l = 9$ and $l = 10$ amount to 0.01 eV and for the K shell they are even smaller. Thus it can safely be assumed that higher angular momenta will contribute with less than 0.1 eV. Higher-order correlation is also estimated to less than 0.1 eV since it scales as $1/Z$ compared to the leading correlation contribution. Here we have extended the calculations in Ref. [3] to atoms from $Z = 31$ to 100. Since the correlation calculations are very tedious and further the result changes smoothly with Z, see Figs. 2–4, only a few elements have been calculated. From the results for krypton, xenon, lead, and plutonium, which are displayed in Tables II–IV, all other elements have been obtained by extrapolation. Indeed magnetic correlation energy gives a sizable contribution at high Z.

TABLE II. Contributions to $1s$, $2p_{1/2}$, and $2p_{3/2}$ ionization energies for $Z = 82$ (eV). Each individual contribution is corrected for finite nuclear size.

Level	$1s$	$2p_{1/2}$	$2p_{3/2}$
Coulomb	88498.39	15268.33	13079.67
Magnetic	-355.02	-69.26	-46.11
Retardation (order ω^2)	26.50	7.27	7.25
Higher-order ret. ($> \omega^2$)	6.80	-0.12	3.04
Coulomb correlation	2.09	3.23	3.10
Breit correlation	2.01	0.81	0.54
Auger plus core-core	0.14	-3.39	-1.99
Hydrogenlike self-energy	-225.64	-3.88	-5.17
Self-energy screening	11.94	2.74	2.50
Nuclear polarization	0.10	0.00	0.00
Vacuum pol. (Uehling) $\alpha(Z\alpha)$	48.34	0.50	-0.23
Electronic correction to Uehling	-0.28	-0.04	-0.02
Vacuum pol. $\alpha(Z\alpha)^3$	-2.05	-0.03	0.01
Vac. pol. (Källèn & Sabry) $\alpha^2(Z\alpha)$	0.37	0.00	0.00
Total level energy	88013.69	15206.16	13042.57

TABLE III. Contributions to the $K\alpha_1$ transition energy for Z=36, 82, 92, 94, 100 (eV). Each individual contribution is corrected for finite nuclear size.

Z	36	82	92	94	100
Coulomb	12677.63	75418.73	99101.59	104456.38	121956.17
Magnetic	-21.34	-308.91	-459.97	-496.27	-619.87
Retardation (order ω^2)	1.21	19.24	28.05	30.06	36.62
Higher-order ret. ($>\omega^2$)	0.05	3.76	6.61	7.32	9.74
Coulomb correlation	-1.27	-1.01	-0.85	-0.80	-0.71
Breit correlation	0.36	1.47	1.87	1.95	2.20
Auger plus core-core	1.78	2.13	2.02	2.00	1.94
Hydrogenlike self-energy	-12.76	-220.47	-344.11	-375.42	-486.45
Self-energy screening	0.74	9.44	15.11	16.62	22.24
Nuclear polarization		0.10	1.08		
Vacuum pol. (Uehling) $\alpha(Z\alpha)$	1.28	48.57	89.56	101.10	145.28
Electronic correction to Uehling		-0.25	-0.43	-0.48	-0.67
Vacuum pol. $\alpha(Z\alpha)^3$	-0.01	-2.05	-4.39	-5.08	-7.82
Vac. pol. (Källèn & Sabry) $\alpha^2(Z\alpha)$	0.01	0.37	0.68	0.77	1.10
Total transition energy	12647.68	74971.12	98436.84	103738.16	121059.77
Experiment	12648.01	74970.01	98431.45	103734.40	121095.00
Experiment minus theory	0.33	-1.11	-5.38	-3.76	35.23
Experimental precision	0.05	0.17	0.28	0.60	15.00

B. Auger and core-core effects

Relaxation and correlation are, however, not the only many-body effects. Important remaining effects have earlier been given names as Coster-Kronig fluctuations and Auger effects. Since the situation regarding the names of the different contributions is somewhat confusing it is perhaps appropriate to define precisely the classification used here.

In second-order perturbation theory there is a class of contributions which involve two core electrons and one excited state at the intermediate level

$$\sum_{r,\mathrm{exc}} \sum_{a,b,\mathrm{core}} \frac{\langle ab|V_{12}|rh_{\mathrm{hole}}\rangle\langle rh_{\mathrm{hole}}|V_{12}|ab\rangle}{\varepsilon_a+\varepsilon_b-\varepsilon_r-\varepsilon_{\mathrm{hole}}}. \quad (1)$$

Expression (1) divides naturally into two subclasses. One is just a contribution to the relaxation. This is when either $|a\rangle$ or (or $|b\rangle$) is equal to the hole state, $|h\rangle$, and further the excited state, $|r\rangle$, has the same angular symmetry as $|b\rangle$ (or $|a\rangle$). The full relaxation can either be obtained by treating such admixtures to all orders, which was the method used in Ref. [3], or by performing a full DF calculation where all the electrons are allowed to ad-

TABLE IV. Contribution to the $K\alpha_2$ transition energy for Z=36, 82, 92, 94, 100 (eV). Each individual contribution is corrected for finite nuclear size.

Z	36	82	92	94	100
Coulomb	12623.85	73230.06	95276.28	100197.09	116112.59
Magnetic	-20.37	-285.76	-420.36	-452.27	-559.57
Retardation (order w^2)	1.21	19.23	28.09	30.13	36.82
Higher-order ret. ($>w^2$)	0.09	6.92	12.50	13.94	19.05
Coulomb correlation	-1.28	-1.14	-1.04	-1.04	-0.98
Breit correlation	0.34	1.20	1.44	1.50	1.65
Auger plus core-core	2.27	3.53	4.18	3.92	3.73
Hydrogenlike self-energy	-12.92	-221.75	-343.60	-374.13	-481.32
Self-energy screening	0.78	9.20	14.07	15.31	19.71
Nuclear polarization		0.10	1.06		
Vacuum pol. (Uehling) $\alpha(Z\alpha)$	1.28	47.84	87.50	98.57	140.61
Electronic correction to Uehling		-0.24	-0.39	-0.43	-0.59
Vacuum pol. $\alpha(Z\alpha)^3$	-0.01	-2.01	-4.26	-4.92	-7.51
Vac. pol. (Källèn & Sabry) $\alpha^2(Z\alpha)$	0.01	0.37	0.67	0.75	1.06
Total transition energy	12595.25	72807.53	94656.13	99528.43	115285.26
Experiment	12595.44	72805.33	94650.72	99524.63	115319.00
Experiment minus theory	0.19	-2.21	-5.41	-3.80	33.74
Experimental precision	0.06	0.24	0.56	1.00	15.00

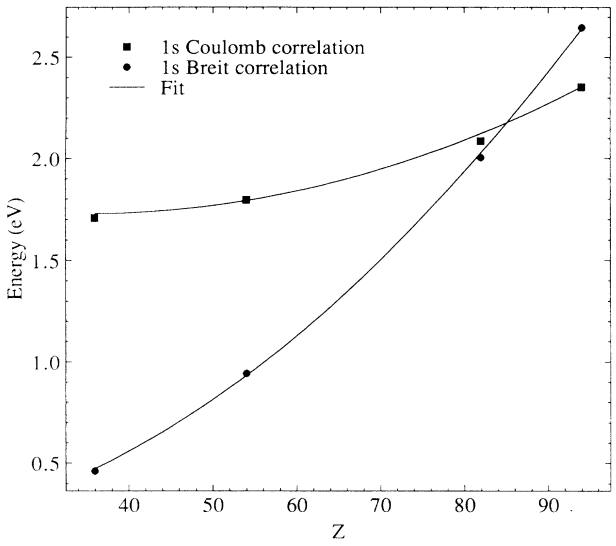

FIG. 2. $1s$ Breit and Coulomb correlation energies (eV).

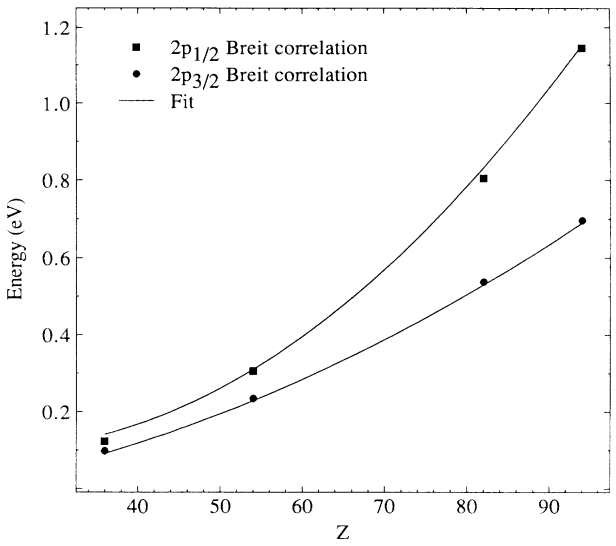

FIG. 4. $2p_{1/2}$ and $2p_{3/2}$ Breit correlation energy (eV).

just to the presence of the hole. As discussed in the beginning of Sec. II the latter method is used in this work.

It is the remaining contributions to (1) which are subject to a rather confusing labeling. The effects when both $|a\rangle$ and $|b\rangle$ are less tightly bound than the hole state $|h\rangle$, i.e., $|\varepsilon_a| < |\varepsilon_h|$ and $|\varepsilon_b| < |\varepsilon_h|$ are often treated separately. In the case when the principal quantum number for $|h\rangle$ is the same as for $|a\rangle$ or $|b\rangle$ the effect is sometimes classified as Coster-Kronig fluctuations in correspondence with the experimentally observed Coster-Kronig transitions. However, since only virtual transitions are considered even energetically forbidden fluctuations, i.e., $|\varepsilon_a + \varepsilon_b| < |\varepsilon_h|$, may sometimes be included in the Coster-Kronig results. Super Coster-Kronig fluctuations refer to the case when all three principal quantum numbers are the same. Although the Coster-Kronig fluctuations constitute an important subclass of effects there

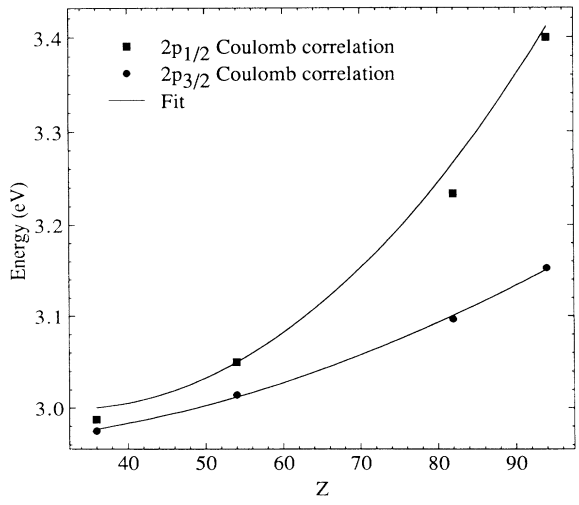

FIG. 3. $2p_{1/2}$ and $2p_{3/2}$ Coulomb correlation energy (eV).

are other important contributions to (1) and we have chosen a somewhat different classification scheme.

As in the earlier work on xenon [3] the contributions where $|\varepsilon_a + \varepsilon_b| < |\varepsilon_h|$ will be called Auger effects and when $|\varepsilon_a + \varepsilon_b| > |\varepsilon_h|$ we refer to core-core contributions in correspondence with the usual nomenclature for calculations on valence states. This separation is natural since for the Auger effects the intermediate state is autoionizing, which is not the case for the core-core effects. Thus the treatment of the latter involves no special problems while the calculation of the former requires an integration over a pole in the energy spectrum. The pole is treated by a method suggested in Ref. [38]. The matrix elements, obtained numerically, are fitted to a polynomial which make possible an analytical calculation of the integral. It should be noted that all contributions in (1) are included in the present calculation.

Coster-Kronig fluctuations were identified to give sizable contributions for $2s$ holes as early as 1981 in the pioneering work of Chen and co-workers [36, 39]. Although the core-core and Auger shifts are larger for $2s$ or $3p$ electrons, they are not negligible for $1s$ and, especially not, for $2p$ electrons as shown in Tables II–IV. For the latter hole states, however, one must be careful to include simultaneously the shifts not covered by the Coster-Kronig definition which are often of the same order of magnitude or, as for the case of a $1s$ or $2p_{3/2}$ hole, give the whole contribution [3]. The inclusion of both the core-core and Auger contribution is also very important to get values which are smooth functions of Z. As some of the above calculation are rather time-consuming, we have performed them on a limited number of elements. Although the individual contributions sometimes vary enough to make an extrapolation somewhat uncertain, the sum of the core-core and Auger shifts is well behaved (Fig. 5) and possible to extrapolate, except for the L_2 shell (Fig. 6) around $Z = 92$. The problem for the $2p_{1/2}$ level is due to the fact that for the impor-

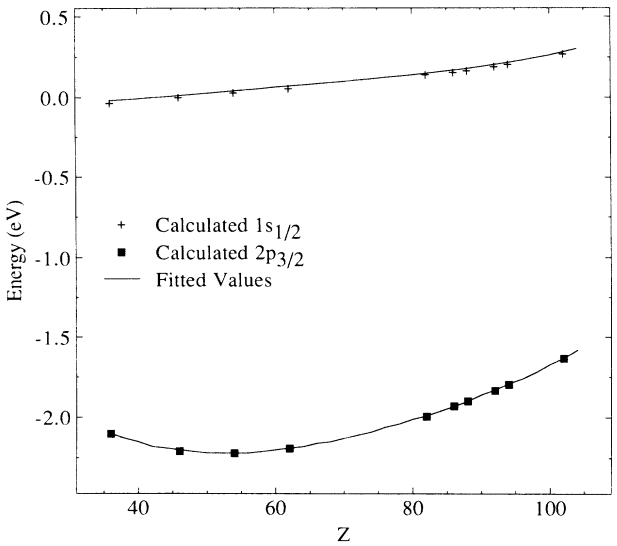

FIG. 5. $1s$ and $2p_{3/2}$ core-core and Auger contribution (eV).

tant admixture of a double vacancy with holes in $2p_{3/2}$ and $3d_{3/2}$ the constant part of the energy denominator $(\varepsilon_{3d_{3/2}} + \varepsilon_{2p_{3/2}} - \varepsilon_{2p_{1/2}})$ passes through zero somewhere around $Z = 92$. The subsequent switch from a core-core type of effect to an Auger contribution leads to a discontinuity in the contribution as a function of Z as shown in Fig. 6. We thus made separate fits for the low-Z and the high-Z part for the L_2 shell. In order to simplify further this part of the calculation we did not recouple the angular momenta of the outer shell with the one of the inner hole.

In Ref. [3] the core-core contributions were iterated to all orders. That improved the agreement with experiment with one order of magnitude for transitions involving a $2s$ hole which have a very large shift due to this effect. For the $K\alpha$ transitions the situation is less dramatic and higher-order core-core effects contribute with at most a few tenths of an electron volt. As mentioned above the extrapolation of the core-core and Auger effects requires the sum of the contributions, at least for the $2p_{1/2}$ hole. Since the iteration of Auger effects is not within reach at present and since the accuracy of the present calculation is around 1 eV up to $Z = 82$, and less for higher Z, the higher-order core-core effects are not included in the results.

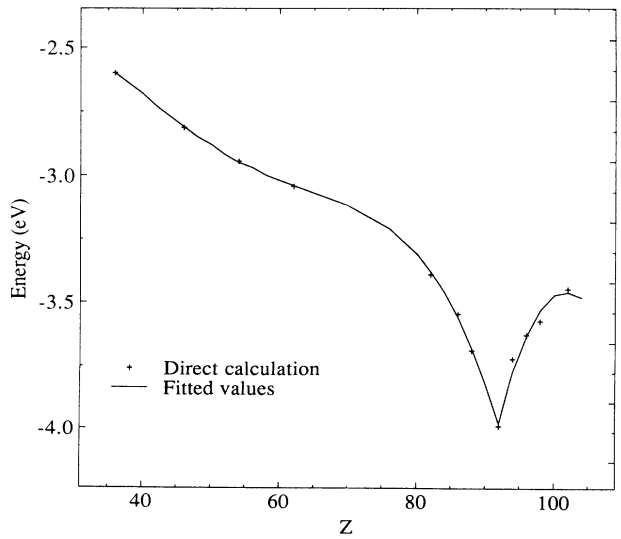

FIG. 6. $2p_{1/2}$ core-core and Auger contribution (eV).

C. QED effects

The next main difficulty in the present calculation lies in the evaluation of radiative corrections. For the vacuum polarization contributions, potential of order $\alpha(Z\alpha)$—the Uehling potential—of order $\alpha(Z\alpha)^3$, and of order $\alpha^2(Z\alpha)$—the Källèn and Sabry potential—have been used in first-order perturbation with Dirac-Fock wave functions, accounting for both the finite nuclear size and screening corrections. Numerical results obtained through this procedure have been checked against one-electron results of Ref. [19] for the two first contributions and against Ref. [40] for the latter and found to be accurate to better than 0.1 eV.

The Uehling potential can be corrected further for many-electron effects. The expression of this potential involves the charge density. In all earlier calculations of inner-shell energies, this charge density was taken as the proton density. Here we also computed a correction where the nuclear charge density is replaced by the electrons' charge density. This correction is very small except for very high Z and is very time-consuming. It has been evaluated for all elements with atomic number larger than 82.

For $1s$, $2s$, $2p_{1/2}$, and $2p_{3/2}$ shells we used one-electron self-energies from Refs. [41,42]. For ns, $np_{1/2}$, $np_{3/2}$, and $nd_{3/2}$ shells, $5 \geq n \geq 3$, we used a recent evaluation by Mohr and Kim [43]. For shells with $n \geq 5$, an n^3 scaling has been used to get self-energy corrections. It has been shown [43] that for $n > 3$, such a scaling reproduces very accurately direct evaluation. Precise accounting for the finite nuclear size in the evaluation of all radiative corrections is really essential in the heavy-atom region. We have corrected ns and $np_{1/2}$ self-energy for the finite nuclear size as in Ref. [19].

To account for the so-called screening correction to the self-energy, for which there is no effective potential valid to all orders in $Z\alpha$, an approximate method based on semiclassical arguments has been used. This method provides an effective potential to correct the lowest order in $Z\alpha$ of the self-energy for changes in the electronic density at the nucleus. Very recently a similar potential has been formally derived from QED [44]. This method has been extensively checked against experiment at low and medium Z in two- [45, 46] and three-electron ions [47]. For two-electron ions this method produces results in good agreement with those obtained [48,49] by the use of the Kabir and Salpeter equation and $1/Z$ expansion to correct for changes in the electronic density at the nucleus and to evaluate two-electron Bethe logarithms. In a recent calculation [51] in a three-electron system

the agreement was found to be of the order of 1.5% of the value. This method also yields results in reasonable agreement with direct evaluation of the screened K-shell self-energy by Desiderio and Johnson using a relativistic Hartree-Fock wave function [50], although a precise comparison is difficult, because of strong numerical noise in their values. In other calculations done for very heavy elements (a complete set of references on previous calculation of K and L transitions can be found in [52]) the self-energy screening correction was evaluated using an effective Z method which lacks rigorous justification and has been found to overestimate the screening corrections. Recently direct calculations of the screening correction on heavy ions have been reported [21, 22]. For the ground state of lithiumlike uranium we find in Ref. [21] a self-energy screening value of -11.41 eV while the method used here gives -10.76 eV [47]. This represents only a 6% change. We have used, to be very conservative, 20% of the self- energy screening as an error estimate. In Table II we give the contribution to ionization energies for lead. Values for the different contributions described above are listed in Tables III and IV for some elements.

III. COMPARISON WITH EXPERIMENTS

Differences between all available experimental results for $K\alpha_1$ and $K\alpha_2$ transition energies and this calculation are shown in Figs. 7 and 8, respectively, with experimental error bars and theoretical uncertainties. The theoretical uncertainty is a combination of the uncertainty of one-electron calculations with extended nucleus (mainly due to an uncertainty in the nuclear radius) and of a fraction of the self-energy screening correction as discussed in Sec. II C. For the lighter elements the latter uncertainty dominates and the estimated error scales as Z^3. For the heavier elements the error scales roughly as $Z^{14/3}$ because of its nuclear origin. Since some nuclear sizes are much better known than others, this uncertainty does not vary smoothly with Z, leading to the small spikes in Figs. 7 and 8. In the near future, when the uncertainty on the self-energy screening will have been reduced, it should be possible to use "electronic" rather than muonic x rays to measure nuclear charge radii.

Theoretical energies and the differences with individual experimental values for all the (Z, A) pairs available are displayed in Table V for $K\alpha_1$ and Table VI for $K\alpha_2$. A simple inspection of Figs. 7 and 8, and of Tables V and VI, shows that the agreement is compatible with combined theoretical and experimental uncertainties for $Z < 90$. For many of the highest Z, however, the discrepancy between experiment and theory can reach 35 or 40 eV, while experimental and theoretical error bars are 15 and 5 eV, respectively. Obviously it should also be

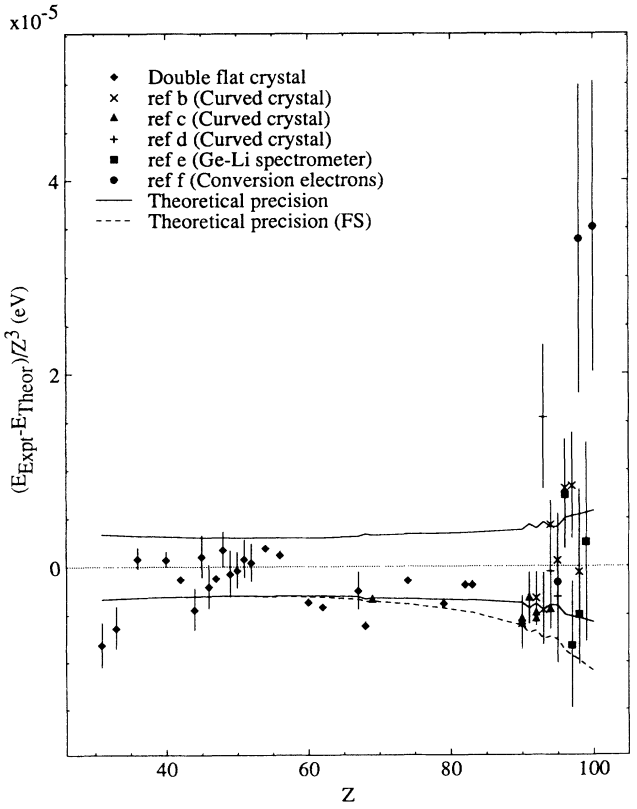

FIG. 7. Experimental-theoretical energy differences for $K\alpha_1$. The dashed curve represents a more realistic theoretical lower bound, due to a likely overevaluation of the effect of the finite nuclear size on the self-energy (see text at the end of the conclusion).

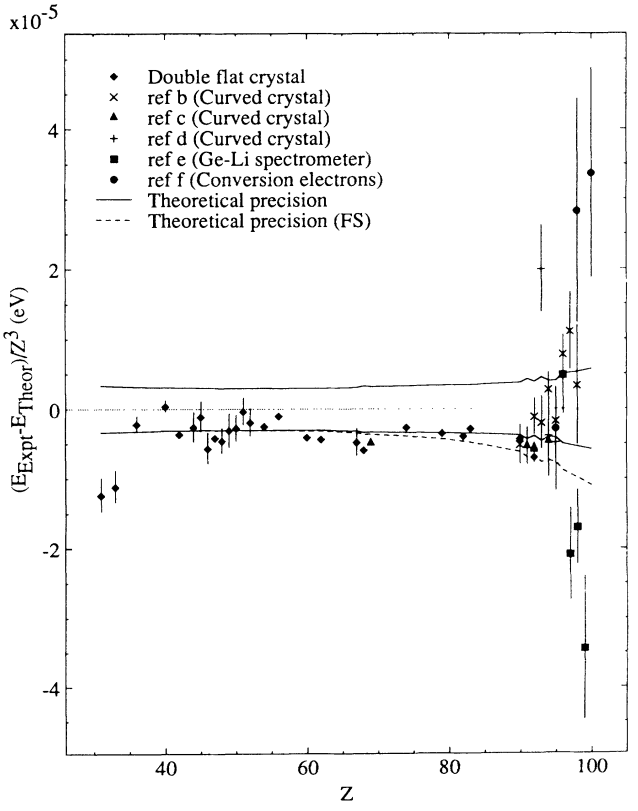

FIG. 8. Experimental-theoretical energies differences for $K\alpha_2$. The dashed curve represents a more realistic theoretical lower bound, due to a likely overevaluation of the effect of the finite nuclear size on the self-energy (see text at the end of the conclusion).

noted that some experiments for the same isotope disagree ($Z = 93$—for both lines—and $Z = 98$ for the $K\alpha_1$ line), and also that experiments for close isotopes are in disagreement (the $A = 250$ and 251 isotopes of $Z = 98$). It is possible, although unlikely, that strong local variation of the nuclear radius of those highly deformed nuclei, or strong increase in the nuclear polarization effects due to the existence of low-lying nuclear levels, could explain the discrepancy between adjacent isotopes or between experiment and theory. However, that would not explain the situation for einsteinium ($Z = 99$), where the $K\alpha_1$ shows very good agreement, while the $K\alpha_2$ disagrees by several standard deviations.

It should also be noted that variation of the transition energy is of the order of 50 eV/fm at $Z = 92$ and 100 eV/fm at $Z = 100$. If real, the discrepancy of 35 eV on fermium would amount to a change of 0.35 fm in the mean-square radius of the nucleus. This is very unlikely. Calculations of the nuclear size and deformation parameter in fermium have been done by Guet [53] and give values in close agreement with the one we used here.

The status and role of nuclear polarization in the comparison between theory and experiment at high Z is not clear either. From the work of Plunien *et al.* [54] we learn that in ^{238}U the nuclear polarization contributes +1 eV to the transition energy. This actually increases

TABLE V. Theoretical energies and comparison with experimental values for $K\alpha_1$ (eV). $\Delta E = E_{\text{expt}} - E_{\text{theor}}$, "Expt. unc." is the experimental uncertainty and "Theor. unc." the theoretical one. References: a, Ref. [56], absolute double flat-crystal measurements; b, Ref. [57]; c, Ref. [58]; d, Ref. [59], curved-crystal measurement using standard lines (all experimental values have been corrected for new fundamental constants and new standard line); e, Ref. [60], Ge-Li spectroscopy; f, Refs. [24, 61–64], conversion electron spectroscopy; g, Ref. [65] measurements relative to silver $K\alpha$ updated to its most recent value; h, T. Mooney (private communication), absolute double flat-crystal measurement.

Z	A	$K\alpha_1$ (Theor.)	$K\alpha_1$ (Expt.)	ΔE	Expt. unc.	Theor. unc.	Ref.
31		9251.92	9251.68	-0.24	0.07	0.1	h
33		10543.50	10543.27	-0.23	0.08	0.1	h
36		12647.68	12648.01	0.33	0.05	0.1	h
40		15774.87	15774.92	0.05	0.05	0.2	h
42		17479.44	17479.35	-0.09	0.01	0.2	g
44		19279.51	19279.14	-0.37	0.18	0.3	g
45		20216.00	20216.10	0.10	0.20	0.3	g
46		21177.25	21177.06	-0.20	0.22	0.3	g
47		22163.01	22162.89	-0.12	0.03	0.3	a
48		23173.75	23173.95	0.20	0.19	0.3	g
49		24209.80	24209.72	-0.08	0.28	0.4	g
50		25271.37	25271.33	-0.04	0.23	0.4	g
51		26358.72	26358.83	0.11	0.25	0.4	g
52		27472.12	27472.18	0.06	0.27	0.4	g
54		29778.43	29778.74	0.31	0.05	0.5	a
56		32193.00	32193.22	0.22	0.07	0.5	a
60		37361.47	37360.69	-0.78	0.07	0.6	a
62		40119.41	40118.43	-0.98	0.06	0.7	a
67		47547.78	47547.03	-0.74	0.58	0.9	a
68		49129.10	49127.18	-1.91	0.12	1.1	a
69	169	50742.55	50741.42	-1.13	0.09	1.1	c
74	Nat	59319.34	59318.77	-0.57	0.05	1.4	a
79	197	68806.28	68804.41	-1.87	0.22	1.7	a
82	Nat	74971.12	74970.01	-1.11	0.17	1.9	a
83	209	77109.90	77108.82	-1.07	0.20	2.0	a
90	232	93351.56	93347.26	-4.30	0.2	2.7	a
			93347.28	-4.28	2	2.7	b
			93347.58	-3.98	0.6	2.7	c
91	231	95868.75	95866.26	-2.49	2	3.3	c
92	233	98437.92	98433.66	-4.26	0.5	3.0	c
	238	98436.84	98432.96	-3.88	0.5	3.0	c
			98431.45	-5.38	0.3	3.0	a
			98434.24	-2.59	2	3.0	b
93	237	101059.80	101056.22	-3.58	3	3.7	b
			101072.28	12.48	6	3.7	d
94	239	103738.16	103734.40	-3.76	0.6	3.3	c
			103737.77	-0.39	5	3.3	d
	244	103736.59	103740.20	3.61	2	3.3	b

TABLE V. *(Continued).*

Z	A	$K\alpha_1$ (Theor.)	$K\alpha_1$ (Expt.)	ΔE	Expt. unc.	Theor. unc.	Ref.
95	241	106473.37	106470.72	-2.65	6	3.5	d
			106472.00	-1.37	6	3.5	f
	243	106472.65	106473.18	0.53	3	3.5	b
96	245	109266.37	109273.00	6.63	5	4.4	e
	248	109264.94	109272.16	7.22	2	4.4	b
97	249	112119.49	112127.14	7.65	5	4.7	b
	250	112118.97	112111.48	-7.49	6	4.7	e
98	250	115035.63	115035.11	-0.52	8	5.0	b
			115031.00	-4.63	5	5.0	e
	251	115035.06	115067.00	31.94	15	5.0	f
99	251	118015.53	118018.00	2.47	10	5.4	e
100	254	121059.77	121095.00	35.23	15	5.8	f

TABLE VI. Theoretical energies and comparison with experimental values for $K\alpha_2$ (eV). $\Delta E = E_{\text{expt}} - E_{\text{theor}}$, "Expt. unc." is the experimental uncertainty and "Theor. unc." the theoretical one. References: a, Ref. [56], absolute double flat-crystal measurements; b, Ref. [57]; c, Ref. [58]; d, Ref. [59], curved crystal measurement using standard lines (all experimental values have been corrected for new fundamental constants and new standard line); e, Ref. [60], Ge-Li spectroscopy; f, Refs. [24, 61–64], conversion electron spectroscopy; g, Ref. [65] measurements relative to silver $K\alpha$ updated to its most recent value; h, T. Mooney (private communication), absolute double flat crystal measurement.

Z	A	$K\alpha_2$ (Theor.)	$K\alpha_2$ (Expt.)	ΔE	Expt. unc.	Theor. unc.	Ref.
31		9225.21	9224.84	-0.37	0.07	0.1	h
33		10507.90	10507.50	-0.40	0.08	0.1	h
36		12595.25	12595.44	0.19	0.05	0.1	h
40		15690.62	15690.65	0.03	0.05	0.2	h
42		17374.53	17374.27	-0.26	0.01	0.2	g
44		19150.68	19150.46	-0.21	0.18	0.3	g
45		20073.74	20073.65	-0.10	0.20	0.3	g
46		21020.66	21020.12	-0.54	0.22	0.3	g
47		21990.70	21990.27	-0.43	0.03	0.3	a
48		22984.52	22984.02	-0.50	0.19	0.3	g
49		24002.35	24002.00	-0.36	0.28	0.4	g
50		25044.35	25044.01	-0.34	0.23	0.4	g
51		26110.78	26110.75	-0.04	0.25	0.4	g
52		27201.79	27201.53	-0.26	0.27	0.4	g
54		29458.59	29458.21	-0.38	0.05	0.5	a
56		31816.73	31816.57	-0.16	0.07	0.5	a
60		36848.32	36847.46	-0.87	0.07	0.6	a
62		39524.34	39523.34	-1.00	0.06	0.7	a
67		46701.33	46699.92	-1.41	0.58	0.9	a
68		48223.35	48221.55	-1.81	0.12	1.1	a
69	169	49774.18	49772.61	-1.58	0.09	1.1	c
74		57982.39	57981.35	-1.05	0.05	1.4	a
79	197	66992.31	66990.64	-1.67	0.22	1.7	a
82		72807.53	72805.33	-2.21	0.17	1.9	a
83	209	74817.72	74816.12	-1.60	0.20	2.0	a
90	232	89960.00	89956.93	-3.07	0.2	2.7	a
			89956.31	-3.69	2	2.7	b
			89956.81	-3.19	0.7	2.7	c
91	231	92287.27	92283.29	-3.98	2	3.3	c
92	233	94657.21	94652.69	-4.51	0.5	3.0	c
	238	94656.13	94651.79	-4.34	0.5	3.0	c
			94650.72	-5.41	0.6	3.0	a
			94655.27	-0.86	2	3.0	b
93	237	97069.80	97068.25	-1.54	3	3.7	b
			97085.89	16.10	5	3.7	d

TABLE VI. *(Continued).*

Z	A	$K\alpha_2$ (Theor.)	$K\alpha_2$ (Expt.)	ΔE	Expt. unc.	Theor. unc.	Ref.
94	239	99528.43	99524.63	-3.80	1	3.3	c
			99525.33	-3.11	5	3.3	d
	244	99526.89	99529.23	2.34	2	3.3	b
95	241	102033.31	102029.29	-4.02	6	3.5	d
			102031.00	-2.31	5	3.5	f
	243	102032.60	102031.21	-1.38	3	3.5	b
96	245	104584.60	104589.00	4.40	5	4.4	e
	248	104583.20	104590.19	7.00	2	4.4	b
97	249	107183.96	107194.17	10.21	5	4.7	b
	250	107183.46	107164.49	-18.97	6	4.7	e
98	250	109833.89	109837.15	3.26	8	5.0	b
			109818.00	-15.89	5	5.0	e
	251	109833.33	109860.00	26.67	15	5.0	f
99	251	112534.30	112501.00	-33.30	10	5.4	e
100	254	115285.26	115319.00	33.74	15	5.8	f

the difference between experiment and theory. The nuclear polarization can be invoked only in cases where this difference is positive. In a more recent paper more precise values for the nuclear polarization have been calculated for lead and uranium [55]. We have included those values in all our tables. Finally we give some calculated values for elements for which we have not found any precise experiments, mostly in the rare-earth region (Table VII).

IV. CONCLUSIONS

In conclusion, the use of the latest developments in MCDF calculations and relativistic many-body perturbation theory have enabled us to compute $K\alpha$ transition energies in medium- and high-Z atoms to high accuracy. It has enabled us to show that some experimental data are inconsistent, while the most reliable ones are in rather good agreement with theory. The good quality of the prediction in the low-Z region shows that our evaluation of the correlation contributions and of the Auger and core-core shifts is adequate. The good agreement in the thorium-plutonium area is a proof that most QED and relativistic corrections are well accounted for. However, the high scatter of some experimental data in the fermium region precludes further conclusions from this study. In order to understand QED in high electric fields, it is then very important that precise and reliable measurements of the $K\alpha$ transitions for $Z \geq 90$ can be repeated in the near future. A more detailed study of the role of the nuclear polarization as well as more measurements of the nuclear radii are also needed.

TABLE VII. Predictions of $K\alpha$ transition energies for some elements for which no high precision measurements have been done (eV). NC stands for not calculated.

Z	$K\alpha_1$	$K\alpha_2$
53	NC	28317.76
61	38725.68	38172.79
63	41543.38	40903.61
64	42997.66	42310.52
65	44482.96	43745.67
66	45999.74	45209.40
70	52389.50	51355.01

Note added. Upon completion of this work we learned [66] that the values we used for the finite nuclear size correction to the self -energy from Ref. [19] are probably too large by $\approx 30\%$. These correction terms have been computed independently by two groups following the method of Refs. [22] and [67]. The new correction values can lead to a reduction of theoretical transition energies by ≈ 0.6 eV in lead, ≈ 1.7 eV in uranium, and ≈ 5.3 eV in fermium. This should improve the agreement between theory and the very precise experimental values at $Z = 90$, 92, and 94, and for several other elements in the transuranic region. Since these new calculations have been performed only for one or two elements and are not yet available, we have not corrected the present values. This problem should not affect elements $Z \leq 70$ for which this correction is negligible.

ACKNOWLEDGMENTS

This work was carried out partly using the computational facility at the National Institutes for Standards and Technology. One of us (P. I.) is very indebted to Dr. R. D. Deslattes, Dr. J. P. Desclaux, Dr. E. Kessler, Dr. P. J. Mohr, Dr. G. Soff, Dr. Y.-K. Kim, and Professor W. R. Johnson for many useful discussions, suggestions, and comments which have been of great help for the completion of this work. P. I. also wishes to thank the Direction du secteur Mathématiques et Physique de Base du CNRS for having provided computer time at the CIRCE and a RS/6000 workstation, and Dr. R. D. Deslattes (Quantum Metrology Division, NIST) for his kind hospitality during most of this work. E. L. is grateful to Dr. A.-M. Mårtensson-Pendrill for enlightening discussions and for support for this work given by the Swedish Natural Science Research Council (NFR). We also thank Dr. S. A. Blundell for providing us unpublished results for finite-size correction to the self-energy. Laboratoire de Physique Atomique et Nucléaire is "Unité de Recherche Associée au CNRS No. 771."

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