PHYSICAL REVIEW A VOLUME 51, NUMBER 1 JANUARY 1995

Theory of $2s_{1/2}$-$2p_{3/2}$ transitions in highly ionized uranium

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(Received 7 July 1994)

Structure and QED effects for $2s_{1/2}$-$2p_{3/2}$ transitions in lithiumlike, berylliumlike, carbonlike, fluorinelike, and neonlike uranium are calculated and compared with recent measurements. With the exception of berylliumlike uranium, which has poor convergence properties, relatively good agreement with experiment is found.

PACS number(s): 31.15.Ar, 31.25.−v, 31.30.Jv

I. INTRODUCTION

Recently, high-precision measurements of the $2s_{1/2}$-$2p_{3/2}$ energy differences in lithiumlike U^{89+} through neonlike U^{82+} were made at an electron-beam ion trap (SuperEBIT) at Lawrence Livermore National Laboratory [1]. These measurements were compared with multiconfiguration Dirac-Fock (MCDF) calculations and discrepancies ranging from 2 eV to 8 eV were found. For the case of lithiumlike uranium, much better agreement was found with theoretical values obtained by combining many-body perturbation theory (MBPT) calculations of the atomic structure [2] with *ab initio* quantum electrodynamic (QED) corrections [3]. Since MBPT is not as flexible as MCDF calculations, it has not been applied to the other ions studied in Ref. [1]. The purpose of this paper is to extend the MBPT calculations from lithiumlike ions to berylliumlike, carbonlike, fluorinelike, and neonlike ions. With the exception of berylliumlike uranium, for which MBPT converges poorly, much better agreement with experiment is obtained. For berylliumlike uranium, an alternative approach such as relativistic configuration interaction (CI) [4] is needed to solve the many-body problem accurately.

The plan of this paper is as follows. In Sec. II we present the MBPT formulas for energy levels of alkali-metal-like, halogenlike, and particle-hole excitations of closed-shell ions, along with the definition of the model potentials used to start our calculations. In Sec. III we discuss our treatment of QED corrections. Finally, in Sec. IV, the results of our calculations are presented and compared with experiment and with other calculations.

II. FORMALISM

One disadvantage of MBPT as compared with MCDF calculations is that each distinct electronic configuration must be treated separately. In the present work, we consider three cases: one electron outside a closed shell (lithiumlike), one hole in a closed shell (fluorinelike), and a particle-hole excitation of a closed shell (berylliumlike, carbonlike, and neonlike). We discuss the MBPT formulas for each of these three cases in turn. It should be noted that certain states of boronlike and nitrogenlike ions could also be treated as one-electron states but, in the experiments we are considering, a second core electron is also excited.

A. One-particle MBPT

While MBPT has been applied previously to alkali-metal-like systems [5] starting from a Hartree-Fock potential, in the present calculation we start from a local model potential $U(r)$. Therefore, we briefly reprise MBPT for this case. A lowest-order valence state vector $|0_v\rangle$ is given by

$$|0_v\rangle = a_v^\dagger |0_c\rangle, \qquad (2.1)$$

where $|0_c\rangle$ is the state vector for the filled core. Here, $v \equiv (n_v, \kappa_v, m_v)$ designates the quantum numbers of the valence state. The lowest-order energy for the valence electron is

$$E^{(0)} = \epsilon_v. \qquad (2.2)$$

In the present discussion, we suppress the energy of the core since it cancels in the $2s_{1/2}$-$2p_{3/2}$ energy difference. The quantity ϵ_v in Eq. (2.2) is the valence eigenvalue of the Dirac equation

$$h(\mathbf{r})\, \varphi_i(\mathbf{r}) = \epsilon_i\, \varphi_i(\mathbf{r})\,, \qquad (2.3)$$

where the Dirac Hamiltonian $h(\mathbf{r})$ includes the interaction of the electron with both the nuclear potential $V_{\rm nuc}(r)$ and the model potential $U(r)$,

$$h(\mathbf{r}) = c\,\boldsymbol{\alpha}\cdot\mathbf{p} + (\beta-1)c^2 + V_{\rm nuc}(r) + U(r). \qquad (2.4)$$

The first-order correction to the valence energy is [6]

$$E^{(1)} = \Delta_{vv}, \qquad (2.5)$$

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where Δ_{ij} represents the frequently occurring combination

$$\Delta_{ij} = (V_{\mathrm{HF}} - U)_{ij} = \langle \varphi_i | V_{\mathrm{HF}} - U | \varphi_j \rangle . \tag{2.6}$$

Here, V_{HF} is the Hartree-Fock potential, which is defined by its matrix elements:

$$(V_{\mathrm{HF}})_{ij} \overset{\mathrm{def}}{=} \sum_a \left[g_{iaja} - g_{iaaj} \right] , \tag{2.7}$$

where the sum extends over occupied core orbitals a. The quantity g_{ijkl} in Eq. (2.7) is a Coulomb matrix element:

$$g_{ijkl} = \int \frac{d^3r_1 d^3r_2}{|\mathbf{r}_1 - \mathbf{r}_2|} \varphi_i^\dagger(\mathbf{r}_1)\varphi_k(\mathbf{r}_1)\varphi_j^\dagger(\mathbf{r}_2)\varphi_l(\mathbf{r}_2). \tag{2.8}$$

Its antisymmetrized form is denoted by

$$\tilde{g}_{ijkl} = g_{ijkl} - g_{ijlk}. \tag{2.9}$$

The second-order energy $E^{(2)}$ is given by [6]

$$E^{(2)} = \sum_{amn} \frac{g_{vamn}\tilde{g}_{mnav}}{\epsilon_m + \epsilon_n - \epsilon_a - \epsilon_v} + \sum_{abm} \frac{g_{abmv}\tilde{g}_{mvab}}{\epsilon_m + \epsilon_v - \epsilon_a - \epsilon_b} - \left[\sum_{am} \frac{\Delta_{am}\tilde{g}_{mvav}}{\epsilon_m - \epsilon_a} + \text{c.c.} \right] - \sum_{i \neq v} \frac{\Delta_{vi}\Delta_{iv}}{\epsilon_i - \epsilon_v}. \tag{2.10}$$

The indices a and b in the above sums refer to core orbitals, the indices n and m refer to virtual orbitals, and the index i refers to both core and virtual orbitals. The sums over virtual states n and m include excited bound states and continuum states. Virtual positron states are not included in the sums. In Eq. (2.10), the symbol c.c. denotes the complex conjugate of the preceding expression in the square bracket.

It is possible, when working with a local potential, to account for the first-order Coulomb correction $E^{(1)}$, the instantaneous Breit interaction $B^{(1)}$, and the frequency dependent corrections to the Breit interaction $\Delta B^{(1)}(k)$ by working in Feynman gauge [7]. This is done by replacing the Coulomb matrix element in Eq. (2.8) with

$$g_{ijkl}(k) = \mathrm{Re} \left\{ \int \frac{d^3r_1 d^3r_2}{|\mathbf{r}_1 - \mathbf{r}_2|} \varphi_i^\dagger(\mathbf{r}_1)\alpha_\mu \varphi_k(\mathbf{r}_1)\varphi_j^\dagger(\mathbf{r}_2)\alpha^\mu \varphi_l(\mathbf{r}_2) e^{ik|\mathbf{r}_1 - \mathbf{r}_2|} \right\} , \tag{2.11}$$

where

$$k = \frac{|\epsilon_i - \epsilon_k|}{\hbar c} = \frac{|\epsilon_j - \epsilon_l|}{\hbar c}. \tag{2.12}$$

The three corrections, taken together, are denoted by $F^{(1)}$:

$$F^{(1)} \overset{\mathrm{def}}{=} E^{(1)} + B^{(1)} + \Delta B^{(1)}(k) = \sum_a \tilde{g}_{vava}(k) - U_{vv}. \tag{2.13}$$

The final correction considered in the present MBPT calculation is the correlation correction to the Breit interaction $B^{(2)}$. This correction is obtained by replacing

$$g_{ijkl} \to g_{ijkl} + b_{ijkl}$$

in $E^{(2)}$, where b_{ijkl} is the matrix element of the instantaneous Breit interaction, and linearizing the resulting expression in b_{ijkl} [5].

B. One-hole MBPT

The formalism for one-hole systems is almost identical to the one-particle case. In the one-hole case, the lowest-order state vector for a state with quantum numbers $a' = (n_a, \kappa_a, -m_a)$ is given by

$$|0_{a'}\rangle = (-1)^{j_a - m_a} a_a |0_c\rangle , \tag{2.14}$$

with $a = (n_a, \kappa_a, m_a)$. The factor $(-1)^{j_a - m_a}$ is needed to make a_a into a proper tensor operator. The only difference between the formulas in this case and those for the one-particle case is that $v \to a$ and each of the previous formulas enters with the opposite sign. We use the one-hole formalism to calculate the structure of fluorinelike uranium.

C. Particle-hole MBPT

The remaining states considered can all be described as particle-hole excitations of a closed-shell ion in which a core electron a is raised to an excited state v, coupled (in the jj scheme) to give an eigenstate of total angular momentum $|JM\rangle_{av} \equiv |j_a j_v, JM\rangle$:

$$\begin{aligned} |JM\rangle_{av} &= \sum_{m_a m_v} (-1)^{j_a - m_a} \langle j_a {-m_a} j_v m_v | JM \rangle a_a a_v^\dagger |0_c\rangle \\ &\equiv F_{av} a_a a_v^\dagger |\, 0_c\rangle . \end{aligned} \tag{2.15}$$

The phase and the minus sign in front of m_a in the 3-j symbol are required because a is a hole state. In Ref. [8], MBPT for particle-hole states has been treated through third order for the case in which the starting potential is a Hartree-Fock potential. In the present case, where $U(r)$ is an arbitrary local potential, the lowest-order energy is given by

$$E^{(0)} = \epsilon_v - \epsilon_a , \tag{2.16}$$

and the first-order energy is given by

$$E^{(1)} = \Delta_{vv} - \Delta_{aa} + F_{av}F_{bw}\tilde{g}_{awvb}. \tag{2.17}$$

The operator F_{bw} differs from F_{av} only in that the sum over $m_a m_v$ is replaced by a sum over $m_b m_w$. The expression for the second-order energy is relatively lengthy, so we break it into parts:

$$E_A^{(2)} = F_{av}F_{bw}\delta_{ab}\sum_{mcd}\frac{g_{cdvm}\tilde{g}_{wmcd}}{\epsilon_m+\epsilon_v-\epsilon_c-\epsilon_d}, \tag{2.18}$$

$$E_B^{(2)} = F_{av}F_{bw}\sum_{mn}\frac{g_{awmn}\tilde{g}_{mnbv}}{\epsilon_m+\epsilon_n-\epsilon_a-\epsilon_v}, \tag{2.19}$$

$$E_C^{(2)} = -F_{av}F_{bw}\delta_{ab}\sum_{mnc}\frac{g_{wcmn}\tilde{g}_{mnvc}}{\epsilon_m+\epsilon_n-\epsilon_v-\epsilon_c}, \tag{2.20}$$

$$E_D^{(2)} = -F_{av}F_{bw}\sum_{mc}\frac{\tilde{g}_{macv}\tilde{g}_{wcbm}}{\epsilon_a+\epsilon_m-\epsilon_c-\epsilon_v}, \tag{2.21}$$

$$E_E^{(2)} = F_{av}F_{bw}\sum_{cd}\frac{g_{cdvb}\tilde{g}_{wacd}}{\epsilon_a+\epsilon_v-\epsilon_c-\epsilon_d}, \tag{2.22}$$

$$E_F^{(2)} = \left[F_{av}F_{bw}\sum_{mc}\frac{\tilde{g}_{cwmv}\tilde{g}_{macb}}{\epsilon_m-\epsilon_c}+\text{c.c.}\right], \tag{2.23}$$

$$E_G^{(2)} = F_{av}F_{bw}\sum_{mc}\frac{\tilde{g}_{cavm}\tilde{g}_{wmbc}}{\epsilon_m+\epsilon_v-\epsilon_a-\epsilon_c}, \tag{2.24}$$

$$E_H^{(2)} = F_{av}F_{bw}\delta_{vw}\sum_{mcd}\frac{g_{cdbm}\tilde{g}_{macd}}{\epsilon_m+\epsilon_a-\epsilon_c-\epsilon_d}, \tag{2.25}$$

$$E_I^{(2)} = F_{av}F_{bw}\delta_{vw}\sum_{mnc}\frac{g_{camn}\tilde{g}_{mncb}}{\epsilon_m+\epsilon_n-\epsilon_a-\epsilon_c}, \tag{2.26}$$

$$E_{\Delta 1}^{(2)} = F_{av}F_{bw}\left[\sum_i\frac{\Delta_{ai}\tilde{g}_{wivb}}{\epsilon_i-\epsilon_a}+\sum_i\frac{\Delta_{wi}\tilde{g}_{aibv}}{\epsilon_i-\epsilon_v}+\text{c.c.}\right], \tag{2.27}$$

$$E_{\Delta 2}^{(2)} = F_{av}F_{bw}\left\{\delta_{ab}\sum_i\frac{\Delta_{wi}\Delta_{iv}}{\epsilon_v-\epsilon_i}+\delta_{vw}\sum_i\frac{\Delta_{ai}\Delta_{ib}}{\epsilon_i-\epsilon_a}\right.$$
$$+\left[\delta_{vw}\sum_{mc}\frac{\Delta_{mc}\tilde{g}_{camb}}{\epsilon_m-\epsilon_c}\right.$$
$$\left.\left.+\delta_{ab}\sum_{mc}\frac{\Delta_{mc}\tilde{g}_{cwmv}}{\epsilon_c-\epsilon_m}+\text{c.c.}\right]\right\}. \tag{2.28}$$

A number of features of $E^{(2)}$ are worth noting. First, the terms involving δ_{ab} are easily shown to be identical to the expression for the second-order energy for a one-particle state. Second, the terms involving δ_{vw} reproduce the second-order energy for a one-hole state. Furthermore, the terms $E_D^{(2)}$, $E_F^{(2)}$, $E_G^{(2)}$, $E_{\Delta 1}^{(2)}$ are random-phase approximation corrections to the energy. The Breit interaction is calculated just as it was in the one-particle case; the resulting expression for the correlation correction to the Breit interaction is very lengthy. The particle-hole formalism will be applied to berylliumlike, carbonlike, and neonlike ions.

D. Model potentials

We use two different model potentials to start our MBPT calculations. The corresponding difference in energy at a given level of approximation is a measure of the convergence of our calculations. The first potential $U_A(r)$ is taken to be the direct part of the Hartree-Fock potential for a closed-shell atom except for lithiumlike ions, where it is taken to be the monopole part of the entire HF potential. Specifically, U_A is defined by

$$U_A(r) = \begin{cases} 2v_0(1s,r)+v_0(2s,r), & \text{for Li-like ions,}\\ 2v_0(1s,r)+2v_0(2s,r), & \text{for Be-like ions,}\\ 2v_0(1s,r)+2v_0(2s,r)+ & \\ 2v_0(2p_{1/2},r), & \text{for C-like ions,}\\ 2v_0(1s,r)+2v_0(2s,r)+ & \\ 2v_0(2p_{1/2},r)+4v_0(2p_{3/2},r), & \text{for F- and Ne-like ions,}\end{cases} \tag{2.29}$$

where

$$v_0(a,r) = \frac{1}{r}\int_0^r[G_a^2(r')+F_a^2(r')]dr'$$
$$+\int_r^\infty[G_a^2(r')+F_a^2(r')]\frac{dr'}{r'}. \tag{2.30}$$

Here, $G_a(r)$ and $F_a(r)$ are the large and small components of the radial Dirac function for state a. The potential $U_A(r)$ was used in Ref. [9] for calculations of the Lamb shift. The second potential $U_B(r)$ is a Hartree-type potential, defined by

$$U_B(r) = U_A(r) - \begin{cases} v_0(1s,r), & \text{for Li-like ions,}\\ v_0(2s,r), & \text{for Be-like ions,}\\ v_0(2p_{1/2},r), & \text{for C-like ions,}\\ v_0(2p_{3/2},r), & \text{for F- and Ne-like ions.}\end{cases} \tag{2.31}$$

Since $v_0(n,r) \to 1/r$ for large r, the effective charge at large distances is $Z-N$ for the potential $U_A(r)$ and $Z-N+1$ for $U_B(r)$. Here, N is the number of electrons included in the potential U_A; i.e., 3, 4, 6, 10, and 10 for lithiumlike, berylliumlike, carbonlike, fluorinelike, and neonlike ions, respectively. The potentials $U_{A,B}(r)$ and the corresponding core orbitals are calculated self-consistently.

There are, of course, any number of model potentials that could be used. As long as MBPT converges, however, the choice of potential is, in principle, immaterial. However, because we do not go beyond second order in perturbation theory here, we obtain slightly different energies starting from different potentials. We use the difference in calculated energies as a measure of the convergence of our MBPT calculations.

III. QUANTUM ELECTRODYNAMIC CORRECTIONS

At high nuclear charge, QED corrections are known to contribute a substantial fraction to the energy levels so

TABLE I. MBPT and QED contributions to the $2s_{1/2}$-$2p_{3/2}$ transition energy for lithiumlike, berylliumlike, carbonlike, fluorinelike, and neonlike uranium evaluated starting from the potential U_A: units in a.u.

Term	Li-like	Be-like	C-like	F-like	Ne-like
$E^{(0)}$	163.9406	163.9885	164.7607	165.9570	165.9570
$F^{(1)}$	1.3960	2.4276	3.8185	4.3211	5.7267
$E^{(2)}$	-0.0150	0.4412	-0.0277	-0.0683	-0.0579
$B^{(2)}$	0.0081	0.0576	0.0096	0.0006	0.0011
RM+MP	-0.0017	-0.0020	-0.0019	-0.0017	-0.0019
MBPT	165.3280	166.9129	168.5592	170.2087	171.6250
SE	-1.9871	-1.9730	-1.9358	-1.8812	-1.8812
UP	0.5698	0.5654	0.5537	0.5366	0.5366
WK+HO	-0.0278	-0.0276	-0.0270	-0.0262	-0.0262
QED	-1.4450	-1.4352	-1.4091	-1.3709	-1.3709
Total	163.8830	165.4777	167.1501	168.8378	170.2541

it is important to treat these corrections in a consistent manner. One of the advantages of using MBPT based on local model potentials is that it is possible to understand the origin of the formulas of MBPT from the S-matrix approach to QED, and that this same approach leads to QED formulas. The QED corrections are dominated by the one-loop Lamb shift evaluated in whatever external potential is used. It is now straightforward to carry out such calculations [3,9,10]. Since the two model potentials used in this work have asymptotic charges that differ by unity, one can see qualitatively that the two calculations of the Lamb shift will lead to different results. This is because the Lamb shift scales as Z^4 so that a difference of a factor of $4/Z$ is expected. For uranium ions, these differences are several percent of the Lamb shift. Thus to obtain highly accurate values, correlation corrections to the Lamb shift must also be considered [3]. Since we ignore such corrections here, we expect our QED corrections to be accurate to a few percent only.

IV. CALCULATIONS

In this work, the following $2s$-$2p_{3/2}$ transitions are considered:

$$\text{Li-like:}\quad 2s - 2p_{3/2},$$

$$\text{Be-like:}\quad 2s^2\ (J=0) - 2s2p_{3/2}\ (J=1),$$

$$\text{C-like:}\quad 2s^2 2p_{1/2}^2\ (J=0) - 2s2p_{1/2}^2 2p_{3/2}\ (J=1),$$

$$\text{F-like:}\quad 2s^2 2p_{1/2}^2 2p_{3/2}^3\ (J=3/2) \\ -2s2p_{1/2}^2 2p_{3/2}^4\ (J=1/2),$$

$$\text{Ne-like:}\quad 2s^2 2p_{1/2}^2 2p_{3/2}^3 3s\ (J=1) \\ -2s2p_{1/2}^2 2p_{3/2}^4 3s\ (J=0).$$

These are transitions identified in the EBIT spectrum [1]. The self-consistent determination of the potentials $U_{A,B}(r)$, the core orbitals $\varphi_a(\mathbf{r})$, and the valence orbital $\varphi_v(\mathbf{r})$ was carried out using finite difference methods. The effect of finite nuclear size was built into all of the orbitals by choosing $V_{\mathrm{nuc}}(r)$ to be the potential of a finite charge distribution. The distribution was assumed to have a quadrupole shape, with parameters determined from muonic atom studies [11]. The MBPT calculations were carried out using a B-spline basis set for electrons confined to a cavity of finite radius $R = 1$ a.u. as described in Ref. [12]. Since only single and double summations over excited states are encountered, a relatively large basis set was employed, with 50 basis functions for each angular momentum state up to $\ell = 9$. A fine radial grid with 500 points was used, and extrapolation methods were used to carry out partial wave expansions completely. We do not quote numerical errors for our MBPT calculations, since such errors are much smaller than the errors resulting from uncalculated terms (dominated by $E^{(3)}$). We calculate QED corrections using the same potentials used in the MBPT calculations. The method of calculation has been described previously in Ref. [9]. Higher-order QED corrections are taken from the tables of Johnson and Soff [13].

In Tables I and II, we present the results of our calculations starting from potentials U_A and U_B, respectively, for the five ions under consideration. The contributions $E^{(0)}$, $F^{(1)}$, $E^{(2)}$, and $B^{(2)}$ are evaluated using the formulas written out in the preceding section. The contribution listed in the row RM+MP is the sum of the reduced-mass and mass-polarization corrections. Since we include the reduced-mass correction explicitly, we must use the infinite-mass Rydberg constant to convert our theoretical values from atomic units to eV. The five contributions to ionic structure are summed to give the values listed in the row MBPT. The row labeled SE contains values of the electron self-energy evaluated in the potential $V_{\mathrm{nuc}}(r) + U_{A,B}(r)$, and the row UP gives the corresponding Uehling potential contribution to the vacuum-polarization energy. The row labeled WK+HO gives the sum of the Wichmann-Kroll (WK) and higher-order (HO) corrections taken from Ref. [13]. Hydrogenic

TABLE II. MBPT and QED contributions to the $2s_{1/2}$-$2p_{3/2}$ transition energy for lithiumlike, berylliumlike, carbonlike, fluorinelike, and neonlike uranium evaluated starting from the potential U_B: units in a.u.

Term	Li-like	Be-like	C-like	F-like	Ne-like
$E^{(0)}$	163.8866	163.9406	164.3856	165.6826	165.6826
$F^{(1)}$	1.4505	2.4790	4.2032	4.6008	6.0237
$E^{(2)}$	-0.0182	0.4912	-0.0395	-0.0698	-0.0708
$B^{(2)}$	0.0082	0.0655	0.0092	-0.0051	-0.0053
RM+MP	-0.0017	-0.0020	-0.0019	-0.0017	-0.0019
MBPT	165.3254	166.9743	168.5566	170.2068	171.6283
SE	-2.0018	-1.9871	-1.9547	-1.8943	-1.8943
UP	0.5744	0.5698	0.5595	0.5408	0.5408
WK+HO	-0.0280	-0.0278	-0.0273	-0.0264	-0.0264
QED	-1.4554	-1.4450	-1.4224	-1.3799	-1.3799
Total	163.8700	165.5293	167.1342	168.8269	170.2484

values of the WK and HO corrections from this reference are scaled by the ratio of the present value of the Uehling potential correction to its hydrogenic value. The sum of the three QED corrections is given in the row labeled QED. Finally, the MBPT and QED contributions are summed to give the theoretical energy intervals in the row labeled "Total."

We find that the MBPT values of the energies obtained in the two different potentials agree to the level of 0.01 a.u. (0.3 eV) except for the poorly converged case of berylliumlike uranium, where the difference is about 0.06 a.u. (1.6 eV). These differences could be reduced by considering third- and higher-order MBPT corrections. The corresponding difference between the QED contributions calculated in the two potentials is also about 0.01 a.u. for all of the ions considered. To reduce the QED differences, one must account for correlation corrections to self-energy and vacuum polarization. Such corrections are expected to contribute values that are roughly $1/Z$ of the Lamb shift, ($\approx$0.01 a.u. or 0.3 eV). Additionally, we ignore corrections to the energy interval from nuclear polarizability which are estimated to be $\approx$ 0.2 eV [14]. All of the omitted corrections contribute at the level of the experimental uncertainty.

In Table III, we compare our calculations in the two potentials with results of MCDF calculations and experimental values given in Ref. [1]. The values listed under ΔU_A, ΔU_B and ΔMCDF are the differences between the respective theoretical values and experiment. With the exception of the cases of berylliumlike and neonlike uranium, the differences ΔU_A and ΔU_B range from 0.1 to 0.5 eV, reducing the discrepancy of MCDF calculations with experiment, ΔMCDF, by an order of magnitude.

For berylliumlike uranium, a large-scale relativistic CI calculation has been carried out [15] giving the value 4539.89 eV (166.838 a.u.) for the structure contribution and -38.25 eV (-1.406 a.u.) for the QED correction, leading to a theoretical prediction of 4501.64 eV (165.432 a.u.) for the $2p_{3/2}$-$2s_{1/2}$ energy interval. This CI value differs from experiment by 0.08 eV. The QED values used in the CI calculation are values obtained in potential U_B weighted by the CI expansion coefficients.

Because neonlike uranium has relatively good convergence properties, the discrepancy with experiment of almost 2 eV is puzzling, particularly since the neighboring fluorinelike ion agrees fairly well with experiment. We consider the explanation of this situation an important challenge.

In conclusion, we have found that second-order MBPT calculations of atomic structure combined with *ab initio* calculations of the one-loop QED corrections suffices to determine the energies of lithiumlike, carbonlike, and fluorinelike uranium at the 0.5 eV level of accuracy. For berylliumlike uranium, the convergence of the MBPT is poor so this level of accuracy is not obtained. However, for berylliumlike uranium, a relativistic CI calculation leads to results in close agreement with experiment. To improve the comparison for the remaining ions, particularly neonlike uranium, it will be necessary to include third- and higher-order MBPT corrections, correlation corrections to the Lamb shift, and corrections for nuclear polarization. Each of these interesting corrections contributes at the level of the error in the present experiment. Therefore, to make more refined calculations

TABLE III. Comparison of MBPT and MCDF calculations of the $2s_{1/2}$-$2p_{3/2}$ transition energy for lithiumlike, berylliumlike, carbonlike, fluorinelike, and neonlike uranium with experiment: units in eV.

	U_A	U_B	MCDF	Expt.	ΔU_A	ΔU_B	ΔMCDF
Li-like	4459.49	4459.13	4461.7	4459.37 ± 0.27	0.12	-0.24	2.3
Be-like	4502.88	4504.28	4505.3	4501.72 ± 0.21	1.16	2.56	3.6
C-like	4548.39	4547.96	4552.3	4548.32 ± 0.16	0.07	-0.36	4.0
F-like	4594.31	4594.02	4599.8	4593.83 ± 0.12	0.48	0.19	6.0
Ne-like	4632.85	4632.70	4638.9	4630.93 ± 0.26	1.92	1.77	8.0

worthwhile, we strongly encourage more accurate measurements of transitions in uranium and other heavy ions.

ACKNOWLEDGMENTS

We would like to thank Euripides Avgoustoglou, Peter Beiersdorfer, Steve Blundell, and Dan Plante for helpful conversations. Particular thanks are due to Mau Hsiung Chen for providing us with results of unpublished CI calculations. This research was supported in part by NSF Grant No. PHY-92-04089 and DOE Contract No. W-7405-ENG-48. W.R.J. and J.S. would like to acknowledge the hospitality of Lawrence Livermore National Laboratory.

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