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A Dirac-Fock-Slater approach to atomic structure for highly charged ions

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A very rapid, but accurate, fully relativistic method for calculating the atomic-structure data needed in determining collision strengths for highly charged ions is developed. A more rapid quasirelativistic approximation to this approach is also described. Results for oscillator strengths and energies are compared with those by mostly more elaborate programs for neonlike and nickel-like ions and generally good agreement is obtained.

I. INTRODUCTION

Ions with large values for the nuclear-charge number Z are becoming of increased interest in the study of high-temperature plasmas, partially due to the quest to develop ultrashort-wavelength lasers. In fact, soft x-ray lasing has recently been achieved in high-temperature plasmas using neonlike[1,2] and nickel-like ions.[3] For such ions with $Z \gtrsim 30$ relativistic interactions have significant effect on the radial functions, so that they should be included directly in the zeroth-order Hamiltonian in obtaining accurate results. Several rather elaborate fully relativistic atomic structure programs based on the use of the Dirac equation now exist.[4-7] These multiconfiguration Dirac-Fock programs tend to be much more time consuming to use than the corresponding multiconfiguration Hartree-Fock programs. This occurs largely as a consequence of the j dependence of the radial functions in a fully relativistic treatment, which results in a factor of 2 (except for s orbitals) more radial functions and typically an order of magnitude more radial (Slater) integrals required in diagonalizing the Hamiltonian. Moreover, each radial function has two components, the so-called "large" and "small" components. Although the use of such elaborate relativistic programs in determining quantities such as the energy levels and radiative rates required for most plasma applications may no longer be prohibitively time consuming with the use of supercomputers; this is often not the case for the analogous relativistic calculations of collision rates. The reason for this is that, to determine a collision rate, the corresponding cross section must be calculated for several impact-electron energies, and for each of these the scattering matrix elements must be determined for many initial and final values for the angular momenta of the free electron. Moreover, collision rates for many thousands of transitions are needed in some applications. Thus there is a need for very efficient, high-speed approaches for relativistic calculations of collision cross sections. The purpose of the present work is to develop approximate relativistic and quasirelativistic atomic-structure approaches and corresponding computer programs for providing the appropriate atomic-structure input for the rapid cross-section programs described in the accompanying paper.[8] These programs are designed to make very rapid, but accurate, calculations for ions that have lost at least half their electrons, i.e., that satisfy $Z > 2N$, where N is the number of bound electrons per ion. This appears to be satisfied for the plasmas of principal interest for x-ray-laser research, as well as for many other plasmas.

In Sec. II the theory of the present approach for atomic structure is outlined. Then in Sec. III results for neonlike and nickel-like ions by this method are compared with those by other mostly more elaborate programs to determine the accuracy of the approach.

II. OUTLINE OF THEORY

A. Summary of general features

As is standard in multiconfiguration relativistic programs, in treating an ion with N bound electrons we use basis states $\Phi_\nu(1,2,\ldots,N)$ that are single-configuration-state functions (CSF). These are antisymmetric sums of products of N one-electron Dirac spinors $u_{n\kappa m}$ that are solutions of the Dirac equation for a central potential $V(r)$,

$$u_{n\kappa m}=\frac{1}{r}\begin{bmatrix} P_{n\kappa}(r) & \chi_{\kappa m}(\theta,\phi,\sigma) \\ iQ_{n\kappa}(r) & \chi_{-\kappa m}(\theta,\phi,\sigma)\end{bmatrix}, \tag{1}$$

where $P_{n\kappa}$ and $Q_{n\kappa}$ are the large and small components of the radial function, respectively, the $\chi_{\kappa m}$ are the usual spin-angular-momentum functions

$$\chi_{\kappa m}(\theta,\phi,\sigma)=\sum_{m_l,m_s} C(l\tfrac{1}{2}m_l m_s;jm)Y_{lm_l}(\theta,\phi)\delta(m_s|\sigma)\,, \tag{2}$$

and the relativistic quantum number κ has the values

$$\kappa=l,\quad j=l-\tfrac{1}{2};\quad \kappa=-(l+1),\quad j=l+\tfrac{1}{2}\,. \tag{3}$$

In forming the Φ_ν, the standard jj coupling scheme is followed, e.g., Grant *et al.*[5] In fact, the angular package of Grant *et al.*[5] is used in the present program. In this coupling scheme the j values of all the electrons in a subshell $n_r l_r j_r$ are coupled together to form the total angular momentum J_r of the subshell. Then these are successively coupled together starting with the lowest subshell to form the total angular momentum J for the ion. By the lower of the two subshells $n_1 l_1 j_1$ and $n_2 l_2 j_2$, one means the one with the smaller n value; or if $n_1 = n_2$, the one with the smaller l value; or if $n_1 l_1 = n_2 l_2$, the one with the smaller j value.

The approximate ion wave functions are given by

$$\psi = \sum_{\nu=1}^{N_{\mathrm{CSF}}} b_\nu \Phi_\nu \ , \tag{4}$$

where the mixing coefficients b_ν are obtained by diagonalizing the Hamiltonian H. This is assumed to be given by

$$H = \sum_{i=1}^{N} H_D(i) + \sum_{\substack{i,j \\ i<j}}^{N} \frac{2}{r_{ij}} \ , \tag{5}$$

where $H_D(i)$ is the single-electron Dirac Hamiltonian for a pure Coulomb potential $-2Z/r_i$ due to the nucleus of the ion. In Eq. (5) energies are in rydbergs and distances are in units of the Bohr radius a_0. In general, the number N_{CSF} of single-configuration-state functions included in Eq. (4) is at least all those in a complex, i.e., having the same set of n values, parity, and J value; however, in cases where there are states with additional n values that are very nearby or overlapping in energy, these can be included.

In diagonalizing H given by Eq. (5) we add and subtract the electron-electron electrostatic contributions $V^{ee}(r_i)$ to the central potentials $V(r_i)$, so that H is written

$$H = \sum_{i=1}^{N} H_D'(i) - \sum_{i=1}^{N} V^{ee}(r_i) + \sum_{\substack{i,j \\ i<j}}^{N} \frac{2}{r_{ij}} \ , \tag{6}$$

where

$$H_D'(i) = H_D(i) + V^{ee}(r_i) \ . \tag{7}$$

This $H_D'(i)$ is the single-electron Dirac Hamiltonian with the central potential $V(r_i)$, where

$$V(r_i) = -\frac{2Z}{r_i} + V^{ee}(r_i) \ . \tag{8}$$

Since the Φ_ν are antisymmetric products of the Dirac spinors $u_{n\kappa m}$, which are eigenfunctions of H_D', the first term on the right-hand side of Eq. (6) contributes only to the diagonal matrix elements and gives a contribution equal to the sum of the N energy eigenvalues $\varepsilon_{n\kappa}$ of the N spinors contained in Φ_ν. Also the second term $-\sum_i V^{ee}(r_i)$ contributes only to the diagonal matrix elements, if we restrict the mixing to the states in a complex. However, if we include mixing with additional states, it contributes to the off-diagonal matrix elements between states with the same angular functions, but differing n values. Of course, the final term contributes to both diagonal and nondiagonal matrix elements, with the general form of the contribution being given by sums over λ of products of angular parts and so-called Slater integrals

$$R^{\lambda}(ab,cd) = 2\int_0^\infty \int_0^\infty [P_{n_a\kappa_a}(r_1)P_{n_c\kappa_c}(r_1) + Q_{n_a\kappa_a}(r_1)Q_{n_c\kappa_c}(r_1)] \times \frac{r_<^{\lambda}}{r_>^{\lambda+1}} [P_{n_b\kappa_b}(r_2)P_{n_d\kappa_d}(r_2) + Q_{n_b\kappa_b}(r_2)Q_{n_d\kappa_d}(r_2)]\,dr_1\,dr_2 \ , \tag{9}$$

where $r_<$ ($r_>$) is the lesser (greater) of r_1 and r_2.

B. Determination of the radial functions

The coupled Dirac radial equations determining the $P_{n\kappa}$ and $Q_{n\kappa}$ in Eq. (1) are

$$\left[\frac{d}{dr} + \frac{\kappa}{r}\right] P_{n\kappa} = \frac{\alpha}{2}\left[\varepsilon_{n\kappa} - V + \frac{4}{\alpha^2}\right] Q_{n\kappa} \ , \tag{10}$$

and

$$\left[\frac{d}{dr} - \frac{\kappa}{r}\right] Q_{n\kappa} = \frac{\alpha}{2}(V - \varepsilon_{n\kappa}) P_{n\kappa} \ , \tag{11}$$

where, as in Eq. (5), distances are in units of a_0, and ε and V are in rydbergs. One can use Eq. (10) to express $Q_{n\kappa}$ in terms of $P_{n\kappa}$ and substitute this in Eq. (11) to obtain the second-order differential equation for the large component

$$\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + V - \frac{\alpha^2}{4}(\varepsilon_{n\kappa} - V)^2 - \frac{\alpha^2}{4}\left[1 + \frac{\alpha^2}{4}(\varepsilon_{n\kappa} - V)\right]^{-1} \left[\frac{dV}{dr}\right] \left[\frac{1}{P_{n\kappa}}\frac{dP_{n\kappa}}{dr} + \frac{\kappa}{r}\right] \right] P_{n\kappa} = \varepsilon_{n\kappa} P_{n\kappa} \ , \tag{12}$$

where use was made of the fact that

$$\kappa(\kappa+1)=l(l+1)\ . \tag{13}$$

Equation (12) has an appearance like the usual nonrelativistic Schrödinger equation, except that it has a much more complicated effective potential. Thus, except for special considerations for small r discussed, for example, in Sec. 7-17 of Cowan,[9] similar numerical procedures can be used in solving it, as in a nonrelativistic approach. The radial part of the Hartree-Fock relativistic (HFR) version of Cowan's widely used program[9] corresponds to solving Eq. (12), with κ replaced by its average over j value -1, so that the large component becomes independent of j. Then the small component is neglected and the large component normalized as though it were the total radial function. Our procedure has been simply to use the radial part of Cowan's HFR program, modified so that it does not make the approximation $\kappa=-1$ and also modified to simultaneously obtain $Q_{n\kappa}$. The latter is readily done because, as seen from Eq. (10), $Q_{n\kappa}$ is essentially given by the final term in the effective potential of Eq. (12). Of course, we also use the correct fully relativistic normalization

$$\int_0^\infty [P_{n\kappa}^2(r)+Q_{n\kappa}^2(r)]dr=1\ . \tag{14}$$

In addition, in order to obtain $Q_{n\kappa}$ with sufficient accuracy at large Z, we found it necessary to keep separate the $-2Z/r$ nuclear contribution to $V(r)$ and determine its contribution to $dV(r)/dr$ analytically. Also we started the calculations with a mesh size $\frac{1}{8}$ the value for the initial mesh size usually used with Cowan's program. Specifically, we used

$$\Delta\rho_{\text{init}}=3.125\times10^{-4},\quad \rho=4\left[\frac{2Z}{9\pi^2}\right]^{1/3} r\ . \tag{15}$$

This did not add very much to the computing time because a linear mesh is used with a doubling of the interval size every 40 points, which only added 120 points to a total usually of 640 points. Actually, in providing the atomic-structure data for collision strengths, we stop the doubling at the largest mesh size that satisfies Eq. (16) of Ref. 8.

Except for the details we have just mentioned regarding the numerical solution of Eqs. (10) and (11), the approach we have described is mostly quite standard. The principal manner in which we obtain speed in our calculations is through our choice for the central potential $V(r)$, which we discuss next.

C. Choice for the potential

For the central potential $V(r)$ in Eqs. (10)–(12) we use the Dirac-Fock-Slater potential. That is, we use the relativistic version of the Hartree-Fock-Slater potential introduced by Slater[10] and discussed, for example, in Sec. 7-11 of Ref. 9, except that we use the Kohn-Sham[11] value for the coefficient of the exchange term. Specifically, this potential is given by

$$V(r)=-\frac{2Z}{r}+V_c(r)-\left[\frac{24}{\pi}\rho\right]^{1/3}\ , \tag{16}$$

where the first term is the potential due to the nucleus, and the remaining part is the electron-electron contribution previously called $V^{ee}(r)$ in Eq. (8). The part of this called $V_c(r)$ is the spherically averaged classical potential due to the bound electrons,

$$V_c(r)=\sum_{n',\kappa'} w_{n'\kappa'}\int_0^\infty \frac{2}{r_>}[P_{n'\kappa'}^2(r_2)+Q_{n'\kappa'}^2(r_2)]dr_2\ , \tag{17}$$

where $w_{n'\kappa'}$ is the occupation of subshell $n'\kappa'=n'l'j'$. The summation in Eq. (17) is over all occupied subshells and $r_>$ is the greater of r and r_2. The final term in Eq. (16) is the exchange energy of an electron in a free-electron gas of density ρ averaged over all possible momenta of the electron. Following Slater,[10] we use for ρ the number density of electrons at distance r from the nucleus. The spherically averaged value for this is

$$\rho(r)=\frac{1}{4\pi r^2}\sum_{n',\kappa'} w_{n'\kappa'}[P_{n'\kappa'}^{(2)}(r)+Q_{n'\kappa'}^2(r)]\ . \tag{18}$$

We note that if $w_{n'\kappa'}$ were replaced by $w_{n\kappa}-1$ when $n'\kappa'=n\kappa$, then the potential given by Eq. (17) would be the relativistic version of the Hartree potential. The undesirable feature that self-interaction is included in V_c is at least partially cancelled out by the fact that self-exchange energy is also included because Eq. (18) also includes the contribution from all the electrons, including all those in subshell $n\kappa$.

In addition, a single mean configuration with fractional occupation numbers is used in determining the potential given by Eqs. (16)–(18) for a given class of transitions. The prescription we generally use in determining this mean configuration is that the occupation of the active electron is split approximately equally between initial and final subshells. For example, in obtaining the structure results required for calculations of collision strengths for transitions in neonlike ions between the ground level, which has the configuration $1s_{1/2}^2 2s_{1/2}^2 2p_{1/2}^2 2p_{3/2}^4$, and excited levels in which there is a single electron with $n=3$, an appropriate choice of the mean configuration is

$$1s_{1/2}^2 2s_{1/2}^{1.9} 2p_{1/2}^{1.9} 2p_{3/2}^{3.7} 3s_{1/2}^{0.1} 3p_{1/2}^{0.1} 3p_{3/2}^{0.1} 3d_{3/2}^{0.1} 3d_{5/2}^{0.1}\ . \tag{19}$$

Actually most of our calculations were instead done using

$$1s_{1/2}^2 2s_{1/2}^{1.8} 2p_{1/2}^{1.8} 2p_{3/2}^{3.6} 3s_{1/2}^{0.16} 3p_{1/2}^{0.16} 3p_{3/2}^{0.16} 3d_{3/2}^{0.16} 3d_{5/2}^{0.16}\ . \tag{20}$$

The reason for this is that it was planned to also use the same potential in treating $n=3$ to $n=3$ transitions. However, as will be discussed further in Sec. III A, use of slightly different choices for the mean configuration, such as use of Eqs. (19) or (20), generally has a small effect on the results. The effect of using a slightly different distribution among the upper subshells of a fixed total occupation of the upper subshells is almost undetectable; for example, the effect of using a distribution proportional to the statistical weights of the upper subshells instead of equal distribution, as in Eqs. (19) or (20).

We emphasize that, as discussed previously in connection with the diagonalization of the Hamiltonian and determination of the mixing coefficients, our calculations are generally multiconfiguration calculations in which at least the mixing between all states in a complex is included. The single mean configuration is used solely in determining the potential. However, this, coupled with use of Eqs. (16)–(18), has many advantages. In particular, the potential is then the same for all electrons, so all orbitals are automatically orthogonal and the calculations are much more rapid than with a program such as that of Grant *et al.*[5] or Desclaux[4] in which full multiconfiguration Dirac-Fock calculations are made. We also use this same potential for the free electrons in collision-strength calculations, as discussed in Ref. 8.

It should be pointed out that the relativistic code RELAC of Klapisch *et al.*[12] has similar advantages deriving from use of the same potential for all electrons, in their case a so-called parametric potential rather than a Dirac-Fock-Slater potential. Also we mention that use of a single mean configuration in determining the potential, such as Eqs. (19) or (20), is frequently done at the Lawrence Livermore National Laboratory in conjunction with use of the relativistic programs of Refs. 6 and 7.

D. Quasirelativistic approach

In addition to the fully relativistic (FR) approach we have described, we have a quasirelativistic (QR) option in our program. This corresponds to simply solving Eq. (12) for $P_{n\kappa}$, normalizing it as though it were the total radial function

$$\int_0^\infty [P_{n\kappa}^{\mathrm{QR}}(r)]^2 dr = 1 \quad (\text{QR approach}) , \tag{21}$$

and then omitting $Q_{n\kappa}$ everywhere, such as in Eqs. (9), (17), and (18). Thus this approach is similar to the HFR approach of Cowan,[9] except that the further approximation of using $\kappa = -1$, which has the simplifying effect of making the radial functions independent of j, is not made. It was very easy to modify the radial part of Cowan's program[9] to obtain these QR radial functions and this was the first version of our program that was obtained. It was thought initially that this would be somewhat faster than a fully relativistic program, but it turns out that the QR option is only about 5–10 % more rapid than the FR option of our program. This occurs because, as noted previously, the small component $Q_{n\kappa}$ is essentially calculated anyway in determining the final term in the effective potential of Eq. (12). Also, the angular part of the calculations is unaltered and the same number of radial integrals occur; they are just slightly simpler when the $Q_{n\kappa}$ part is omitted. Thus it would appear that there is little point in using the QR approach, even though, as indicated by the numerical results given in Sec. III, this approach is rather accurate even for large Z when transitions involving 1s orbitals are not of interest, as is the case for Ne-like and Ni-like ions. However, it turns out that the QR approach is useful in obtaining collision strengths when it is coupled with an additional approximation for the free electrons discussed in the accompanying paper.[8]

E. Fitting to Z

In studying a large portion of an isoelectronic sequence; for example, all neonlike ions with $22 \leq Z \leq 92$, it is convenient to be able to obtain approximate mixing coefficients and transition energies for all Z after making detailed calculations for only a few Z values. We are able to do this by using procedures like those applied previously by one of us (R.E.H.C.) to Cowan's atomic-structure code[9] and used in Ref. 13. Specifically, the matrix elements of the Hamiltonian are calculated in detail for a few Z values. For the purpose of discussion, let us say six, which is typical. Then the six values for each matrix element are fitted to a power series in Z with six terms. The results of the fits are then used in performing the diagonalization of the Hamiltonian for each Z to obtain the corresponding mixing coefficients and energy roots. The procedure requires practically no more time than that required for the detailed calculations for the six Z values and is almost as accurate as direct calculations for all Z.

In this connection it is of interest to note that on a Cray XMP supercomputer at the MFE Computer Center at Livermore, California, the CPU time in seconds, required for the present quasirelativistic and fully relativistic options of the program to make the complete atomic-structure calculations for the 36 $n=3$ excited levels plus the ground level in neonlike ions, is given by

$$t_{\mathrm{CPU}}(\mathrm{sec}) = 1.9 + N_Z \times 3.5 \quad (\text{QR approach}) , \tag{22}$$

and

$$t_{\mathrm{CPU}}(\mathrm{sec}) = 1.9 + N_Z \times 3.8 \quad (\text{FR approach}) . \tag{23}$$

In these expressions the first term is the time required for the angular part, which is the same for both QR and FR approaches and is done only once in considering many Z values. N_Z is the number of Z values for which detailed calculations are made. For the situation discussed above this would be six. The final numbers are the time required to do the detailed radial part for each value of Z, which is less for the QR approach. Since the fitting procedure takes essentially no time, the total CPU time required to do a very large portion of the isoelectronic sequence (assuming $N_Z = 6$) is only about 23 sec with the QR approach and 25 sec with the FR approach. Further improvements in speed are expected to be achieved in future work.

Of course, with this fitting procedure one does not have the orbitals for each Z, but this is often not necessary. For example, this is the case for the applications to inner-shell ionization of Na-like, Li-like, and Cu-like ions considered in Refs. 14–16. It is also the case for oscillator strengths, if one makes similar fits of the radial transition matrix elements to a power series in Z; or for collision strengths, if one uses the factorized form and fits the radial part to a power series in Z. The latter is discussed in more detail in the accompanying paper.[8]

III. NUMERICAL RESULTS AND DISCUSSION

In order to test the accuracy of the present approach we have calculated the radiative oscillator strengths f

with retardation effects ignored, that is, by the formula

$$f_{ij}=\frac{\Delta E_{if}}{3g_i}\sum_{M_f,M_i}\left|\left\langle\psi_f\left|\sum_{\alpha}\mathbf{r}_\alpha\right|\psi_i\right\rangle\right|^2 , \tag{24}$$

where ψ_i and ψ_f are initial and final antisymmetrized ion wave functions of the form given by Eq. (4), the sum is over the initial and final magnetic quantum numbers of the ion, ΔE_{if} is the transition energy in rydbergs, and g_i is the statistical weight of the initial lower level. The results for f and ΔE are then compared with those calculated with the elaborate multiconfiguration Dirac-Fock program of Grant *et al.*,[5] considered as a standard. Also, comparisons with results obtained by other programs are included when available. In running the program of Grant *et al.*,[5] we generally used the average-level (AL) option in which the average of the energies of the levels in a complex was minimized in each run. In fact, all results compared in the tables were obtained with the inclusion of the mixing among all the states in a complex, i.e., with a common set of n values, parity, and J value.

A. Results for neonlike ions

Values for the oscillator strengths for transitions between the ground-state level and the excited-state levels with $n=3$ in neonlike ions with $Z=26$, 47, 56, 74, and 92 are compared in Table I. The transitions are indicated by the upper levels ordered according to energy and labeled by the basis state making the dominant contribution using the following abbreviations:

$$(2p_{3/2}3l_j)_J=(1s_{1/2}^2 2s_{1/2}^2 2p_{1/2}^2 2p_{3/2}^3 3l_j)_J , \tag{25}$$

$$(2p_{1/2}3l_j)_J=(1s_{1/2}^2 2s_{1/2}^2 2p_{1/2} 2p_{3/2}^4 3l_j)_J , \tag{26}$$

and

$$(2s_{1/2}3l_j)_J=(1s_{1/2}^2 2s_{1/2} 2p_{1/2}^2 2p_{3/2}^4 3l_j)_J . \tag{27}$$

The unstarred QR and FR results are the present quasirelativistic and fully relativistic values obtained using Eq. (20), while the starred energies are corresponding values obtained using Eq. (19). By comparing FR and FR* values one sees that the results are not very sensitive to the precise occupation numbers used in the mean configuration determining the electron-electron contribution to the potential, especially for high Z, where the electron-electron interaction becomes less important relative to the potential due to the nuclear charge.

In addition to the results obtained by the program of Grant *et al.*[5] obtained for a point nuclear charge and with retardation omitted, which are labeled G in Table I, we have included results labeled G^*, which are obtained with inclusion of retardation, i.e., without making the assumption that the wavelength of the photon is very large compared with the size of the ion. One sees that the effect of retardation is rather small in all cases, but, as expected, is generally more important for large Z. Also results labeled G^{**} by that program are included. In addition to retardation, these include the effects of the relativistic two-body Breit interaction and the quantum electrodynamic (QED) corrections due to self-energy and vacuum polarization. Also, the effect of a finite nuclear size with a Fermi charge distribution[17] is included. The most important of these in affecting oscillator strengths is the Breit interaction. This interaction is only included perturbatively in the structure calculations. That is, its contributions to the matrix elements of the Hamiltonian are included before the final diagonalization. Thus it affects only the energies and mixing coefficients. Since the former are always affected by less than 1%, usually much less, the principal effect on f values is through the effect on the mixing coefficients. However, the comparison of G^* and G^{**} results in Table I indicate that this effect is generally small. It tends to be greatest for weak transitions to an upper level that lies close in energy to the upper level of a strong transition, so that slight differences in the method of calculation can affect the mixing of the two levels sufficiently to provide an appreciable change in the f value for the weaker transition. The best example of this occurs for $Z=56$ for the weak transition to the $(2p_{1/2}3s_{1/2})_1$ level, which lies between the upper levels of two very strong transitions.

Also included in Table I for $Z=26$ and 74 are results by the semirelativistic so-called Hartree-Fock-relativistic (HFR) program of Cowan,[9] as given in Ref. 18, and the results calculated using hydrogenic basis states plus screening (HBS) constants, also given in Ref. 18. In addition, HFR values calculated the same way as in Ref. 18, that is, using the same scale factors for the Slater integrals, are also given for $Z=47$, 56, and 92. Moreover, for $Z=56$ we could include values labeled R that were calculated by Reed[19] using the relativistic program of Hagelstein and Jung,[6] which includes the Breit interaction, QED corrections, and finite nuclear size.

All of these results for f values are seen to be in quite close agreement, except that the HFR and HBS results differ appreciably from the other results for some transitions when Z is very large. Presumably this is largely due to omission of the j dependence in the radial functions in those calculations. Also there is the noticeable trend among the QR, FR, FR*, and G values that the agreement between FR, FR*, and G results increases with Z, while that between QR and FR results decreases with Z. The former is expected because the difference in the physics of the FR, FR*, and G calculations is solely in the treatment of the electron-electron contribution $V^{ee}(r)$ to the central potential. Since $V^{ee}(r)$ becomes smaller relative to the nuclear contribution as Z increases, the effect of this on f values decreases as Z increases. Of course, the quasirelativistic approximations made in the QR approach discussed in Sec. II D increase in significance as Z increases and relativistic effects became more important. Thus one expects the differences between QR and FR results to increase with Z. Nevertheless, one sees that, even for $Z=92$, the QR results for oscillator strengths appear to be quite good.

In Tables II–IV a comparison of energies relative to the ground-state level is made for the 36 excited levels with $n=3$ for a sample of neonlike ions with $Z=26$, 56, and 92. Here the labeling is as in Table I. The energy ordering is according to FR, FR*, and G results, which always agree in that respect. Of course, retardation, in the sense used previously regarding oscillator strengths, has no meaning here. The results labeled HJ are from Ref. 6 and are obtained with the same program that was used for the results labeled R from Ref. 19. As noted previously, that program includes the QED corrections, the effect of a finite nuclear size, and the Breit interaction. However, the latter is obtained for the limit $\omega=0$. All of these effects increase with Z. In most cases the Breit contribution is the most important, but for cases involving holes in the $2s_{1/2}$ subshell the contribution from the QED corrections is comparable. The effect of the finite nuclear size is negligible for $Z=26$, is still small (less than about

TABLE I. Comparison of oscillator strengths for neonlike ions. Upper levels are ordered according to energy and are designated by the pure *jj* coupled state making the dominant contribution using the abbreviations of Eqs. (25)–(27). The following labeling is used: QR and FR are present quasirelativistic and fully relativistic results using Eq. (20) in determining the potential. FR* differs from FR only in that Eq. (19) is used in place of Eq. (20). *G*, *G**, and *G*** are results obtained with the program of Grant *et al.* (Ref. 5) without retardation; with retardation; and with retardation plus Breit interaction, QED corrections, and finite nuclear size; respectively. HFR and HBS are results obtained using Cowan's (Ref. 9) HFR program and using hydrogenic basis states, respectively. R are results of Reed (Ref. 19) obtained using the relativistic program of Hagelstein and Jung (Ref. 6).

Z = 26

	$(2p_{3/2}3s_{1/2})_1$	$(2p_{1/2}3s_{1/2})_1$	$(2p_{3/2}3d_{3/2})_1$	$(2p_{3/2}3d_{5/2})_1$	$(2p_{1/2}3d_{3/2})_1$	$(2s_{1/2}3p_{1/2})_1$	$(2s_{1/2}3p_{3/2})_1$
QR	0.1093	0.0919	0.0097	0.6140	2.5326	0.0369	0.2875
FR	0.1081	0.0922	0.0098	0.5900	2.5516	0.0358	0.2880
FR*	0.1102	0.0937	0.0099	0.6095	2.5514	0.0358	0.2868
G	0.1051	0.0890	0.0076	0.6049	2.3779	0.0342	0.2648
G*	0.1051	0.0888	0.0074	0.6036	2.3743	0.0343	0.2642
G**	0.1047	0.0896	0.0072	0.5900	2.3844	0.0337	0.2638
HFR	0.121	0.103	0.010	0.682	2.582	0.039	0.322
HBS	0.116	0.099	0.010	0.659	2.651	0.041	0.344

Z = 47

	$(2p_{3/2}3s_{1/2})_1$	$(2p_{1/2}3s_{1/2})_1$	$(2p_{3/2}3d_{3/2})_1$	$(2p_{3/2}3d_{5/2})_1$	$(2p_{1/2}3d_{3/2})_1$	$(2s_{1/2}3p_{1/2})_1$	$(2s_{1/2}3p_{3/2})_1$
QR	0.1262	0.1010	0.0003	2.0531	1.5905	0.1214	0.3273
FR	0.1239	0.0971	0.0001	2.0460	1.5797	0.1210	0.3253
FR*	0.1250	0.0978	0.0001	2.0557	1.5828	0.1207	0.3248
G	0.1223	0.0957	0.0003	2.0013	1.5491	0.1165	0.3132
G*	0.1222	0.0947	0.0004	1.9839	1.5420	0.1166	0.3097
G**	0.1232	0.0947	0.0005	1.9897	1.5305	0.1166	0.3050
HFR	0.1238	0.1156	0.0005	2.0336	1.6826	0.1084	0.3647

Z = 56

	$(2p_{3/2}3s_{1/2})_1$	$(2p_{3/2}3d_{3/2})_1$	$(2p_{3/2}3d_{5/2})_1$	$(2p_{1/2}3s_{1/2})_1$	$(2p_{1/2}3d_{3/2})_1$	$(2s_{1/2}3p_{1/2})_1$	$(2s_{1/2}3p_{3/2})_1$
QR	0.1304	0.0066	2.3117	0.0214	1.4733	0.1083	0.3268
FR	0.1268	0.0057	2.2688	0.0534	1.4477	0.1128	0.3232
FR*	0.1278	0.0058	2.2798	0.0508	1.4511	0.1123	0.3229
G	0.1256	0.0065	2.2320	0.0457	1.4299	0.1086	0.3138
G*	0.1254	0.0073	2.2026	0.0452	1.4208	0.1088	0.3084
G**	0.1267	0.0083	2.1624	0.0897	1.4066	0.1114	0.3025
R	0.1369	0.0068	2.326	0.0564	1.475	0.1050	0.3121
HFR	0.1217	0.0079	2.2865	0.0000	1.6042	0.0867	0.3744

Z = 74

	$(2p_{3/2}3s_{1/2})_1$	$(2p_{3/2}3d_{3/2})_1$	$(2p_{3/2}3d_{5/2})_1$	$(2p_{1/2}3s_{1/2})_1$	$(2s_{1/2}3p_{1/2})_1$	$(2p_{1/2}3d_{3/2})_1$	$(2s_{1/2}3p_{3/2})_1$
QR	0.1527	0.0640	2.3918	0.0280	0.3962	1.0370	0.2899
FR	0.1451	0.0599	2.3787	0.0266	0.4196	0.9725	0.2829
FR*	0.1460	0.0603	2.3847	0.0269	0.4186	0.9759	0.2826
G	0.1441	0.0611	2.3413	0.0269	0.4081	0.9726	0.2772
G*	0.1441	0.0648	2.2827	0.0260	0.4068	0.9600	0.2676
G**	0.1456	0.0704	2.2783	0.0256	0.4809	0.8756	0.2609
HFR	0.127	0.064	2.225	0.062	0.306	1.319	0.364
HBS	0.078	0.065	2.474	0.028	0.802	1.047	0.534

Z = 92

	$(2p_{3/2}3s_{1/2})_1$	$(2p_{3/2}3d_{3/2})_1$	$(2p_{3/2}3d_{5/2})_1$	$(2p_{1/2}3s_{1/2})_1$	$(2s_{1/2}3p_{1/2})_1$	$(2p_{1/2}3d_{3/2})_1$	$(2s_{1/2}3p_{3/2})_1$
QR	0.2045	0.1297	2.3564	0.0306	0.2985	0.9947	0.2143
FR	0.1893	0.1197	2.3393	0.0287	0.2768	0.9517	0.2041
FR*	0.1902	0.1202	2.3445	0.0289	0.2768	0.9535	0.2039
G	0.1878	0.1202	2.3087	0.0288	0.2725	0.9498	0.2012
G*	0.1886	0.1271	2.2143	0.0272	0.2725	0.9299	0.1882
G**	0.1895	0.1356	2.2020	0.0268	0.2775	0.9177	0.1834
HFR	0.1496	0.1167	2.0645	0.0928	0.1851	1.4323	0.3187

0.5 eV) for $Z=56$, but has become equal to about 25–30 % of the total difference between G and G^{**} values for levels with $2s_{1/2}$ holes for $Z=92$. However, even for $Z=92$, the effect of all these corrections is seen to be somewhat under 1% by comparing G and G^{**} values. Nevertheless, it is seen to be sufficient at high Z to switch the energy ordering for a few pairs of very nearby levels.

Although, in general, the agreement between the various results for energies is rather good, one sees, as expected, that, similar to the situation for oscillator strengths, the difference between QR and FR results increases with Z. Also, as expected, the reliability of the HFR results appears to decrease as Z becomes very large.

An interesting aspect of the comparison of energies is that the differences between FR, FR*, and G values are

TABLE II. Comparison of energies (in eV) for excited levels relative to the ground-state level for neonlike iron. Notation is as in Table I except HJ designates Ref. 6.

Upper Level	QR	FR	FR*	G	G**	HJ	HFR
$(2p_{3/2}3s_{1/2})_2$	724.22	723.91	725.22	724.62	724.17	725.82	724.98
$(2p_{3/2}3s_{1/2})_1$	726.24	725.92	727.22	726.58	726.13	727.75	726.74
$(2p_{1/2}3s_{1/2})_0$	737.57	736.86	738.19	737.55	736.80	738.57	737.66
$(2p_{1/2}3s_{1/2})_1$	738.87	738.17	739.50	738.81	738.04	739.79	738.76
$(2p_{3/2}3p_{1/2})_1$	754.40	754.17	755.46	754.95	754.48	756.03	755.98
$(2p_{3/2}3p_{1/2})_2$	758.00	757.80	759.05	758.55	758.09	759.52	758.93
$(2p_{3/2}3p_{3/2})_3$	759.73	759.45	760.72	760.23	759.68	761.12	760.54
$(2p_{3/2}3p_{3/2})_1$	760.86	760.60	761.85	761.35	760.88	762.29	761.52
$(2p_{3/2}3p_{3/2})_2$	762.70	762.43	763.67	763.14	762.65	764.05	763.14
$(2p_{3/2}3p_{3/2})_0$	768.58	768.14	769.40	769.28	768.71	769.70	768.67
$(2p_{1/2}3p_{1/2})_1$	770.82	770.22	771.50	770.95	770.18	771.75	771.14
$(2p_{1/2}3p_{3/2})_1$	774.12	773.46	774.74	774.19	773.41	774.94	774.14
$(2p_{1/2}3p_{3/2})_2$	774.60	773.92	775.21	774.63	773.79	775.33	774.56
$(2p_{1/2}3p_{1/2})_0$	790.27	789.96	791.15	787.39	786.79	790.57	787.38
$(2p_{3/2}3d_{3/2})_0$	800.49	800.22	801.60	800.90	800.42	801.99	801.65
$(2p_{3/2}3d_{3/2})_1$	801.55	801.27	802.64	802.19	801.63	802.95	802.60
$(2p_{3/2}3d_{5/2})_2$	803.50	803.18	804.54	803.88	803.27	804.77	804.35
$(2p_{3/2}3d_{5/2})_4$	803.67	803.36	804.71	804.06	803.44	804.88	804.44
$(2p_{3/2}3d_{3/2})_3$	804.42	804.14	805.47	804.85	804.28	805.71	805.07
$(2p_{3/2}3d_{3/2})_2$	806.11	805.82	807.14	806.54	805.98	807.42	806.61
$(2p_{3/2}3d_{5/2})_3$	807.27	806.96	808.26	807.66	807.09	808.47	807.66
$(2p_{3/2}3d_{5/2})_1$	812.26	811.88	813.15	812.45	811.81	813.33	812.21
$(2p_{1/2}3d_{3/2})_2$	817.69	817.03	818.39	817.71	816.82	818.41	817.64
$(2p_{1/2}3d_{5/2})_2$	818.49	817.81	819.16	818.50	817.60	819.15	818.40
$(2p_{1/2}3d_{5/2})_3$	819.14	818.44	819.79	819.11	818.22	819.74	818.99
$(2p_{1/2}3d_{3/2})_1$	827.11	826.52	827.69	826.61	825.69	827.53	825.99
$(2s_{1/2}3s_{1/2})_1$	860.77	860.57	861.56	861.58	860.87	861.73	861.52
$(2s_{1/2}3s_{1/2})_0$	867.52	867.39	868.36	867.90	867.24	868.23	867.65
$(2s_{1/2}3p_{1/2})_0$	893.49	893.40	894.34	894.43	893.78	894.44	894.54
$(2s_{1/2}3p_{1/2})_1$	893.99	893.89	894.83	894.96	894.27	894.89	894.98
$(2s_{1/2}3p_{3/2})_2$	896.45	896.28	897.23	897.35	896.60	897.22	897.25
$(2s_{1/2}3p_{3/2})_1$	898.41	898.24	899.18	899.22	898.46	899.09	898.96
$(2s_{1/2}3d_{3/2})_1$	938.73	938.57	939.60	939.63	938.84	939.56	939.74
$(2s_{1/2}3d_{3/2})_2$	938.92	938.75	939.78	939.83	938.99	939.68	939.93
$(2s_{1/2}3d_{5/2})_3$	939.24	939.04	940.07	940.07	939.18	939.92	940.24
$(2s_{1/2}3d_{5/2})_2$	944.25	944.05	945.00	944.99	944.14	944.79	944.65

generally very small (~1 or 2 eV) and almost independent of Z, except for $Z=92$. These differences should be entirely due to the differences in the determination of the electron-electron contribution $V^{ee}(r)$ to the central potential, because, as noted in the discussion of f values, this is the only difference in the physics used. The difference between FR and FR* is simply due to the use of Eqs. (20) or (19) in determining the potential, while G uses the much more elaborate multiconfiguration Dirac-Fock potential. For $Z=92$, the larger differences between G and FR or FR* values of up to about 14 eV, which are seen to occur for levels involving s orbitals, may be due principally to numerical error in our calculations of the small component for s orbitals. However, the percentage error in energies is very small and the corresponding numerical error in line strengths or collision strengths is probably

TABLE III. Comparison of energies (in eV) for excited-state levels relative to the ground-state level for neonlike barium. Notation is as in Table I.

Upper Level	QR	FR	FR*	G	G**	R	HFR
$(2p_{3/2}3s_{1/2})_2$	4571.18	4567.06	4568.29	4568.06	4561.76	4560.42	4560.43
$(2p_{3/2}3s_{1/2})_1$	4576.99	4572.80	4574.02	4573.73	4567.56	4566.23	4565.85
$(2p_{3/2}3p_{1/2})_1$	4666.86	4664.61	4665.76	4665.55	4659.72	4657.62	4656.63
$(2p_{3/2}3p_{1/2})_2$	4670.12	4667.81	4668.95	4668.73	4662.09	4660.00	4659.58
$(2p_{3/2}3p_{3/2})_1$	4774.11	4770.49	4771.67	4771.40	4763.48	4761.68	4763.16
$(2p_{3/2}3p_{3/2})_3$	4774.34	4770.71	4771.89	4771.64	4763.36	4761.61	4763.34
$(2p_{3/2}3p_{3/2})_2$	4782.35	4778.78	4779.94	4779.65	4772.15	4770.32	4770.88
$(2p_{3/2}3p_{3/2})_0$	4819.73	4816.76	4817.89	4816.01	4809.22	4808.93	4805.62
$(2p_{3/2}3d_{3/2})_0$	4884.83	4881.37	4882.63	4882.24	4875.35	4873.33	4872.92
$(2p_{3/2}3d_{3/2})_1$	4892.26	4888.77	4890.01	4889.84	4881.84	4879.62	4879.78
$(2p_{3/2}3d_{3/2})_3$	4896.92	4893.38	4894.59	4894.29	4885.46	4883.10	4883.88
$(2p_{3/2}3d_{3/2})_2$	4900.18	4896.78	4897.99	4897.69	4889.71	4887.57	4886.97
$(2p_{3/2}3d_{5/2})_4$	4918.53	4914.34	4915.59	4915.22	4905.51	4903.30	4905.56
$(2p_{3/2}3d_{5/2})_2$	4922.17	4917.98	4919.22	4918.89	4909.82	4907.74	4908.97
$(2p_{3/2}3d_{5/2})_3$	4929.49	4925.29	4926.50	4926.19	4917.31	4914.98	4915.88
$(2p_{3/2}3d_{5/2})_1$	4951.05	4946.39	4947.52	4946.82	4936.89	4935.39	4936.24
$(2p_{1/2}3s_{1/2})_0$	4974.76	4964.58	4965.96	4965.48	4954.47	4954.00	4966.05
$(2p_{1/2}3s_{1/2})_1$	4979.40	4969.57	4970.91	4970.34	4959.21	4958.59	4969.92
$(2p_{1/2}3p_{1/2})_1$	5071.02	5062.65	5063.95	5063.49	5051.74	5050.46	5063.09
$(2p_{1/2}3p_{1/2})_0$	5102.70	5095.66	5096.91	5095.13	5084.47	5084.42	5090.50
$(2p_{1/2}3p_{3/2})_1$	5177.56	5168.00	5169.32	5168.81	5156.48	5155.47	5168.97
$(2p_{1/2}3p_{3/2})_2$	5181.69	5171.93	5173.25	5172.74	5159.60	5158.60	5172.71
$(2p_{1/2}3d_{3/2})_2$	5299.18	5289.82	5291.19	5290.59	5276.93	5275.65	5288.08
$(2s_{1/2}3s_{1/2})_1$	5297.76	5294.64	5295.60	5295.40	5283.65	5281.48	5288.71
$(2p_{1/2}3d_{3/2})_1$	5318.10	5308.73	5310.00	5309.32	5295.02	5293.80	5306.81
$(2s_{1/2}3s_{1/2})_0$	5316.08	5314.25	5315.18	5314.46	5303.32	5301.43	5306.07
$(2p_{1/2}3d_{5/2})_2$	5325.01	5314.93	5316.32	5315.70	5301.58	5300.33	5313.56
$(2p_{1/2}3d_{5/2})_3$	5328.34	5318.18	5319.55	5318.94	5304.72	5303.24	5316.98
$(2s_{1/2}3p_{1/2})_0$	5393.44	5392.29	5393.16	5392.96	5381.70	5378.73	5384.62
$(2s_{1/2}3p_{1/2})_1$	5396.40	5395.14	5396.01	5395.82	5383.95	5380.94	5387.29
$(2s_{1/2}3p_{3/2})_2$	5501.20	5498.66	5499.56	5499.34	5486.22	5483.44	5491.58
$(2s_{1/2}3p_{3/2})_1$	5505.64	5503.06	5503.95	5503.67	5490.44	5487.70	5495.72
$(2s_{1/2}3d_{3/2})_1$	5617.64	5615.48	5616.42	5616.18	5602.84	5599.90	5606.48
$(2s_{1/2}3d_{3/2})_2$	5622.14	5619.86	5620.79	5620.55	5606.39	5603.47	5610.72
$(2s_{1/2}3d_{5/2})_3$	5643.65	5640.67	5641.64	5641.32	5626.31	5623.52	5632.19
$(2s_{1/2}3d_{5/2})_2$	5655.49	5652.44	5653.34	5653.03	5638.65	5635.80	5643.39

much less than 1%. The fact that we have been able to reproduce exact relativistic hydrogen line strengths for $Z=90$, even for the $1s_{1/2}$-$2p_{1/2}$ and $1s_{1/2}$-$2p_{3/2}$ transitions, to much better than 1% would appear to confirm this.

Experimental values for the energies of many of these levels have been obtained for neonlike ions with Z values in the vicinity of 56 by Beiersdorfer *et al.*[20] and compared with values by the program of Grant *et al.*[5] with QED, Breit, and finite-nuclear-size contributions included. The discrepancies found between theory and experiment were generally of the order of 1 or 2 eV, which is of the same order as the differences between FR, FR*, and G results, and is considerably less than the difference between G and G^{**} results. Thus it appears that the accuracy of our fully relativistic approach is sufficient to war-

TABLE IV. Comparison of energies (in eV) for excited-state levels relative to the ground-state level for neonlike ions with $Z=92$. Notation as in Table I.

Upper Level	QR	FR	FR*	G	G**	HFR
$(2p_{3/2}3s_{1/2})_2$	12890.5	12871.4	12872.7	12877.1	12860.3	12596.1
$(2p_{3/2}3s_{1/2})_1$	12901.9	12882.4	12883.7	12888.1	12872.0	12607.0
$(2p_{3/2}3p_{1/2})_1$	13103.6	13096.7	13097.9	13097.8	13075.8	12777.8
$(2p_{3/2}3p_{1/2})_2$	13108.8	13101.6	13102.8	13102.6	13075.9	12782.2
$(2p_{3/2}3p_{3/2})_1$	14221.9	14204.2	14205.5	14206.0	14167.0	13971.4
$(2p_{3/2}3p_{3/2})_3$	14222.1	14204.5	14205.8	14206.0	14165.4	13971.6
$(2p_{3/2}3p_{3/2})_2$	14236.5	14219.1	14220.4	14220.7	14184.1	13985.4
$(2p_{3/2}3p_{3/2})_0$	14308.2	14295.4	14296.6	14294.9	14262.7	14051.1
$(2p_{3/2}3d_{3/2})_0$	14426.5	14409.6	14411.0	14411.4	14378.5	14092.2
$(2p_{3/2}3d_{3/2})_1$	14445.8	14428.6	14430.0	14430.5	14391.1	14109.3
$(2p_{3/2}3d_{3/2})_3$	14448.5	14431.2	14432.5	14432.8	14389.5	14111.4
$(2p_{3/2}3d_{3/2})_2$	14454.9	14438.4	14439.8	14440.1	14401.6	14117.4
$(2p_{3/2}3d_{5/2})_4$	14688.2	14667.0	14668.4	14668.4	14619.9	14359.5
$(2p_{3/2}3d_{5/2})_2$	14694.8	14673.6	14675.0	14675.3	14630.5	14365.7
$(2p_{3/2}3d_{5/2})_3$	14707.9	14686.6	14688.0	14688.2	14644.2	14378.1
$(2p_{3/2}3d_{5/2})_1$	14746.7	14725.1	14726.3	14726.3	14679.0	14413.5
$(2p_{1/2}3s_{1/2})_0$	16886.6	16820.4	16822.3	16828.3	16764.8	16836.6
$(2p_{1/2}3s_{1/2})_1$	16893.0	16826.6	16828.5	16834.4	16768.1	16842.7
$(2p_{1/2}3p_{1/2})_1$	17097.8	17043.4	17045.2	17046.6	16970.0	17020.1
$(2p_{1/2}3p_{1/2})_0$	17158.1	17110.9	17112.7	17112.7	17043.1	17065.9
$(2s_{1/2}3s_{1/2})_1$	17581.0	17561.9	17563.1	17553.4	17458.5	17504.6
$(2s_{1/2}3s_{1/2})_0$	17623.7	17612.1	17613.3	17602.8	17511.8	17463.9
$(2s_{1/2}3p_{1/2})_0$	17797.9	17790.7	17791.8	17777.4	17678.0	17648.3
$(2s_{1/2}3p_{1/2})_1$	17801.8	17794.3	17795.4	17781.0	17676.1	17651.2
$(2p_{1/2}3p_{3/2})_1$	18222.1	18158.1	18160.0	18161.9	18077.5	18217.7
$(2p_{1/2}3p_{3/2})_2$	18225.3	18160.9	18162.8	18164.7	18076.0	18220.3
$(2p_{1/2}3d_{3/2})_2$	18444.4	18382.1	18384.0	18385.8	18295.1	18351.6
$(2p_{1/2}3d_{3/2})_1$	18474.8	18411.9	18413.8	18415.6	18322.5	18385.8
$(2p_{1/2}3d_{5/2})_2$	18692.5	18626.1	18628.1	18629.7	18535.9	18605.9
$(2p_{1/2}3d_{5/2})_3$	18697.7	18630.9	18632.9	18634.5	18540.2	18612.8
$(2s_{1/2}3p_{3/2})_2$	18918.5	18901.1	18902.3	18888.4	18772.9	18843.4
$(2s_{1/2}3p_{3/2})_1$	18926.8	18909.2	18910.4	18896.5	18781.0	18850.5
$(2s_{1/2}3d_{3/2})_1$	19135.3	19119.8	19121.1	19107.3	18991.6	18974.5
$(2s_{1/2}3d_{3/2})_2$	19145.6	19129.5	19130.7	19116.8	18996.4	18983.9
$(2s_{1/2}3d_{5/2})_3$	19383.4	19363.3	19364.6	19350.5	19225.5	19299.9
$(2s_{1/2}3d_{5/2})_2$	19399.4	19379.0	19380.3	19366.3	19244.7	19246.0

TABLE V. Comparison of oscillator strengths for Ni-like gadolinium. Notation is as in Table I except that now QR and FR results correspond to use of Eq. (29) and FR* results correspond to use of Eq. (30). Also H and Z designate results from Refs. 21 and 23, respectively.

Upper level	QR	FR	FR*	G	G^*	G^{**}	H	Z
$(3d_{3/2}4p_{1/2})_1$	0.110	0.111	0.112	0.110	0.109	0.111	0.121	0.111
$(3d_{5/2}4p_{3/2})_1$	0.286	0.281	0.286	0.274	0.274	0.273	0.305	0.275
$(3d_{3/2}4p_{3/2})_1$	0.033	0.033	0.034	0.032	0.032	0.032	0.036	0.033
$(3p_{3/2}4s_{1/2})_1$	0.374	0.372	0.373	0.357	0.356	0.362	0.384	0.357
$(3d_{5/2}4f_{5/2})_1$	0.014	0.015	0.015	0.011	0.011	0.011	0.016	0.014
$(3d_{5/2}4f_{7/2})_1$	1.092	1.054	1.075	1.082	1.075	1.059	1.09	1
$(3d_{3/2}4f_{5/2})_1$	6.448	6.471	6.489	6.142	6.119	6.123	6.65	6.38
$(3p_{1/2}4s_{1/2})_1$	0.043	0.041	0.042	0.045	0.045	0.043	0.047	
$(3p_{3/2}4d_{3/2})_1$	0.019	0.017	0.018	0.018	0.018	0.017	0.018	
$(3p_{3/2}4d_{5/2})_1$	1.134	1.129	1.126	1.076	1.070	1.060	1.11	
$(3p_{1/2}4d_{3/2})_1$	0.559	0.545	0.544	0.525	0.523	0.511	0.553	
$(3s_{1/2}4p_{1/2})_1$	0.024	0.031	0.031	0.030	0.030	0.035	0.020	
$(3s_{1/2}4p_{3/2})_1$	0.148	0.147	0.147	0.140	0.139	0.138	0.143	

rant an option to include the dominant corrections, that is, the Breit and QED corrections. Then the accuracy should be sufficient for purposes such as line identification work for ions with $Z \gtrsim 2.5N$. However, since the effect of this on energies and mixing coefficients is small, this option should have little effect on collision strengths, which are usually less sensitive to slight changes in mixing coefficients than are f values.

B. Results for nickel-like ions

Nickel-like ions are similar to neonlike ions with a ground-state level having an outer closed $n=3$ shell in place of the closed $n=2$ shell for neonlike ions and they have also been of major interest for x-ray laser research, e.g., Refs. 3, 21, and 22. In Table V we compare results of our calculations of oscillator strengths with those by other approaches for Ni-like gadolinium ($Z=64$). It was thought to be too lengthy to include the energies for all 106 excited levels with $n=4$, but the wavelengths in angstroms for the transitions considered in Table V are given in Table VI. We note that in Table V rows and columns have been interchanged, as compared with Table I, for economy of space.

Again the upper levels are ordered according to energy and are designated by the basis state, making the dominant contribution using the analogs of Eqs. (25)–(27). For example,

$$(3d_{3/2}4f_{5/2})_1=(1s_{1/2}^2 2s_{1/2}^2 2p_{1/2}^2 2p_{3/2}^4 3s_{1/2}^2 3p_{1/2}^2 3p_{3/2}^4 3d_{3/2}^3 3d_{5/2}^6 4f_{5/2})_1 \ . \tag{28}$$

The symbols designating the various sets of data in Tables V and VI have the same meanings as in Tables I–IV, except that now QR and FR results correspond to using the mean configuration

$$1s_{1/2}^2 2s_{1/2}^2 2p_{1/2}^2 2p_{3/2}^4 3s_{1/2}^{1.9} 3p_{1/2}^{1.9} 3p_{3/2}^{3.8} 3d_{3/2}^{3.8} 3d_{5/2}^{5.7} 4s_{1/2}^{0.12} 4p_{1/2}^{0.12} 4p_{3/2}^{0.13} 4d_{3/2}^{0.13} 4d_{5/2}^{0.13} 4f_{5/2}^{0.13} 4f_{7/2}^{0.14} \tag{29}$$

TABLE VI. Comparison of wavelengths (in Å) for nickel-like gadolinium. Notation as in Table V except that λ(expt) represents the experimental results of Ref. 24.

Upper level	λ(QR)	λ(FR)	λ(FR*)	λ(G)	λ(G^{**})	λ(H)	λ(Z)	λ(expt)
$(3d_{3/2}4p_{1/2})_1$	10.897	10.910	10.893	10.899	10.905	10.906	10.87	10.90
$(3d_{5/2}4p_{3/2})_1$	10.760	10.769	10.753	10.759	10.763	10.764	10.73	10.75
$(3d_{3/2}4p_{3/2})_1$	10.465	10.481	10.465	10.471	10.482	10.476	10.45	10.47
$(3p_{3/2}4s_{1/2})_1$	8.982	8.995	8.986	8.986	8.996	8.982	8.98	9.01
$(3d_{5/2}4f_{5/2})_1$	8.874	8.883	8.871	8.873	8.881	8.880	8.76	
$(3d_{5/2}4f_{7/2})_1$	8.758	8.769	8.757	8.761	8.770	8.766	8.75	8.77
$(3d_{3/2}4f_{5/2})_1$	8.495	8.507	8.498	8.509	8.522	8.506	8.49	8.54
$(3p_{1/2}4s_{1/2})_1$	8.088	8.109	8.101	8.102	8.119	8.096		
$(3p_{3/2}4d_{3/2})_1$	7.671	7.679	7.673	7.673	7.684	7.678		
$(3p_{3/2}4d_{5/2})_1$	7.609	7.619	7.613	7.613	7.625	7.618		
$(3p_{1/2}4d_{3/2})_1$	7.000	7.014	7.008	7.009	7.025	7.013		
$(3s_{1/2}4p_{1/2})_1$	6.901	6.905	6.900	6.900	6.914	6.917		
$(3s_{1/2}4p_{3/2})_1$	6.721	6.726	6.721	6.722	6.736	6.738		

TABLE VII. Comparison of present quasirelativistic (QR) and fully relativistic (FR) values for oscillator strengths and energies relative to the ground level for Ni-like ions with Z=92. Notation as in Table V.

Upper level	f QR	f FR	f FR*	ΔE (eV) QR	ΔE (eV) FR	ΔE (eV) FR*
$(3d_{3/2}4p_{1/2})_1$	0.1914	0.1876	0.1892	3032.5	3028.3	3029.9
$(3d_{5/2}4p_{3/2})_1$	0.2608	0.2542	0.2565	3169.6	3166.1	3167.7
$(3d_{3/2}4p_{3/2})_1$	0.0074	0.0074	0.0074	3362.7	3355.2	3357.0
$(3p_{3/2}4s_{1/2})_1$	0.4224	0.4132	0.4151	3413.1	3405.7	3407.0
$(3d_{5/2}4f_{5/2})_1$	0.0011	0.0008	0.0008	3654.1	3648.9	3650.6
$(3d_{5/2}4f_{7/2})_1$	3.3999	3.3643	3.3832	3716.6	3710.4	3712.0
$(3d_{3/2}4f_{5/2})_1$	5.0765	5.0714	5.0797	3891.4	3882.3	3883.9
$(3p_{3/2}4d_{3/2})_1$	0.1111	0.1061	0.1061	4095.9	4089.2	4090.4
$(3p_{3/2}4d_{5/2})_1$	1.4012	1.3875	1.3858	4168.9	4160.8	4162.0
$(3p_{1/2}4s_{1/2})_1$	0.0489	0.0467	0.0471	4358.6	4340.8	4342.4
$(3s_{1/2}4p_{1/2})_1$	0.2530	0.2464	0.2465	4849.8	4846.7	4848.0
$(3p_{1/2}4d_{3/2})_1$	0.3471	0.3354	0.3347	5050.4	5033.4	5034.9
$(3s_{1/2}4p_{3/2})_1$	0.0993	0.0961	0.0960	5189.0	5182.8	5184.2

in determining the central potential with Eqs. (16)–(18), while FR* corresponds to our fully relativistic results obtained using

$$1s_{1/2}^{2}2s_{1/2}^{2}2p_{1/2}^{2}2p_{3/2}^{4}3s_{1/2}^{1.95}3p_{1/2}^{1.95}3p_{3/2}^{3.9}3d_{3/2}^{3.9}3d_{5/2}^{5.8}4s_{1/2}^{0.07}4p_{1/2}^{0.07}4p_{3/2}^{0.07}4d_{3/2}^{0.07}4d_{5/2}^{0.07}4f_{5/2}^{0.07}4f_{7/2}^{0.08} \tag{30}$$

in determining the central potential. The sets of values labeled by H and Z refer to results from Refs. 21 and 23, while the experimental wavelengths are from Ref. 24. One sees that, in general, the agreement between the various sets of results is good and there are no special surprises as compared with the analogous results for neonlike ions discussed rather thoroughly previously. The one noticeable difference is that, since the results for Ni-like ions correspond to one additional step upward in n values, the relativistic effects are less pronounced than for neonlike ions of corresponding Z. Hence, the Breit and QED corrections are less important than for neonlike ions and the effect of a finite nuclear size is essentially negligible for $Z=64$. Also one would expect QR results to be better for Ni-like ions. Partly for this reason we give QR, FR, and FR* results for f values and the corresponding transition energies in Table VII for $Z=92$. Results by the program by Grant *et al.*[5] could not be included because we were unable to get the program to converge for this case. As expected, FR and FR* results are very close and one sees that indeed the QR and FR results are also close with a maximum deviation of only 4.7% for f values, except for the very weak transition to the $(3d_{5/2}4f_{5/2})_1$ level. Thus it appears that the QR approach is quite a good approximation for highly charged Ni-like ions with essentially any value of Z.

IV. SUMMARY AND CONCLUSIONS

A relatively simple Dirac-Fock-Slater atomic-structure approach and associated computer programs have been developed for the purpose of rapidly providing the atomic-structure results required for large-scale, rapid calculations of the atomic data for ions with $Z>2N$ needed for the modeling of high-temperature plasmas such as those in x-ray laser research. For this regime the approach appears to be very accurate, as well as rapid, from comparisons of oscillator strengths and energies with results by other more elaborate approaches. In fact, it appears to be sufficiently accurate to warrant an option to include the Breit interaction and the vacuum polarization and self-energy QED corrections, which we plan on doing in a future work. However, we expect this to have little effect on collision strengths and, since it would increase the computing time, we would probably usually not use this option in generating the atomic-structure data for collision strengths, which is the main objective of our work. We have also developed a slightly more rapid quasirelativistic approximation to the present approach that appears to be quite accurate even for very high Z, especially for Ni-like ions. However, since it saves only about 5% or 10% in computer time, it appears to be of little practical value, except when coupled with an additional approximation in determining collision strengths, as discussed in Sec. II D of the accompanying paper.[8]

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