Fully relativistic and quasirelativistic distorted-wave methods for calculating collision strengths for highly charged ions

Hong Lin Zhang, Douglas H. Sampson, and Ajaya K. Mohanty*

Department of Astronomy, The Pennsylvania State University, University Park, Pennsylvania 16802

(Received 26 October 1988; revised manuscript received 6 February 1989)

A rapid fully relativistic distorted-wave method for calculating collision strengths for highly charged ions is described. A more rapid quasirelativistic approximation in which the average over j value -1 is used for the relativistic quantum number κ for the free electrons is also discussed. Very rapid, but accurate, procedures for obtaining results for a given class of transitions for a large portion of an isoelectronic sequence by using fits to Z after making detailed calculations for only a few values of Z are described. Results by the present methods are compared with more elaborate relativistic distorted-wave calculations by other workers, principally for neonlike and nickel-like ions, but also comparisons for He-like, Li-like, and Na-like ions are discussed. In addition, comparisons with a few experimental results for neonlike barium could be made. Generally very good agreement is obtained with all these data.

I. INTRODUCTION

The purpose of the present paper is to develop a very rapid, but accurate approach for calculating electron-impact cross sections or, equivalently, collision strengths, for excitation of highly charged ions with moderate to very high values for the nuclear charge number Z. The motivation for the work is to provide the immense amount of collision data needed for applications to very-high-temperature plasmas. In such plasmas, often ions of very high Z are of interest, especially in the plasmas involved in research to develop x-ray lasers.[1] For $Z \gtrsim 30$, relativistic effects have a significant effect on the radial functions, so that a relativistic approach, i.e., an approach based on the Dirac equation, is desirable, rather than simply treating all relativistic effects as a perturbation. However, due to the dependence of the radial functions on j in a fully relativistic treatment, there is about an order of magnitude more scattering radial matrix elements than in a nonrelativistic treatment, and it is the number of these quantities that principally determines the length of the calculations. Even in a nonrelativistic treatment the calculations tend to be lengthy, because in order to determine the collision rate, the cross section or collision strength must be known for several impact-electron energies, and for each energy one must determine the scattering matrix elements for many initial and final values for the angular momenta of the free electron. In addition, particularly for relatively high-density plasmas, such as the laser-produced plasmas used in x-ray laser research, transitions between excited states are important so that collision rates for thousands of transitions are sometimes needed for treating a particular case (single Z value) and many values of Z are of interest. Thus there is an acute need for the development of very rapid, accurate relativistic collision-strength approaches, as we attempt to do here. It should be mentioned that several rather elaborate fully relativistic distorted-wave pro-

grams now exist.[2-4] A new, very rapid program using a relativistic treatment of the bound electrons and a nonrelativistic treatment of the free electrons[5] is most like the present one in the emphasis on speed and similarity of some techniques. The present approach is designed for moderate to very high-Z ions satisfying $Z > 2N$, where N is the number of bound electrons per ion. It uses the atomic structure provided by the program described in the accompanying paper.[6] We note that some preliminary results for neonlike ions obtained with the quasirelativistic version of the present approach have been reported in Ref. 7.

In Sec. II the theory of the present approach is outlined. Then in Sec. III, results obtained with it are compared with results calculated by more elaborate procedures. These comparisons are made principally for neonlike and nickel-like ions, but comparisons for He-like, Li-like, and Na-like ions are also discussed. In the case of neonlike barium, comparison could also be made with a few experimental results.

II. OUTLINE OF THEORY

A. General features

In outlining the theory of the present work we will sometimes refer to equations in the closely related accompanying paper[6] on relativistic atomic structure. In doing so Eq. (X) of that paper will be called Eq. (I.X).

The relativistic cross section $Q(i\text{-}f)$ for the transition $i\text{-}f$ can be expressed in terms of the collision strength $\Omega(i\text{-}f)$ by the relation

$$Q(i\text{-}f) = \frac{\pi a_0^2}{k^2 g_i} \Omega(i\text{-}f) , \tag{1}$$

where a_0 is the Bohr radius, k is the relativistic wave number of the impact electron, and g_i is the statistical weight of the initial level of the N-electron target ion.

The relation between k, the relativistic momentum p, and kinetic energy ε of the impact electron is

$$k^2 = \frac{p^2 a_0^2}{\hbar^2} = \varepsilon \left[1 + \frac{\alpha^2}{4} \varepsilon \right] , \qquad (2)$$

where α is the fine-structure constant $e^2/(\hbar c)$ and ε is in rydbergs. For the highly charged ions of interest here, unitarization should be unnecessary. Then the relativistic distorted-wave expression for the collision strength can be written

$$\Omega(i\text{-}f) = 8 \sum_J (2J+1) \sum_{\kappa,\kappa'} \left| \left\langle \Psi_i \left| \sum_{\substack{q,k \\ q<k}}^{N+1} \frac{1}{r_{qk}} \right| \Psi_f \right\rangle \right|^2 , \qquad (3)$$

where κ and κ' are the initial and final relativistic quantum numbers for the free electron. Since the customary procedure of using unsubscripted quantum numbers for the free electron is being followed here, κ is related to the initial orbital and total angular momentum quantum numbers l and j for the free electron by Eqs. (I.3). Similarly, the relations

$$\kappa' = l', \quad j' = l' - \tfrac{1}{2}, \quad \kappa' = -(l'+1), \quad j' = l' + \tfrac{1}{2} \qquad (4)$$

apply for the final state of the free electron. The Ψ_i and Ψ_f in Eq. (3) are the initial and final antisymmetric wave functions for the total $(N+1)$-electron system consisting of the target ion plus the free electron. For example,

$$\Psi_i = \frac{1}{(N+1)^{1/2}} \sum_{p=1}^{N} (-1)^{N+1-p}$$

$$\times \sum_{M_t,m} C(J_t j M_t m ; JM) \Psi_{\beta_t J_t}(x_p^{-1})$$

$$\times u_{\varepsilon l j m}(x_p) , \qquad (5)$$

with an analogous expression applying for Ψ_f in which β_t', J_t'; M_t', ε', l', j', and m' replace the corresponding unprimed quantities. Here x_p designates the space and spin coordinates for electron p and x_p^{-1} means the space and spin coordinates of all the N electrons other than p. The $\Psi_{\beta_t J_t}$ and $\Psi_{\beta_t' J_t'}$ are the initial and final target-ion wave functions of the kind given by Eq. (I.4). The J_t and J_t' indicate the initial and final total momentum quantum numbers for the target ion, so they play the role

previously played by J in Ref. 6, while here J designates the total angular momentum quantum number for the entire $(N+1)$-electron system. The β_t and β_t' represent all quantum numbers, in addition to J_t and J_t', that are required to specify the initial and final states, respectively, of the target ion. The $u_{\varepsilon l j m}$ in Eq. (5) is the distorted-wave Dirac spinor or orbital for a free electron in a central potential $V(r)$ due to the target ion. In particular, analogous to Eq. (I.1),

$$u_{\varepsilon l j m}(x) \equiv u_{\varepsilon \kappa m} = \frac{1}{r} \begin{bmatrix} P_{\varepsilon \kappa}(r) & \chi_{\kappa m}(\theta,\phi,\sigma) \\ i Q_{\varepsilon \kappa}(r) & \chi_{-\kappa m}(\theta,\phi,\sigma) \end{bmatrix} , \qquad (6)$$

where the $\chi_{\kappa m}$ are the usual spin-angular-momentum functions given by Eq. (I.2), and the large and small components $P_{\varepsilon \kappa}$ and $Q_{\varepsilon \kappa}$ satisfy the coupled Dirac equations

$$\left[\frac{d}{dr} + \frac{\kappa}{r} \right] P_{\varepsilon \kappa} = \frac{\alpha}{2} \left[\varepsilon - V + \frac{4}{\alpha^2} \right] Q_{\varepsilon \kappa} \qquad (7)$$

and

$$\left[\frac{d}{dr} - \frac{\kappa}{r} \right] Q_{\varepsilon \kappa} = -\frac{\alpha}{2} (\varepsilon - V) P_{\varepsilon \kappa} . \qquad (8)$$

These are like Eqs. (I.10) and (I.11) for bound orbitals, except that ε is positive and is the kinetic energy of the electron in rydbergs when $r \to \infty$.

We note that the Ψ_i given by Eq. (5) has the same form as the wave function for an $(N+1)$-electron ion with an N-electron core and a single electron in a high subshell. An analogous statement applies for Ψ_f. Thus, as far as the angular part is concerned, the matrix element in Eq. (3) is of the same form[8] as occurs in atomic-structure calculations for an $(N+1)$-electron ion when one determines the off-diagonal matrix elements of the electron-electron electrostatic interaction prior to the diagonalization of the Hamiltonian. Therefore, in evaluating the right-hand side of Eq. (3), we could simply use the angular part of the relativistic atomic-structure code of Grant et al.,[9] except that a few modifications had to be made, such as allowing the outer electron (free electron in our case) to have much larger angular momenta than occur in ordinary atomic-structure calculations. Also the radial part is similar to that of atomic-structure calculations and takes the form of Slater integrals similar to Eq. (I.9). Specifically, there are "direct" terms

$$D^\lambda(n_a l_a j_a \varepsilon l j ; n_a' l_a' j_a' \varepsilon' l' j') = \int_0^\infty \int_0^\infty [P_{n_a l_a j_a}(r_1) P_{n_a' l_a' j_a'}(r_1) + Q_{n_a l_a j_a}(r_1) Q_{n_a' l_a' j_a'}(r_1)]$$

$$\times \frac{r_<^\lambda}{r_>^{\lambda+1}} [P_{\varepsilon l j}(r_2) P_{\varepsilon' l' j'}(r_2) + Q_{\varepsilon l j}(r_2) Q_{\varepsilon' l' j'}(r_2)] dr_1 dr_2 , \qquad (9)$$

and "exchange" terms

$$E^\lambda(n_a l_a j_a \varepsilon l j ; n_a' l_a' j_a' \varepsilon' l' j') = \int_0^\infty \int_0^\infty [P_{n_a l_a j_a}(r_1) P_{\varepsilon' l' j'}(r_1) + Q_{n_a l_a j_a}(r_1) Q_{\varepsilon' l' j'}(r_1)]$$

$$\times \frac{r_<^\lambda}{r_>^{\lambda+1}} [P_{\varepsilon l j}(r_2) P_{n_a' l_a' j_a'}(r_2) + Q_{\varepsilon l j}(r_2) Q_{n_a' l_a' j_a'}(r_2)] dr_1 dr_2 , \qquad (10)$$

where $r_<$ ($r_>$) is the lesser (greater) of r_1 and r_2. Here we made the dependence on l and j explicit partly because an approximation that removes the dependence of the free-electron radial functions on j, and hence reduces the number of radial integrals of the form given by Eqs. (9) and (10) by a factor of 4 (except when l and/or $l'=0$), will be considered later in Sec. II D.

In the evaluation of Eq. (3) it is assumed that all orbitals bound and free are orthogonal. This and a completely consistent treatment of exchange between bound and free electrons are automatically obtained in the present approach because the central potential used in Eqs. (7) and (8) is exactly the same as that used in Eqs. (I.10) and (I.11) for the bound electrons. That is, we use the same Dirac-Fock-Slater potential given by Eqs. (I.16)–(I.18) coupled with use of a mean configuration, such as the one given by Eq. (I.19), for both bound and free electrons.

B. Numerics of the free-electron radial functions

One can use Eq. (7) to substitute for $Q_{\varepsilon\kappa}$ in Eq. (8), thereby obtaining a second-order differential equation for $P_{\varepsilon\kappa}$ analogous to Eq. (I.12). However, for the continuum radial functions it is convenient to go a step further, following Hagelstein and Jung,[4] and make the substitution for $P_{\varepsilon\kappa}$

$$F_{\varepsilon\kappa}(r)=a_P^{-1/2}(r)P_{\varepsilon\kappa}(r) , \tag{11}$$

where

$$a_P(r)=\frac{\alpha}{2}\left[\varepsilon-V(r)+\frac{4}{\alpha^2}\right] . \tag{12}$$

Then one obtains

$$\frac{d^2}{dr^2}F_{\varepsilon\kappa}(r)+\omega(r)F_{\varepsilon\kappa}(r)=0 , \tag{13}$$

where

$$\omega(r)=a_P(r)a_Q(r)-\frac{l(l+1)}{r^2}-\frac{\kappa}{r}\frac{1}{a_P(r)}\frac{d}{dr}a_P(r)$$
$$-\frac{3}{4}\left[\frac{1}{a_P(r)}\frac{d}{dr}a_P(r)\right]^2+\frac{1}{2}\frac{1}{a_P(r)}\frac{d^2}{dr^2}a_P(r) , \tag{14}$$

in which

$$a_Q(r)=\frac{\alpha}{2}[\varepsilon-V(r)] . \tag{15}$$

In writing the second term on the right-hand side of Eq. (14), we used the fact that $\kappa(\kappa+1)=l(l+1)$. The advantage of solving Eq. (14) rather than the analog of Eq. (I.12) for the free electrons is that $\omega(r)$ does not depend on $F_{\varepsilon\kappa}$, in contrast to the effective potential in Eq. (I.12), which does depend on $P_{n\kappa}$. For bound orbitals, use of Eq. (I.12), rather than the analog of Eqs. (13) and (14), does not tend to increase the difficulty in obtaining a solution because the bound orbitals also enter the Dirac-Fock-Slater potential given by Eqs. (I.16)–(I.18), which must be determined self-consistently with the solution of Eq.

(I.12) anyway.

As in the solution of Eq. (I.12) discussed in the accompanying paper,[6] we separate out the nuclear contribution $-2Z/r$ to the central potential and evaluate its contribution to dV/dr and d^2V/dr^2, analytically. Also, we start out with the mesh size given by Eq. (I.15) and double the mesh size every 40 points until we stop at the largest Δr by this procedure that satisfies

$$\Delta r \leq \frac{1}{4\varepsilon_{max}^{1/2}} , \tag{16}$$

where ε_{max} is the largest energy (in rydbergs) being considered in the calculations. Then we continue with this fixed Δr, usually for a total of 1800 points. Although only every fourth point is used in calculating the radial-scattering matrix elements, Eq. (16) ensures that we have a sufficient number of points per cycle to obtain accuracy at large r, where the radial functions are approximately oscillatory. The appropriate normalization for the free-electron radial functions is considered in the Appendix and is given by Eq. (A20).

C. Procedures for minimizing the number of radial integrals

For most cases the length of the calculations of collision strengths is principally determined by the number of radial wave functions and radial matrix elements or integrals. Hence it is important to keep this number to a minimum. In addition to the other convenient aspects of using the same potential in determining the orbitals of all the electrons, this helps to minimize the number of radial integrals in treating complex ions. This occurs because, in contrast to some multiconfiguration treatments, the bound-electron contribution to Eqs. (9) and (10) is then the same for all transitions in which the same orbital transition $n_al_aj_a$-$n_a'l_a'j_a'$ enters, which can be very large for complex ions. Of course, the free-electron contribution to Eqs. (9) and (10) differs for each different initial and final free-electron energy. In order to minimize this effect we use the following procedure: In considering a given class of transitions, such as all the $n=2$ to $n=3$ transitions in neonlike ions, we calculate results for a fixed set of scattered-electron energies (usually six) beginning near zero and spanning the range needed to obtain accurate collision rates. For each of these we calculate results for three impact-electron energies spanning the range of transition energies for the class of transitions being considered. Then we interpolate on these three sets of results for Eqs. (9) and (10) to get the values for the correct transition energy for each particular transition in the complex ion. When the factorized form for the collision strength discussed in Sec. II E below is used, the interpolation is done on the Q^λ, see Eq. (17) below. Since the radial integrals and the Q^λ vary smoothly and quite slowly with energy, this procedure works very well and leads to a large reduction in the number of radial integrals occurring in the treatment of complex ions. This procedure, which was briefly described in Ref. 7, is similar to that used in Ref. 5. However, our interpolation method, which was taken from the program by Bottcher,[10] is a nonlinear scheme that may be superior to the

one used in Ref. 5 because, in contrast to Ref. 5, we never find it necessary to use more than three energy points to obtain numerical accuracy.

As is well known, the partial-wave contributions to Eq. (3) can be significant for very large values for the initial and final angular momenta of the free electron, especially for high impact-electron energies and optically allowed transitions with $\Delta n = 0$. Our procedure for optically allowed transitions, those for which the electric-dipole oscillator strength is nonzero, is to make detailed calculations out to some value $l = l_0$ and use the rapid Coulomb-Bethe approximation[11] for $l > l_0$, where l_0 is chosen to be about 10 for near-threshold energies for excitation from levels with $n \leq 2$ and slightly higher for excitation from higher levels. The value used for l_0 is increased as energy is increased, with a maximum value of 40 being used for very high impact-electron energies. In this approximation l_0 is assumed to be sufficiently large that exchange contributions can be neglected for $l > l_0$, and only the first nonvanishing matrix element of the expansion of the interaction between bound and free electrons, that is, the matrix element of the $r_< / r_>^2$ term, needs to be retained. Moreover, it is assumed that $r_<$ is the radial coordinate of the bound electron and $r_>$ is that of the free electron. Then the contribution from $l > l_0$ factors into a part proportional to the oscillator strength or line strength and a free electron part, e.g., Eqs. (38)–(48) of Ref. 12. For the former part we use the relativistic results calculated with the program of the accompanying paper,[6] but for the latter part we use the nonrelativistic result of Ref. 11. In order to test the accuracy of this procedure we did test cases in which results for collision strengths were calculated using appreciably different values for l_0 and compared. In addition, comparisons were made with results by the much more elaborate relativistic method of Refs. 3 and 13, in which the Coulomb-Bethe approximation is not used. Both of these kinds of comparisons indicate this procedure is accurate; however, eventually we expect to replace the nonrelativistic free-electron part of this procedure with the analogous part calculated relativistically. For transitions that occur only through exchange, the contribution from large l is insignificant. For other non-optically-allowed transitions, the ratio of partial wave contributions for successive l values becomes nearly constant for large l, so that we could use this ratio to estimate the contribution from $l > l_0$ as described in Ref. 14, e.g., Eqs. (10)–(12) of Ref. 14.

D. Quasirelativistic approach with $\kappa = -1$ for the free electrons

Using the quasirelativistic (QR) approach discussed in Sec. II D of Ref. 6 for the atomic-structure input and making the analogous QR approximation for the free electrons, we can calculate collision strengths in what we call the QR approximation. In this approximation the second term in each of the square brackets of Eqs. (9) and (10) is dropped and the P's are normalized as though they were the total radial functions. This normalization is that given by Eq. (I.21) for the bound electrons. The

analogous, appropriate normalization for the free electrons is given in the Appendix by Eq. (A23) if no additional approximations are made. However, for reasons analogous to those discussed in Sec. II D of Ref. 6, this QR approach only saves about 10% in computing time, and hence is of little practical value unless we make an additional approximation for the free electrons. In this approximation we use the average over j value, $\kappa = -1$, for the κ in Eq. (14). Then the free-electron radial functions become independent of j, which reduces the number of free-electron radial functions by approximately a factor of 2 and the number of radial integrals by approximately a factor of 4, and leads to a reduction in computing time by about a factor of 2.5. As discussed further in Sec. III, this procedure is quite accurate. One might expect that this would be the case because a summation over κ and κ' is, of course, equivalent to a summation over l, l', j, and j'. Thus, since j and j' are summed over in Eq. (3), one should expect that using the average over j value, $\kappa = -1$, would be a good approximation for the free electrons. The appropriate normalization for the free-electron radial functions in this case is given by Eqs. (A24) or (A25).

E. Factorization method and fitting to Z

Recently Bar-Shalom et al.[5] have made the important observation that, in general, the various 6-j and 9-j factors entering the exchange and direct scattering matrix elements can be arranged so they contain a common factor that can be factored out and summed over J. The collision strength then factors into the convenient form

$$\Omega = 8 \sum_{\substack{j_a, j'_a \\ j_{a1}, j'_{a1}}} \sum_{\lambda} B^\lambda(j_a j'_a, j_{a1} j'_{a1}) Q^\lambda(j_a j'_a, j_{a1} j'_{a1}) , \quad (17)$$

where we have used the abbreviations $j_a = n_a l_a j_a$, $j'_a = n'_a l'_a j'_a$, $j_{a1} = n_{a1} l_{a1} j_{a1}$, and $j'_{a1} = n'_{a1} l'_{a1} j'_{a1}$. Here the j_{a1} and j_a represent orbitals in the initial target-ion wave function, and j'_{a1} and j'_a orbitals in the final target-ion wave function. A convenient feature of Eq. (17) is that B^λ is a function only of the target-ion quantum numbers and the mixing coefficients plus λ, while the Q^λ contains the radial contribution and depends only on λ and the bound and free orbitals with the summations over the free-electron momenta performed within it.

Thus far, we have coded up the factorization technique only for excitation from the ground-state level of ions such as neonlike and nickel-like ions with closed-shell ground-state configurations. Then the B^λ factors in Eq. (17) take the very simple form of a product of mixing coefficients for the upper level times a $\delta_{\lambda J'_t}$ factor. For example, for excitation of neonlike ions from the ground-state level to an upper $n = 3$ level, U_i,

$$B^\lambda(j_a j'_a, j_{a1} j'_{a1}) = b[U_i, (2l_{a j_a} 3l'_{a j'_a})_{J'_t}]$$

$$\times b[U_i, (2l_{a1 j_{a1}} 3l'_{a1 j'_{a1}})_{J'_t}] \delta_{\lambda J'_t} , \quad (18)$$

where $b[U_i, (2l_{a j_a} 3l'_{a j'_a})_{J'_t}]$ is the mixing coefficient giving the contribution of the state $(2l_{a j_a} 3l'_{a j'_a})_{J'_t}$ to level U_i, and

we have used the abbreviations of Eqs. (I.25)–(I.27). Actually for cases such as this, where the angular part of the calculation is small, we found no improvement in speed using the factorization technique as compared with the usual treatment. However, Bar-Shalom et al.[5] emphasize that the value of the factorization technique is in treating cases, such as transitions between the excited levels with $n = 4$ in Ni-like and Cu-like ions, where there is a huge number of transitions involving a relatively small number of orbital transitions $n_a l_a j_a \text{-} n'_a l'_a j'_a$. Then in the usual treatment the calculations become very lengthy due to the lengthy angular part.

In addition to the great convenience and increase in speed by using the factorization method for such transitions, Eq. (17) is very convenient for another purpose not pointed out in Ref. 5. This is for making very rapid calculations of results for a given class of transitions for many members of an isoelectronic sequence simultaneously with the use of fits to Z. One cannot ordinarily make accurate fits of results for Ω to Z in the case of complex ions because the results can vary suddenly and abruptly as Z changes. The problem is with the mixing coefficients. However, when the factorized form is used, the mixing coefficients are separated off into the B^λ term, which can be treated as part of the atomic-structure part of the calculation. This part of the calculation is very rapid and, in addition, the Z fit procedure discussed in Sec. II E of Ref. 6 can be used. The remaining radial part, the Q^λ part, is much more lengthy to calculate, but the Q^λ's vary in a smooth way with Z. In fact, in the approximation used in much of our earlier work based on use of hydrogenic basis states, e.g., Ref. 15 and references therein, $Z^2 Q^\lambda$ would be independent of Z, and also N. Thus one would expect that fits of the Q^λ to N and Z could readily be made. Recently,[16] in work too lengthy to be included here, we have demonstrated that the latter can be done by considering the $n = 2$ to $n = 3$ and 4 transitions in neonlike ions. In that work, for each of the six values $Z = 22, 30, 42, 56, 74,$ and 92, detailed calculations are made for the same six scattered-electron energies ε_f in the range $0.008 \leq \varepsilon_f \leq 0.75$, where ε_f is in units of Z^2_{eff} Ry with $Z_{\text{eff}} = Z - 7.5$. In each case the Q^λ's are calculated for the three impact-electron energies ε_i in the same units $\varepsilon_i = \varepsilon_f + 0.13$, $\varepsilon_i = \varepsilon_f + 0.197$ and $\varepsilon_i = \varepsilon_f + 0.264$, where 0.13 and 0.264 span the range of transition energies. Then each Q^λ is fit to a power series in Z. These results are then used in Eq. (17) to compute values for Ω for all 71 values of Z in the range $22 \leq Z \leq 92$. In doing this, the values of the Q^λ for the exact energy of each transition are obtained by interpolation, as discussed in Sec. II C. In order to determine the accuracy of this fit procedure, we have made separate detailed calculations for the other Z values, $Z = 26, 36, 47, 64, 79,$ and 82. These indicate that this procedure is accurate to better than 1%. Since the fit procedure requires essentially no computing time, the time required for the calculations is essentially that required for the detailed calculations for the six Z values, and the length of the calculations for the 71 Z values is reduced by over a factor of 10 by this procedure.

III. NUMERICAL RESULTS AND DISCUSSION

Probably the most elaborate and accurate fully relativistic cross-section or collision-strength program presently operating is that of Kim and Desclaux[3] and Kim.[13] We have compared our fully relativistic (FR) results with theirs for numerous transitions involving the valence electron in Li-like ions with $Z = 28$ 54, and Na-like ions with $Z = 54$, for a wide range of impact-electron energies up to 10^4 eV. The agreement is very good, usually within 1% or 2% and the maximum discrepancy is 5.7%. Also, we could make comparison with relativistic distorted-wave results near threshold for excitation from the ground-state level to the $n = 2$ levels in He-like iron and krypton, calculated by Pindzola and Carter.[2] In this case the agreement is to within 5.8% and 3.4% for iron and krypton, respectively. Also, it is interesting to note that our oscillator strengths are to within better than 1% of either their length or velocity results for both iron and krypton. In all of these cases the agreement of our quasirelativistic results with those of these other workers is also good, almost as good as that of our FR results, the maximum discrepancy being about 7%.

By far the most extensive fully relativistic calculations of collision strengths or cross sections that have been published, and with which we next make comparisons, are the relativistic distorted-wave results for neonlike and nickel-like ions obtained with the program of Hagelstein and Jung.[4] In these cases there are large groups of upper states that mix, so the accuracy of the results depends on the accuracy of the mixing coefficients, as well as that of the radial-scattering matrix elements. This is in contrast to the simpler cases we have discussed, where there is no mixing at all in the case of Li-like and Na-like ions, and only the relatively simple mixing of the $(1s_{1/2}2p_{1/2})_1$ and $(1s_{1/2}2p_{3/2})_1$ states (or the $1s2p\ ^3P_1$ and $1s2p\ ^1P_1$ states) in He-like ions. We note that the program of Ref. 4 utilizes a mean configuration in determining the potential like we do, but otherwise uses a multiconfiguration relativistic Hartree-Fock or Dirac-Fock atomic-structure approach, rather than the simpler Dirac-Fock-Slater approach of Ref. 6 used here. Thus it is intermediate in complexity between our program and those of Refs. 2, 3, and 13, which use structure data from the elaborate multiconfiguration Dirac-Fock programs of Grant et al.[9] or Desclaux[17] and a rather sophisticated potential for the free electrons.

A. Results for neon-like ions

Results with the program of Hagelstein and Jung[4] have been given for neonlike ions with $Z = 36, 34, 39, 42,$ and 47 in Ref. 4, and for $Z = 56$ in Ref. 18. In Table I a comparison is made between our results for collision strengths and those of Ref. 4 for $Z = 26$ and 47. Also, for the higher Z values of 74 and 92, a comparison is made between our QR and FR results in order to establish the degree of validity of our QR approach for very high values of Z. The first and second entries for each transition are our QR results with $\kappa = -1$ for the free electrons calculated using the normalizations for the free-electron

TABLE I. Comparison of collision strengths for neonlike ions. Upper levels are designated by the state making the dominant contribution using the abbreviations of Eqs. (I.25)–(I.27). The first and second entries for each transition and Z value are the quasirelativistic results with $\kappa = -1$ for the free electrons obtained using the normalizations given by Eqs. (A24) and (A25), respectively. The third and fourth entries are fully relativistic results by the present approach and by Hagelstein and Jung (Ref. 4), respectively. The numbers in square brackets are powers of 10 by which adjacent entries should be multiplied.

Upper Level	$Z = 26$		$Z = 47$			$Z = 74$			$Z = 92$	
	$\varepsilon_f=100\,\mathrm{eV}$	$\varepsilon_f=2500\,\mathrm{eV}$	$\Delta E(\mathrm{eV})$	$\varepsilon_f=200\,\mathrm{eV}$	$\varepsilon_f=5000\,\mathrm{eV}$	$\Delta E(\mathrm{eV})$	$\varepsilon_f=500\,\mathrm{eV}$	$\varepsilon_f=30000\,\mathrm{eV}$	$\varepsilon_f=800\,\mathrm{eV}$	$\varepsilon_f=50000\,\mathrm{eV}$
$(2p_{3/2}\,3p_{3/2})0$	3.09[-3]	3.22[-3]	3243	6.29[-3]	7.08[-3]	8919	3.13[-3]	3.78[-3]	2.08[-3]	2.59[-3]
	3.11[-3]	3.25[-3]	3243	6.47[-3]	7.31[-3]	8919	3.38[-3]	4.16[-3]	2.35[-3]	3.00[-3]
	2.95[-3]	3.07[-3]	3241	6.52[-3]	7.42[-3]	8912	3.61[-3]	4.60[-3]	2.63[-3]	3.53[-3]
	2.73[-3]	2.93[-3]	3238	6.28[-3]	7.29[-3]					
$(2p_{1/2}\,3p_{1/2})0$	4.40[-2]	5.16[-2]	3373	6.07[-3]	6.84[-3]	9926	1.52[-3]	1.83[-3]	8.27[-4]	1.02[-3]
	4.43[-2]	5.20[-2]	3373	6.26[-3]	7.07[-3]	9926	1.66[-3]	2.03[-3]	9.52[-4]	1.21[-3]
	4.48[-2]	5.28[-2]	3370	6.54[-3]	7.44[-3]	9906	1.82[-3]	2.29[-3]	1.11[-3]	1.46[-3]
	4.16[-2]	5.10[-2]	3366	6.37[-3]	7.40[-3]					
$(2s_{1/2}\,3s_{1/2})0$	1.67[-2]	2.11[-2]	3543	4.40[-3]	5.22[-3]	10243	1.49[-3]	1.91[-3]	8.49[-4]	1.12[-3]
	1.68[-2]	2.13[-2]	3543	4.52[-3]	5.38[-3]	10243	1.61[-3]	2.10[-3]	9.65[-4]	1.30[-3]
	1.71[-2]	2.17[-2]	3542	4.76[-3]	5.71[-3]	10238	1.84[-3]	2.50[-3]	1.20[-3]	1.71[-3]
	1.56[-2]	2.05[-2]	3537	4.61[-3]	5.62[-3]					
$(2p_{3/2}\,3p_{1/2})1$	4.00[-3]	7.46[-4]	3159	6.41[-4]	2.25[-4]	8464	1.92[-4]	3.13[-5]	1.07[-4]	1.82[-5]
	4.03[-3]	7.53[-4]	3159	6.60[-4]	2.34[-4]	8464	2.09[-4]	3.51[-5]	1.23[-4]	2.17[-5]
	4.05[-3]	7.54[-4]	3158	6.68[-4]	2.34[-4]	8459	2.19[-4]	3.45[-5]	1.37[-4]	2.14[-5]
	3.75[-3]	7.45[-4]	3156	6.67[-4]	2.41[-4]					
$(2p_{3/2}\,3p_{3/2})1$	1.53[-3]	2.13[-4]	3208	5.94[-4]	2.03[-4]	8853	2.23[-4]	3.51[-5]	1.39[-4]	2.16[-5]
	1.55[-3]	2.16[-4]	3208	6.11[-4]	2.10[-4]	8853	2.41[-4]	3.92[-5]	1.56[-4]	2.55[-5]
	1.55[-3]	2.15[-4]	3206	6.17[-4]	2.10[-4]	8844	2.47[-4]	3.83[-5]	1.62[-4]	2.47[-5]
	1.43[-3]	2.06[-4]	3203	5.88[-4]	2.04[-4]					
$(2p_{1/2}\,3p_{1/2})1$	1.68[-3]	2.41[-4]	3346	4.72[-4]	1.54[-4]	9882	1.87[-4]	2.79[-5]	1.32[-4]	2.00[-5]
	1.69[-3]	2.43[-4]	3346	4.88[-4]	1.60[-4]	9882	2.06[-4]	3.16[-5]	1.56[-4]	2.47[-5]
	1.67[-3]	2.42[-4]	3342	4.72[-4]	1.57[-4]	9859	1.85[-4]	3.00[-5]	1.24[-4]	2.24[-5]
	1.56[-3]	2.31[-4]	3338	4.60[-4]	1.54[-4]					
$(2p_{1/2}\,3p_{3/2})1$	1.73[-3]	2.60[-4]	3394	5.87[-4]	2.02[-4]	10281	1.35[-4]	2.19[-5]	1.24[-4]	2.21[-5]
	1.75[-3]	2.62[-4]	3394	6.05[-4]	2.10[-4]	10281	1.47[-4]	2.48[-5]	1.42[-4]	2.65[-5]
	1.73[-3]	2.59[-4]	3389	5.91[-4]	2.06[-4]	10257	1.22[-4]	2.05[-5]	1.32[-4]	2.46[-5]
	1.56[-3]	2.44[-4]	3385	5.65[-4]	2.01[-4]					
$(2s_{1/2}\,3s_{1/2})1$	9.92[-4]	1.44[-4]	3528	2.57[-4]	8.02[-5]	10206	1.94[-4]	3.19[-5]	8.22[-5]	1.40[-5]
	1.00[-3]	1.46[-4]	3528	2.66[-4]	8.40[-5]	10206	2.11[-4]	3.60[-5]	9.52[-5]	1.71[-5]
	1.00[-3]	1.46[-4]	3526	2.70[-4]	8.47[-5]	10196	2.27[-4]	3.82[-5]	9.84[-5]	1.72[-5]
	9.17[-4]	1.38[-4]	3521	2.59[-4]	8.26[-5]					
$(2s_{1/2}\,3d_{3/2})1$	1.70[-3]	2.45[-4]	3746	4.80[-4]	1.55[-4]	10915	1.64[-4]	2.46[-5]	9.12[-5]	1.43[-5]
	1.71[-3]	2.46[-4]	3746	4.89[-4]	1.59[-4]	10915	1.73[-4]	2.65[-5]	9.89[-5]	1.61[-5]
	1.70[-3]	2.45[-4]	3744	4.84[-4]	1.57[-4]	10909	1.69[-4]	2.51[-5]	9.67[-5]	1.50[-5]
	1.74[-3]	2.51[-4]	3738	4.92[-4]	1.61[-4]					
$(2p_{3/2}\,3p_{1/2})2$	3.66[-3]	3.31[-3]	3162	1.01[-3]	9.63[-4]	8467	4.40[-4]	5.27[-4]	3.30[-4]	4.46[-4]
	3.68[-3]	3.32[-3]	3162	1.03[-3]	9.79[-4]	8467	4.64[-4]	5.55[-4]	3.57[-4]	4.83[-4]
	3.67[-3]	3.30[-3]	3161	1.03[-3]	9.64[-4]	8463	4.58[-4]	5.29[-4]	3.48[-4]	4.48[-4]
	3.73[-3]	3.50[-3]	3159	1.04[-3]	9.96[-4]					

TABLE I. (Continued).

Upper Level	Z = 26 ε_f=100eV	ε_f=2500eV	Z = 47 ΔE(eV)	ε_f=200eV	ε_f=5000eV	Z = 74 ΔE(eV)	ε_f=500eV	ε_f=30000eV	Z = 92 ε_f=800eV	ε_f=50000eV
$(2p_{3/2}3p_{3/2})_2$	2.98[-3]	3.26[-3]	3214	7.65[-4]	7.83[-4]	8864	2.82[-4]	3.53[-4]	1.79[-4]	2.39[-4]
	3.00[-3]	3.28[-3]	3214	7.81[-4]	7.96[-4]	8864	2.97[-4]	3.71[-4]	1.93[-4]	2.59[-4]
	3.01[-3]	3.27[-3]	3212	7.86[-4]	7.89[-4]	8856	3.00[-4]	3.59[-4]	1.96[-4]	2.46[-4]
	3.08[-3]	3.69[-3]	3210	8.03[-4]	8.44[-4]					
$(2p_{1/2}3p_{3/2})_2$	3.52[-3]	3.70[-3]	3397	8.41[-4]	7.37[-4]	10277	2.62[-4]	2.21[-4]	1.39[-4]	1.01[-4]
	3.54[-3]	3.72[-3]	3397	8.61[-4]	7.50[-4]	10277	2.82[-4]	2.34[-4]	1.58[-4]	1.11[-4]
	3.53[-3]	3.72[-3]	3392	8.54[-4]	7.47[-4]	10250	2.75[-4]	2.30[-4]	1.51[-4]	1.08[-4]
	3.60[-3]	4.17[-3]	3387	8.69[-4]	7.98[-4]					
$(2s_{1/2}3d_{3/2})_2$	2.86[-3]	4.82[-4]	3748	1.18[-3]	1.03[-3]	10923	6.82[-4]	1.15[-3]	4.01[-4]	7.57[-4]
	2.87[-3]	4.85[-4]	3748	1.19[-3]	1.05[-3]	10923	7.06[-4]	1.22[-3]	4.24[-4]	8.27[-4]
	2.86[-3]	4.71[-4]	3747	1.17[-3]	1.01[-3]	10917	6.82[-4]	1.17[-3]	4.02[-4]	7.77[-4]
	2.93[-3]	4.84[-4]	3740	1.18[-3]	1.02[-3]					
$(2s_{1/2}3d_{5/2})_2$	1.45[-2]	3.29[-2]	3767	4.30[-3]	7.49[-3]	11023	1.19[-3]	2.58[-3]	5.70[-4]	1.30[-3]
	1.45[-2]	3.30[-2]	3767	4.34[-3]	7.60[-3]	11023	1.22[-3]	2.72[-3]	5.99[-4]	1.42[-3]
	1.45[-2]	3.30[-2]	3766	4.33[-3]	7.58[-3]	11014	1.21[-3]	2.69[-3]	5.93[-4]	1.39[-3]
	1.42[-2]	3.32[-2]	3758	4.32[-3]	7.68[-3]					
$(2p_{3/2}3p_{3/2})_3$	4.30[-3]	6.35[-4]	3208	1.08[-3]	3.46[-4]	8853	3.73[-4]	5.29[-5]	2.21[-4]	3.13[-5]
	4.34[-3]	6.42[-4]	3208	1.11[-3]	3.59[-4]	8853	4.03[-4]	5.90[-5]	2.49[-4]	3.69[-5]
	4.36[-3]	6.41[-4]	3206	1.13[-3]	3.61[-4]	8844	4.20[-4]	5.77[-5]	2.67[-4]	3.58[-5]
	4.10[-3]	6.15[-4]	3203	1.10[-3]	3.58[-4]					
$(2s_{1/2}3d_{5/2})_3$	3.95[-3]	5.67[-4]	3757	1.10[-3]	3.54[-4]	11008	3.63[-4]	5.35[-5]	1.94[-4]	2.98[-5]
	3.96[-3]	5.70[-4]	3757	1.12[-3]	3.62[-4]	11008	3.81[-4]	5.76[-5]	2.10[-4]	3.35[-5]
	3.96[-3]	5.66[-4]	3755	1.11[-3]	3.55[-4]	11000	3.76[-4]	5.29[-5]	2.07[-4]	2.92[-5]
	4.06[-3]	5.83[-4]	3748	1.14[-3]	3.66[-4]					
$(2p_{1/2}3s_{1/2})_0$	3.02[-4]	5.82[-5]	3270	8.10[-5]	3.00[-5]	9738	2.93[-5]	5.52[-6]	1.97[-5]	3.68[-6]
	3.05[-4]	5.88[-5]	3270	8.39[-5]	3.12[-5]	9738	3.28[-5]	6.24[-6]	2.38[-5]	4.50[-6]
	3.01[-4]	5.84[-5]	3265	7.99[-5]	3.03[-5]	9710	2.95[-5]	5.90[-6]	2.08[-5]	4.25[-6]
	3.03[-4]	6.00[-5]	3262	8.01[-5]	3.09[-5]					
$(2p_{3/2}3d_{3/2})_0$	1.92[-3]	2.39[-4]	3297	5.32[-4]	1.59[-4]	9009	2.02[-4]	2.52[-5]	1.29[-4]	1.59[-5]
	1.93[-3]	2.40[-4]	3297	5.41[-4]	1.63[-4]	9009	2.12[-4]	2.71[-5]	1.39[-4]	1.78[-5]
	1.94[-3]	2.41[-4]	3295	5.47[-4]	1.64[-4]	9000	2.18[-4]	2.75[-5]	1.45[-4]	1.82[-5]
	2.00[-3]	2.46[-4]	3293	5.59[-4]	1.68[-4]					
$(2s_{1/2}3p_{1/2})_0$	2.42[-4]	4.52[-5]	3604	7.54[-5]	2.72[-5]	10360	3.16[-5]	5.09[-6]	2.11[-5]	3.44[-6]
	2.44[-4]	4.58[-5]	3604	7.81[-5]	2.83[-5]	10360	3.48[-5]	5.73[-6]	2.47[-5]	4.16[-6]
	2.43[-4]	4.56[-5]	3603	7.74[-5]	2.81[-5]	10357	3.48[-5]	5.81[-6]	2.57[-5]	4.43[-6]
	2.36[-4]	4.47[-5]	3597	7.71[-5]	2.82[-5]					
$(2p_{3/2}3s_{1/2})_1$	1.85[-3]	8.04[-3]	3089	4.41[-4]	1.33[-3]	8327	2.34[-4]	1.09[-3]	2.75[-4]	1.13[-3]
	1.86[-3]	8.07[-3]	3089	4.48[-4]	1.35[-3]	8327	2.43[-4]	1.14[-3]	2.89[-4]	1.21[-3]
	1.85[-3]	7.98[-3]	3087	4.42[-4]	1.32[-3]	8317	2.30[-4]	1.08[-3]	2.62[-4]	1.11[-3]
	1.96[-3]	8.90[-3]	3085	4.60[-4]	1.42[-3]					
$(2p_{1/2}3s_{1/2})_1$	1.65[-3]	6.55[-3]	3273	4.46[-4]	1.03[-3]	9742	9.64[-5]	1.68[-4]	5.97[-5]	1.03[-4]
	1.66[-3]	6.57[-3]	3273	4.56[-4]	1.04[-3]	9742	1.06[-4]	1.79[-4]	7.04[-5]	1.14[-4]
	1.66[-3]	6.61[-3]	3267	4.37[-4]	1.00[-3]	9714	1.00[-4]	1.74[-4]	6.53[-5]	1.10[-4]
	1.73[-3]	7.30[-3]	3264	4.56[-4]	1.08[-3]					

TABLE I. (Continued).

Upper Level	Z = 26		Z = 47			Z = 74			Z = 92	
	ϵ_f=100eV	ϵ_f=2500eV	ΔE(eV)	ϵ_f=200eV	ϵ_f=5000eV	ΔE(eV)	ϵ_f=500eV	ϵ_f=30000eV	ϵ_f=800eV	ϵ_f=50000eV
$(2p_{3/2}3d_{3/2})_1$	5.76[-3]	1.65[-3]	3302	1.31[-3]	3.87[-4]	9022	7.17[-4]	7.35[-4]	6.28[-4]	9.59[-4]
	5.78[-3]	1.66[-3]	3302	1.34[-3]	3.96[-4]	9022	7.48[-4]	7.76[-4]	6.68[-4]	1.04[-3]
	5.80[-3]	1.66[-3]	3300	1.34[-3]	3.94[-4]	9014	7.33[-4]	7.26[-4]	6.40[-4]	9.59[-4]
	5.98[-3]	1.69[-3]	3297	1.38[-3]	4.06[-4]					
$(2p_{3/2}3d_{5/2})_1$	2.53[-2]	6.09[-2]	3342	2.22[-2]	3.97[-2]	9159	9.81[-3]	2.42[-2]	6.17[-3]	1.58[-2]
	2.53[-2]	6.12[-2]	3342	2.25[-2]	4.03[-2]	9159	1.01[-2]	2.55[-2]	6.50[-3]	1.72[-2]
	2.44[-2]	5.88[-2]	3340	2.24[-2]	4.02[-2]	9149	1.01[-2]	2.54[-2]	6.42[-3]	1.71[-2]
	2.41[-2]	6.05[-2]	3336	2.24[-2]	4.09[-2]					
$(2p_{1/2}3d_{3/2})_1$	9.57[-2]	2.42[-1]	3508	1.54[-2]	2.77[-2]	10470	3.61[-3]	8.70[-3]	1.81[-3]	4.65[-3]
	9.60[-2]	2.43[-1]	3508	1.56[-2]	2.81[-2]	10470	3.74[-3]	9.19[-3]	1.92[-3]	5.09[-3]
	9.68[-2]	2.46[-1]	3503	1.56[-2]	2.80[-2]	10445	3.60[-3]	8.75[-3]	1.88[-3]	4.92[-3]
	9.39[-2]	2.49[-1]	3497	1.54[-2]	2.83[-2]					
$(2s_{1/2}3p_{1/2})_1$	9.43[-4]	1.88[-3]	3606	4.70[-4]	1.05[-3]	10361	7.39[-4]	2.35[-3]	3.14[-4]	1.02[-3]
	9.50[-4]	1.89[-3]	3606	4.80[-4]	1.06[-3]	10361	7.67[-4]	2.47[-3]	3.37[-4]	1.11[-3]
	9.39[-4]	1.84[-3]	3605	4.74[-4]	1.06[-3]	10357	8.22[-4]	2.64[-3]	3.03[-4]	1.02[-3]
	9.57[-4]	2.00[-3]	3599	4.78[-4]	1.07[-3]					
$(2s_{1/2}3p_{3/2})_1$	2.25[-3]	1.33[-2]	3655	8.31[-4]	2.54[-3]	10757	2.18[-4]	1.18[-3]	6.82[-5]	4.39[-4]
	2.26[-3]	1.34[-2]	3655	8.42[-4]	2.58[-3]	10757	2.26[-4]	1.25[-3]	7.41[-5]	4.77[-4]
	2.27[-3]	1.34[-2]	3654	8.42[-4]	2.56[-3]	10750	2.25[-4]	1.21[-3]	7.45[-5]	4.52[-4]
	2.48[-3]	1.43[-2]	3648	8.65[-4]	2.63[-3]					
$(2p_{3/2}3s_{1/2})_2$	1.50[-3]	2.89[-4]	3085	3.75[-4]	1.46[-4]	8319	1.41[-4]	2.55[-5]	9.42[-5]	1.67[-5]
	1.51[-3]	2.92[-4]	3085	3.88[-4]	1.52[-4]	8319	1.54[-4]	2.84[-5]	1.07[-4]	1.95[-5]
	1.53[-3]	2.93[-4]	3082	4.04[-4]	1.54[-4]	8309	1.70[-4]	2.86[-5]	1.26[-4]	2.00[-5]
	1.53[-3]	3.03[-4]	3081	4.04[-4]	1.58[-4]					
$(2p_{3/2}3d_{5/2})_2$	7.38[-3]	8.81[-4]	3318	1.26[-3]	3.42[-4]	9118	5.06[-4]	5.59[-5]	3.13[-4]	3.39[-5]
	7.41[-3]	8.87[-4]	3318	1.29[-3]	3.50[-4]	9118	5.31[-4]	6.01[-5]	3.37[-4]	3.80[-5]
	7.43[-3]	8.86[-4]	3315	1.27[-3]	3.42[-4]	9107	5.24[-4]	5.60[-5]	3.30[-4]	3.40[-5]
	7.72[-3]	9.11[-4]	3312	1.29[-3]	3.47[-4]					
$(2p_{3/2}3d_{3/2})_2$	2.60[-3]	2.18[-4]	3309	1.05[-3]	2.72[-4]	9031	3.13[-4]	2.80[-5]	1.95[-4]	1.69[-5]
	2.61[-3]	2.19[-4]	3309	1.07[-3]	2.78[-4]	9031	3.29[-4]	3.03[-5]	2.12[-4]	1.90[-5]
	2.62[-3]	2.20[-4]	3307	1.08[-3]	2.80[-4]	9022	3.35[-4]	3.00[-5]	2.17[-4]	1.88[-5]
	2.76[-3]	2.27[-4]	3304	1.13[-3]	2.95[-4]					
$(2p_{1/2}3d_{3/2})_2$	3.00[-3]	2.88[-4]	3491	8.63[-4]	2.29[-4]	10443	2.96[-4]	3.19[-5]	1.67[-4]	1.86[-5]
	3.02[-3]	2.90[-4]	3491	8.80[-4]	2.34[-4]	10443	3.13[-4]	3.45[-5]	1.84[-4]	2.12[-5]
	2.99[-3]	2.87[-4]	3487	8.59[-4]	2.30[-4]	10417	2.91[-4]	3.25[-5]	1.60[-4]	1.92[-5]
	3.13[-3]	2.95[-4]	3481	8.86[-4]	2.36[-4]					
$(2p_{1/2}3d_{5/2})_2$	3.99[-3]	4.12[-4]	3503	1.36[-3]	3.87[-4]	10536	4.51[-4]	5.53[-5]	2.36[-4]	3.03[-5]
	4.01[-3]	4.15[-4]	3503	1.39[-3]	3.96[-4]	10536	4.76[-4]	5.97[-5]	2.57[-4]	3.42[-5]
	3.95[-3]	4.06[-4]	3497	1.35[-3]	3.83[-4]	10509	4.42[-4]	5.33[-5]	2.27[-4]	2.85[-5]
	4.12[-3]	4.15[-4]	3492	1.39[-3]	3.95[-4]					
$(2s_{1/2}3p_{3/2})_2$	1.17[-3]	2.23[-4]	3652	3.29[-4]	1.25[-4]	10751	1.10[-4]	2.09[-5]	5.96[-5]	1.28[-5]
	1.18[-3]	2.26[-4]	3652	3.41[-4]	1.30[-4]	10751	1.20[-4]	2.34[-5]	6.95[-5]	1.52[-5]
	1.19[-3]	2.26[-4]	3651	3.52[-4]	1.32[-4]	10744	1.33[-4]	2.39[-5]	8.36[-5]	1.60[-5]
	1.15[-3]	2.22[-4]	3644	3.48[-4]	1.32[-4]					
$(2p_{3/2}3d_{3/2})_3$	4.61[-3]	2.57[-3]	3307	1.28[-3]	9.43[-4]	9026	4.88[-4]	4.25[-4]	3.13[-4]	2.95[-4]
	4.63[-3]	2.58[-3]	3307	1.30[-3]	9.58[-4]	9026	5.09[-4]	4.49[-4]	3.34[-4]	3.21[-4]

TABLE I. (Continued).

Upper Level	Z = 26 ε_f=100eV	Z = 26 ε_f=2500eV	Z = 47 ΔE(eV)	Z = 47 ε_f=200eV	Z = 47 ε_f=5000eV	Z = 74 ΔE(eV)	Z = 74 ε_f=500eV	Z = 74 ε_f=30000eV	Z = 92 ε_f=800eV	Z = 92 ε_f=50000eV
$(2p_{3/2}3d_{5/2})_3$	4.63[-3]	2.55[-3]	3305	1.30[-3]	9.45[-4]	9017	5.12[-4]	4.29[-4]	3.37[-4]	3.00[-4]
	4.84[-3]	2.67[-3]	3301	1.33[-3]	9.72[-4]					
	3.23[-3]	2.78[-3]	3323	8.80[-4]	6.69[-4]	9128	3.23[-4]	2.80[-4]	2.00[-4]	1.89[-4]
	3.25[-3]	2.79[-3]	3323	8.94[-4]	6.79[-4]	9128	3.38[-4]	2.96[-4]	2.14[-4]	2.05[-4]
	3.25[-3]	2.80[-3]	3321	8.94[-4]	6.77[-4]	9118	3.36[-4]	2.94[-4]	2.12[-4]	2.03[-4]
	3.41[-3]	2.91[-3]	3317	9.23[-4]	6.94[-4]					
$(2p_{1/2}3d_{5/2})_3$	3.87[-3]	3.01[-3]	3505	1.07[-3]	7.67[-4]	10541	3.45[-4]	2.61[-4]	1.81[-4]	1.41[-4]
	3.88[-3]	3.02[-3]	3505	1.08[-3]	7.80[-4]	10541	3.62[-4]	2.76[-4]	1.96[-4]	1.54[-4]
	3.86[-3]	3.02[-3]	3500	1.06[-3]	7.73[-4]	10513	3.41[-4]	2.71[-4]	1.76[-4]	1.48[-4]
	4.04[-3]	3.17[-3]	3496	1.09[-3]	8.01[-4]					
$(2p_{3/2}3d_{5/2})_4$	6.48[-3]	6.79[-4]	3315	1.76[-3]	4.70[-4]	9113	6.36[-4]	6.69[-5]	3.92[-4]	4.05[-5]
	6.50[-3]	6.83[-4]	3315	1.79[-3]	4.81[-4]	9113	6.67[-4]	7.19[-5]	4.23[-4]	4.53[-5]
	6.51[-3]	6.79[-4]	3312	1.79[-3]	4.74[-4]	9102	6.64[-4]	6.64[-5]	4.18[-4]	3.98[-5]
	6.83[-3]	6.98[-4]	3308	1.84[-3]	4.89[-4]					

radial functions given by Eqs. (A24) and (A25), respectively. The third entries are our FR results and the fourth entries are the relativistic distorted-wave results of Ref. 4. The largest discrepancies tend to occur either near threshold or for relatively large energies. Thus, although a complete set of comparisons for all final electron energies ε_f considered by Hagelstein is available from the authors, in the interest of brevity only the results for the lowest and highest values of ε_f are given here. Also for similar reasons only results for two final electron energies, one very small and one rather large, are given for $Z = 74$ and 92. Moreover, in order to conserve additional space the transition energies for $Z = 26$ and 92 are not included because they are given in Tables II and IV of Ref. 6.

In making the calculations of the FR and QR values given in Table I, the mean configuration given by Eq. (I.20) was used in determining the potential. Perhaps Eq. (I.19) would have been a better choice, but it would have made little difference. Test calculations for $Z = 26$, where the effect should be largest, indicated use of Eq. (I.19) leads to collision strengths within 1% of those obtained with Eq. (I.20) in most cases. Considerably the largest deviation was about 4% near threshold for the fairly weak optically allowed transition to the $(2s_{1/2}3p_{3/2})_1$ level. We note that QR results without the further approximation $\kappa = -1$ for the free electrons are not included in the table. The reason for this is that this method is of little value because it saves only about 10% in computing time compared with the FR approach, and it is no more reliable than the QR approach with the additional approximation of $\kappa = -1$ for the free electrons, which saves about a factor of 2.5 in computing time compared with the FR approach. Thus, hereafter, when we discuss QR results we mean those obtained with the additional approximation of using $\kappa = -1$ in Eq. (14) for the free electrons.

Inspection of Table I indicates that the results are essentially as one should expect. Except for a very slight effect on mixing coefficients due to inclusion of the Breit interaction in the atomic-structure part of the programs of Ref. 4, the differences between their collision strengths and our FR results should be a consequence of the use of different electron-electron contributions to the potentials used in determining the radial functions. The importance of this should decrease as Z increases, and the magnitude of the electron-electron contribution decreases relative to the nuclear contribution. Indeed, the maximum discrepancy between our FR results and those of Ref. 4 decreases from about 11% for $Z = 26$ to about 7% for $Z = 47$, and the agreement of our FR values with those of Reed[18] obtained with the program of Ref. 4 for $Z = 56$ appears to be even somewhat better. In fact, the comparisons shown in Fig. 1, in which our FR results are hardly distinguishable from Reed's, are typical.

Also in the figure recent experimental results of Marrs et al.[19] are included. In addition, they give results for the sum of the three transitions to the even-parity levels with $J = 0$ for impact-electron energies of 5.7 and 8.2 keV. Our estimates by interpolation to these energies are that our FR values are about 2% above Reed's and are

about 6% above and 12% below the experimental values for 5.7 and 8.2 keV, respectively.

With regard to QR results, we expect them to be close to the FR values for low Z, where relativistic effects are not very important, so that use of QR approximations to these effects should introduce little error. As Z increases one expects the deviations of the QR values from the FR values to increase. Inspection of the results given in Table I indicates that this does generally occur. Nevertheless, the QR results with the normalization given by Eq. (A25) are seen to still be quite close to the FR values for $Z = 74$ and they are even within 25% of the FR results for $Z = 92$. In fact, for $Z = 92$ they are within 15% of the FR results for all but four transitions, three of which are very weak. The most significant deviations are from about 20 to 24 % for the moderately strong transition to the $(2s_{1/2}3s_{1/2})_0$ level.

We note that the QR results with the normalization of Eq. (A25) were not included in Fig. 1 because they are too close to the FR values. However, in one exceptional case for neonlike barium the QR results do differ by a large factor from our FR results and the relativistic re-
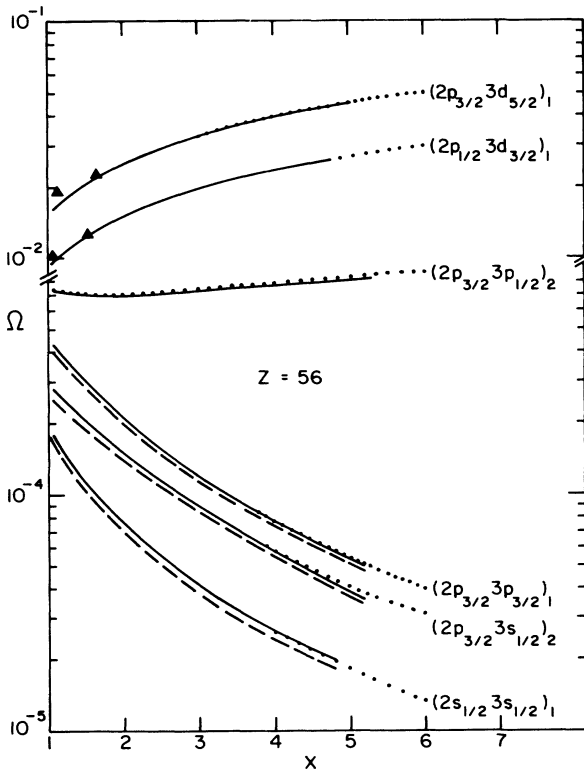
sults of Reed.[18] This is for excitation to the $(2p_{1/2}3s_{1/2})_1$ level, where the QR results are about 30% or 35% lower near threshold and approach a value more than 50% lower for high energies. As discussed in Sec. III A of the accompanying paper,[6] the upper level of this weak transition lies between the upper levels of two strong transitions. Hence, slight differences in the method of calculation can affect the mixing of the upper level of the weak transition with those of the strong transitions sufficiently to have a large effect on the oscillator strength and collision strength for the weak transition. In fact, probably our FR results and Reed's results are also appreciably in error for this transition, although less so than the QR results, because the corresponding oscillator strengths given in Table I of Ref. 6 differ appreciably from the result of the program by Grant et al.[9] with inclusion of the Breit interaction.

Finally we mention that our earlier results[20] for neonlike ions based on the use of hydrogenic basis states and screening constants are mostly within 15% or 20% of the present values for iron, with discrepancies of 30% or slightly more in a few cases. As Z increases and the nuclear contribution to the potential becomes more dominant, the agreement improves, but then, for $Z \gtrsim 50$, it decreases due presumably to the neglect of relativistic effects on the radial functions in Ref. 20. Thus, although the agreement is, for the most part, still quite good at $Z = 74$, the earlier results of Ref. 20 differ from the present FR values by amounts up to a factor of 2 or more in a few cases.

B. Results for nickel-like ions

We can also compare our results with those of Hagelstein[21] for nickel-like gadolinium $(Z = 64)$. This is done in Table II, where the four entries for each transition are obtained by the same approaches as the corresponding entries in Table I. In this case the potential used in our FR and QR calculations was determined using the mean configuration given by Eq. (I.29). Again, and for similar reasons to those discussed in connection with Table I, we give results only for two energies. Also, in the interest of brevity, we have given results only for excitation of a $3d_{3/2}$ or $3d_{5/2}$ electron, which are the cases of most practical interest; however, the comparisons for excitation of $3s_{1/2}$, $3p_{1/2}$, and $3p_{3/2}$ electrons to $n = 4$ levels and for all the energies considered by Hagelstein[21] are available upon request from the authors. It should be mentioned that here, as in the calculations discussed previously for neonlike ions, we have only included all the mixing among states in a complex, i.e., having the same set of n values, parity, and J value, in order to be consistent with the calculations with which comparisons were being made. However, as noted by Goldstein et al.,[22] the $n = 4$ levels with holes in the $3s$ and $3p$ subshells overlap in energy the $n = 5$ levels with holes in the $3d$ subshells. Thus it may be necessary to include mixing with the latter in order to obtain accurate results for excitation to some of the $n = 4$ levels.

One sees that the agreement between the present results and those of Hagelstein is generally good and is

FIG. 1. Comparison of collision strengths as a function of impact electron energy in threshold units X for various transitions in neonlike barium. Present FR results, ———; present QR results using Eq. (A24) for the normalization of the free-electron radial functions, — — —; relativistic distorted-wave results of Reed (Ref. 18) , . . . ; experimental results of Marrs et al. (Ref. 19), ▲.

TABLE II. Comparison of collision strengths for nickel-like ions with Z = 64. Abbreviations like that given by Eq. (I.28) are used in designating the upper levels. The first and second entries for each transition are the quasirelativistic results with $\kappa=-1$ for the free electrons obtained using the normalizations given by Eqs. (A24) and (A25), respectively. The third and fourth entries are fully relativistic results by the present approach and by Hagelstein (Ref. 21), respectively. The numbers in square brackets are powers of 10 by which adjacent entries should be multiplied.

Upper Level	ΔE(eV)	ε_f(eV) 160	ε_f(eV) 2500	Upper Level	ΔE(eV)	ε_f(eV) 160	ε_f(eV) 2500	Upper Level	ΔE(eV)	ε_f(eV) 160	ε_f(eV) 2500
$(3d_{5/2}4d_{5/2})_0$	1288	3.82[-3]	3.80[-3]	$(3d_{3/2}4d_{3/2})_0$	1341	5.80[-2]	6.11[-2]	$(3d_{3/2}4s_{1/2})_1$	1062	3.62[-4]	1.29[-4]
	1288	3.89[-3]	3.87[-3]		1341	5.90[-2]	6.24[-2]		1062	3.69[-4]	1.31[-4]
	1287	3.72[-3]	3.71[-3]		1340	5.98[-2]	6.34[-2]		1060	3.80[-4]	1.32[-4]
	1287	3.51[-3]	3.60[-3]		1340	5.64[-2]	6.17[-2]		1062	3.80[-4]	1.32[-4]
$(3d_{5/2}4d_{3/2})_1$	1262	1.90[-3]	6.50[-4]	$(3d_{5/2}4d_{5/2})_1$	1275	1.26[-3]	3.93[-4]	$(3d_{3/2}4d_{3/2})_1$	1300	1.12[-3]	3.50[-4]
	1262	1.93[-3]	6.62[-4]		1275	1.28[-3]	4.00[-4]		1300	1.14[-3]	3.57[-4]
	1262	1.95[-3]	6.66[-4]		1274	1.28[-3]	4.00[-4]		1298	1.14[-3]	3.56[-4]
	1262	1.95[-3]	6.86[-4]		1275	1.23[-3]	3.92[-4]		1299	1.09[-3]	3.50[-4]
$(3d_{3/2}4d_{5/2})_1$	1309	1.31[-3]	4.17[-4]	$(3d_{5/2}4s_{1/2})_2$	1029	2.23[-3]	2.86[-3]	$(3d_{3/2}4s_{1/2})_2$	1063	1.67[-3]	1.99[-3]
	1309	1.33[-3]	4.25[-4]		1029	2.25[-3]	2.88[-3]		1063	1.69[-3]	2.00[-3]
	1307	1.31[-3]	4.21[-4]		1028	2.24[-3]	2.85[-3]		1061	1.69[-3]	2.01[-3]
	1308	1.33[-3]	4.41[-4]		1030	2.32[-3]	2.99[-3]		1063	1.74[-3]	2.11[-3]
$(3d_{5/2}4d_{3/2})_2$	1268	1.79[-3]	9.84[-4]	$(3d_{5/2}4d_{5/2})_2$	1280	3.46[-3]	4.27[-3]	$(3d_{3/2}4d_{3/2})_2$	1305	2.25[-3]	2.74[-3]
	1268	1.81[-3]	9.96[-4]		1280	3.49[-3]	4.30[-3]		1305	2.27[-3]	2.76[-3]
	1268	1.81[-3]	9.82[-4]		1279	3.47[-3]	4.26[-3]		1303	2.26[-3]	2.76[-3]
	1267	1.89[-3]	1.09[-3]		1280	3.77[-3]	4.82[-3]		1304	2.36[-3]	2.94[-3]
$(3d_{3/2}4d_{5/2})_2$	1313	1.91[-3]	1.42[-3]	$(3d_{5/2}4s_{1/2})_3$	1028	8.35[-4]	3.00[-4]	$(3d_{5/2}4d_{3/2})_3$	1270	1.28[-3]	3.51[-4]
	1313	1.93[-3]	1.43[-3]		1028	8.51[-4]	3.05[-4]		1270	1.30[-3]	3.58[-4]
	1311	1.93[-3]	1.44[-3]		1027	8.45[-4]	3.05[-4]		1269	1.31[-3]	3.58[-4]
	1311	1.97[-3]	1.49[-3]		1029	8.47[-4]	3.05[-4]		1269	1.36[-3]	3.84[-4]
$(3d_{5/2}4d_{5/2})_3$	1280	1.65[-3]	4.76[-4]	$(3d_{3/2}4d_{3/2})_3$	1301	1.51[-3]	4.38[-4]	$(3d_{3/2}4d_{5/2})_3$	1315	1.16[-3]	3.07[-4]
	1280	1.67[-3]	4.85[-4]		1301	1.53[-3]	4.47[-4]		1315	1.17[-3]	3.14[-4]
	1278	1.69[-3]	4.87[-4]		1299	1.48[-3]	4.36[-4]		1313	1.17[-3]	3.12[-4]
	1279	1.65[-3]	4.84[-4]		1299	1.47[-3]	4.39[-4]		1313	1.22[-3]	3.36[-4]
$(3d_{5/2}4d_{3/2})_4$	1267	1.87[-3]	9.04[-4]	$(3d_{5/2}4d_{5/2})_4$	1281	1.25[-3]	4.67[-4]	$(3d_{3/2}4d_{5/2})_4$	1312	1.76[-3]	8.13[-4]
	1267	1.90[-3]	9.16[-4]		1281	1.27[-3]	4.74[-4]		1312	1.78[-3]	8.25[-4]
	1266	1.89[-3]	9.13[-4]		1280	1.30[-3]	4.77[-4]		1310	1.78[-3]	8.21[-4]
	1267	1.99[-3]	9.81[-4]		1280	1.27[-3]	4.89[-4]		1310	1.89[-3]	8.88[-4]
$(3d_{5/2}4d_{5/2})_5$	1276	2.47[-3]	7.26[-4]	$(3d_{3/2}4p_{3/2})_0$	1181	2.46[-4]	9.66[-5]	$(3d_{5/2}4f_{5/2})_0$	1395	1.09[-3]	3.26[-4]
	1276	2.51[-3]	7.40[-4]		1181	2.50[-4]	9.83[-5]		1395	1.10[-3]	3.29[-4]
	1275	2.57[-3]	7.50[-4]		1179	2.45[-4]	9.70[-5]		1394	1.11[-3]	3.31[-4]
	1276	2.55[-3]	7.54[-4]		1179	2.40[-4]	9.93[-5]		1394	1.15[-3]	3.44[-4]
$(3d_{3/2}4p_{1/2})_1$	1138	2.16[-3]	4.54[-3]	$(3d_{5/2}4p_{3/2})_1$	1152	4.24[-3]	1.04[-2]	$(3d_{3/2}4p_{3/2})_1$	1185	8.23[-4]	1.25[-3]
	1138	2.18[-3]	4.58[-3]		1152	4.27[-3]	1.05[-2]		1185	8.33[-4]	1.27[-3]
	1136	2.16[-3]	4.59[-3]		1152	4.21[-3]	1.04[-2]		1183	8.35[-4]	1.27[-3]
	1137	2.13[-3]	4.69[-3]		1152	4.46[-3]	1.13[-2]		1183	8.33[-4]	1.33[-3]
$(3d_{5/2}4f_{5/2})_1$	1397	3.07[-3]	1.37[-3]	$(3d_{5/2}4f_{7/2})_1$	1416	3.07[-2]	4.94[-2]	$(3d_{3/2}4f_{5/2})_1$	1460	1.66[-1]	2.76[-1]
	1397	3.10[-3]	1.38[-3]		1416	3.09[-2]	4.98[-2]		1460	1.67[-1]	2.78[-1]
	1396	3.13[-3]	1.40[-3]		1414	2.99[-2]	4.82[-2]		1457	1.68[-1]	2.80[-1]
	1396	3.22[-3]	1.40[-3]		1414	3.00[-2]	4.95[-2]		1458	1.65[-1]	2.80[-1]
$(3d_{5/2}4p_{1/2})_2$	1101	8.47[-4]	3.22[-4]	$(3d_{3/2}4p_{1/2})_2$	1135	6.82[-4]	2.24[-4]	$(3d_{5/2}4p_{3/2})_2$	1151	6.33[-4]	2.27[-4]
	1101	8.62[-4]	3.28[-4]		1135	6.96[-4]	2.29[-4]		1151	6.44[-4]	2.31[-4]

TABLE II. (Continued).

Upper Level	ΔE(eV)	ε_f(eV) 160	ε_f(eV) 2500	Upper Level	ΔE(eV)	ε_f(eV) 160	ε_f(eV) 2500	Upper Level	ΔE(eV)	ε_f(eV) 160	ε_f(eV) 2500
	1101	8.68[-4]	3.30[-4]		1134	6.75[-4]	2.26[-4]		1150	6.57[-4]	2.33[-4]
	1101	8.37[-4]	3.30[-4]		1134	6.80[-4]	2.32[-4]		1151	6.46[-4]	2.39[-4]
$(3d_{3/2}4p_{3/2})2$	1187	4.12[-4]	1.34[-4]	$(3d_{5/2}4f_{5/2})2$	1401	3.15[-3]	8.66[-4]	$(3d_{5/2}4f_{7/2})2$	1404	1.83[-3]	4.37[-4]
	1187	4.21[-4]	1.37[-4]		1401	3.18[-3]	8.76[-4]		1404	1.85[-3]	4.42[-4]
	1185	4.23[-4]	1.38[-4]		1399	3.22[-3]	8.84[-4]		1402	1.82[-3]	4.32[-4]
	1186	4.20[-4]	1.42[-4]		1400	3.37[-3]	9.20[-4]		1403	1.96[-3]	4.55[-4]
$(3d_{3/2}4f_{7/2})2$	1435	3.12[-3]	8.71[-4]	$(3d_{3/2}4f_{5/2})2$	1437	1.69[-3]	4.13[-4]	$(3d_{5/2}4p_{1/2})3$	1102	1.37[-3]	1.12[-3]
	1435	3.15[-3]	8.82[-4]		1437	1.70[-3]	4.18[-4]		1102	1.39[-3]	1.13[-3]
	1432	3.14[-3]	8.75[-4]		1435	1.67[-3]	4.08[-4]		1102	1.37[-3]	1.12[-3]
	1433	3.32[-3]	9.09[-4]		1435	1.79[-3]	4.28[-4]		1102	1.41[-3]	1.16[-3]
$(3d_{5/2}4p_{3/2})3$	1154	7.92[-4]	6.69[-4]	$(3d_{3/2}4p_{3/2})3$	1185	1.19[-3]	9.93[-4]	$(3d_{5/2}4f_{5/2})3$	1404	2.15[-3]	5.84[-4]
	1154	8.03[-4]	6.75[-4]		1185	1.20[-3]	1.00[-3]		1404	2.17[-3]	5.91[-4]
	1153	8.22[-4]	6.76[-4]		1183	1.21[-3]	1.00[-3]		1402	2.17[-3]	5.77[-4]
	1153	8.29[-4]	6.92[-4]		1184	1.25[-3]	1.05[-3]		1403	2.33[-3]	6.08[-4]
$(3d_{5/2}4f_{7/2})3$	1408	3.64[-3]	4.37[-3]	$(3d_{3/2}4f_{5/2})3$	1440	1.33[-3]	4.44[-4]	$(3d_{3/2}4f_{7/2})3$	1441	3.28[-3]	3.52[-3]
	1408	3.67[-3]	4.40[-3]		1440	1.34[-3]	4.49[-4]		1441	3.30[-3]	3.55[-3]
	1407	3.66[-3]	4.40[-3]		1438	1.36[-3]	3.50[-4]		1438	3.27[-3]	3.65[-3]
	1407	3.76[-3]	4.50[-3]		1438	1.46[-3]	3.82[-4]		1439	3.38[-3]	3.72[-3]
$(3d_{5/2}4p_{3/2})4$	1150	1.13[-3]	3.91[-4]	$(3d_{5/2}4f_{5/2})4$	1405	1.61[-3]	3.57[-4]	$(3d_{5/2}4f_{7/2})4$	1407	2.11[-3]	5.03[-4]
	1150	1.15[-3]	3.99[-4]		1405	1.62[-3]	3.61[-4]		1407	2.13[-3]	5.10[-4]
	1149	1.18[-3]	4.05[-4]		1403	1.66[-3]	3.69[-4]		1405	2.11[-3]	5.01[-4]
	1149	1.20[-3]	4.22[-4]		1404	1.79[-3]	3.90[-4]		1406	2.26[-3]	5.24[-4]
$(3d_{3/2}4f_{5/2})4$	1435	1.87[-3]	4.61[-4]	$(3d_{3/2}4f_{7/2})4$	1442	1.40[-3]	2.99[-4]	$(3d_{5/2}4f_{5/2})5$	1401	1.75[-3]	7.45[-4]
	1435	1.89[-3]	4.67[-4]		1442	1.41[-3]	3.03[-4]		1401	1.77[-3]	7.52[-4]
	1433	1.87[-3]	4.62[-4]		1439	1.40[-3]	2.98[-4]		1400	1.80[-3]	7.56[-4]
	1433	2.03[-3]	4.90[-4]		1440	1.52[-3]	3.16[-4]		1400	1.95[-3]	7.90[-4]
$(3d_{5/2}4f_{7/2})5$	1408	1.18[-3]	3.22[-4]	$(3d_{3/2}4f_{7/2})5$	1438	1.56[-3]	6.48[-4]	$(3d_{5/2}4f_{7/2})6$	1402	2.99[-3]	7.54[-4]
	1408	1.20[-3]	3.25[-4]		1438	1.58[-3]	6.54[-4]		1402	3.02[-3]	7.63[-4]
	1406	1.20[-3]	3.25[-4]		1436	1.54[-3]	6.44[-4]		1401	3.03[-3]	7.58[-4]
	1407	1.32[-3]	3.45[-4]		1436	1.67[-3]	6.71[-4]		1401	3.27[-3]	7.99[-4]

TABLE III. Comparison of collision strengths for nickel-like ions with Z = 92. Notation is as in Table II, but in this case there are no other fully relativistic results available with which to make comparison.

Upper Level	ΔE(eV)	ε_f(eV) 400	10000	Upper Level	ΔE(eV)	ε_f(eV) 400	10000	Upper Level	ΔE(eV)	ε_f(eV) 400	10000
$(3d_{5/2}4d_{5/2})\,0$	3483	7.86[-3]	8.34[-3]	$(3d_{3/2}4d_{3/2})\,0$	3621	1.77[-2]	1.89[-2]	$(3d_{3/2}4s_{1/2})\,1$	2882	1.40[-4]	3.30[-5]
	3483	8.22[-3]	8.78[-3]		3621	1.86[-2]	2.00[-2]		2882	1.47[-4]	3.48[-5]
	3478	8.12[-3]	8.79[-3]		3615	1.94[-2]	2.11[-2]		2875	1.58[-4]	3.53[-5]
$(3d_{5/2}4d_{3/2})\,1$	3367	5.90[-4]	1.36[-4]	$(3d_{5/2}4d_{5/2})\,1$	3441	4.98[-4]	1.09[-4]	$(3d_{3/2}4d_{3/2})\,1$	3571	3.40[-4]	7.12[-5]
	3367	6.14[-4]	1.43[-4]		3441	5.18[-4]	1.14[-4]		3571	3.54[-4]	7.52[-5]
	3364	6.30[-4]	1.43[-4]		3436	5.24[-4]	1.14[-4]		3564	3.38[-4]	7.17[-5]
$(3d_{3/2}4d_{5/2})\,1$	3637	5.11[-4]	1.15[-4]	$(3d_{5/2}4s_{1/2})\,2$	2689	1.09[-3]	1.54[-3]	$(3d_{3/2}4s_{1/2})\,2$	2884	6.65[-4]	8.33[-4]
	3637	5.31[-4]	1.22[-4]		2689	1.11[-3]	1.57[-3]		2884	6.81[-4]	8.52[-4]
	3628	5.20[-4]	1.19[-4]		2685	1.10[-3]	1.53[-3]		2876	6.82[-4]	8.47[-4]
$(3d_{5/2}4d_{3/2})\,2$	3377	8.23[-4]	6.58[-4]	$(3d_{5/2}4d_{5/2})\,2$	3450	1.39[-3]	1.89[-3]	$(3d_{3/2}4d_{3/2})\,2$	3579	5.31[-4]	5.97[-4]
	3377	8.46[-4]	6.75[-4]		3450	1.42[-3]	1.93[-3]		3579	5.45[-4]	6.12[-4]
	3373	8.39[-4]	6.57[-4]		3445	1.40[-3]	1.90[-3]		3572	5.01[-4]	5.45[-4]
$(3d_{3/2}4d_{5/2})\,2$	3644	6.81[-4]	4.99[-4]	$(3d_{5/2}4s_{1/2})\,3$	2687	3.20[-4]	7.64[-5]	$(3d_{5/2}4d_{3/2})\,3$	3380	4.20[-4]	7.07[-5]
	3644	7.02[-4]	5.13[-4]		2687	3.35[-4]	8.02[-5]		3380	4.38[-4]	7.48[-5]
	3635	7.04[-4]	5.14[-4]		2683	3.28[-4]	7.95[-5]		3377	4.38[-4]	7.42[-5]
$(3d_{5/2}4d_{5/2})\,3$	3449	5.84[-4]	1.11[-4]	$(3d_{3/2}4d_{3/2})\,3$	3570	5.50[-4]	1.05[-4]	$(3d_{3/2}4d_{5/2})\,3$	3647	4.16[-4]	7.08[-5]
	3449	6.08[-4]	1.16[-4]		3570	5.76[-4]	1.11[-4]		3647	4.35[-4]	7.49[-5]
	3444	6.17[-4]	1.16[-4]		3563	5.30[-4]	1.05[-4]		3638	4.31[-4]	7.37[-5]
$(3d_{5/2}4d_{3/2})\,4$	3375	6.84[-4]	3.26[-4]	$(3d_{5/2}4d_{5/2})\,4$	3451	4.35[-4]	1.50[-4]	$(3d_{3/2}4d_{5/2})\,4$	3642	6.26[-4]	2.61[-4]
	3375	7.11[-4]	3.37[-4]		3451	4.52[-4]	1.55[-4]		3642	6.51[-4]	2.70[-4]
	3372	7.02[-4]	3.31[-4]		3447	4.67[-4]	1.55[-4]		3633	6.48[-4]	2.66[-4]
$(3d_{5/2}4d_{5/2})\,5$	3444	8.56[-4]	1.65[-4]	$(3d_{3/2}4p_{3/2})\,0$	3357	9.09[-5]	2.32[-5]	$(3d_{5/2}4f_{5/2})\,0$	3648	4.35[-4]	8.91[-5]
	3444	8.93[-4]	1.74[-4]		3357	9.45[-5]	2.44[-5]		3648	4.46[-4]	9.22[-5]
	3439	9.34[-4]	1.77[-4]		3350	9.19[-5]	2.38[-5]		3643	4.52[-4]	9.29[-5]
$(3d_{3/2}4p_{1/2})\,1$	3032	1.59[-3]	3.87[-3]	$(3d_{5/2}4p_{3/2})\,1$	3170	1.44[-3]	4.20[-3]	$(3d_{3/2}4p_{3/2})\,1$	3363	2.30[-4]	1.69[-4]
	3032	1.62[-3]	3.96[-3]		3170	1.47[-3]	4.29[-3]		3363	2.38[-4]	1.75[-4]
	3028	1.57[-3]	3.88[-3]		3166	1.44[-3]	4.19[-3]		3355	2.37[-4]	1.75[-4]
$(3d_{5/2}4f_{5/2})\,1$	3654	1.01[-3]	2.22[-4]	$(3d_{5/2}4f_{7/2})\,1$	3717	3.98[-2]	7.23[-2]	$(3d_{3/2}4f_{5/2})\,1$	3891	5.52[-2]	1.01[-1]
	3654	1.04[-3]	2.30[-4]		3717	4.06[-2]	7.41[-2]		3891	5.62[-2]	1.03[-1]
	3649	1.04[-3]	2.22[-4]		3710	4.03[-2]	7.35[-2]		3882	5.66[-2]	1.04[-1]
$(3d_{5/2}4p_{1/2})\,2$	2831	3.15[-4]	7.61[-5]	$(3d_{3/2}4p_{1/2})\,2$	3027	2.64[-4]	5.50[-5]	$(3d_{5/2}4p_{3/2})\,2$	3168	2.65[-4]	6.05[-5]
	2831	3.29[-4]	8.01[-5]		3027	2.80[-4]	5.85[-5]		3168	2.76[-4]	6.37[-5]
	2831	3.32[-4]	7.98[-5]		3023	2.62[-4]	5.69[-5]		3164	2.85[-4]	6.41[-5]

TABLE III. (Continued).

Upper Level	ΔE(eV)	ε_f(eV) 400	ε_f(eV) 10000	Upper Level	ΔE(eV)	ε_f(eV) 400	ε_f(eV) 10000	Upper Level	ΔE(eV)	ε_f(eV) 400	ε_f(eV) 10000
$(3d_{3/2}4p_{3/2})2$	3367	1.68[-4]	3.57[-5]	$(3d_{5/2}4f_{5/2})2$	3661	8.28[-4]	1.35[-4]	$(3d_{5/2}4f_{7/2})2$	3681	9.95[-4]	1.73[-4]
	3367	1.77[-4]	3.79[-5]		3661	8.50[-4]	1.39[-4]		3681	1.02[-3]	1.79[-4]
	3359	1.80[-4]	3.81[-5]		3656	8.56[-4]	1.39[-4]		3675	1.02[-3]	1.75[-4]
$(3d_{3/2}4f_{5/2})2$	3858	7.22[-4]	1.22[-4]	$(3d_{3/2}4f_{7/2})2$	3875	1.18[-3]	2.27[-4]	$(3d_{5/2}4p_{1/2})3$	2833	6.18[-4]	5.26[-4]
	3858	7.42[-4]	1.26[-4]		3875	1.21[-3]	2.35[-4]		2833	6.38[-4]	5.40[-4]
	3849	7.33[-4]	1.24[-4]		3864	1.18[-3]	2.25[-4]		2833	6.22[-4]	5.26[-4]
$(3d_{5/2}4p_{3/2})3$	3172	2.93[-4]	2.57[-4]	$(3d_{3/2}4p_{3/2})3$	3364	3.92[-4]	3.33[-4]	$(3d_{5/2}4f_{5/2})3$	3666	9.47[-4]	5.07[-4]
	3172	3.03[-4]	2.64[-4]		3364	4.06[-4]	3.43[-4]		3666	9.69[-4]	5.21[-4]
	3169	3.14[-4]	2.62[-4]		3356	4.14[-4]	3.41[-4]		3660	9.68[-4]	5.05[-4]
$(3d_{5/2}4f_{7/2})3$	3690	1.57[-3]	1.92[-3]	$(3d_{3/2}4f_{5/2})3$	3865	8.11[-4]	9.25[-4]	$(3d_{3/2}4f_{7/2})3$	3883	9.87[-4]	6.70[-4]
	3690	1.60[-3]	1.96[-3]		3865	8.27[-4]	9.48[-4]		3883	1.01[-3]	6.88[-4]
	3684	1.60[-3]	1.97[-3]		3856	8.16[-4]	9.38[-4]		3873	1.00[-3]	6.84[-4]
$(3d_{5/2}4p_{3/2})4$	3166	3.70[-4]	9.03[-5]	$(3d_{5/2}4f_{5/2})4$	3667	5.15[-4]	6.64[-5]	$(3d_{5/2}4f_{7/2})4$	3687	8.58[-4]	1.36[-4]
	3166	3.87[-4]	9.51[-5]		3667	5.29[-4]	6.89[-5]		3687	8.81[-4]	1.41[-4]
	3162	4.16[-4]	9.85[-5]		3661	5.38[-4]	6.95[-5]		3681	8.81[-4]	1.38[-4]
$(3d_{3/2}4f_{5/2})4$	3855	7.22[-4]	1.18[-4]	$(3d_{3/2}4f_{7/2})4$	3885	5.22[-4]	7.17[-5]	$(3d_{5/2}4f_{5/2})5$	3660	6.75[-4]	2.99[-4]
	3855	7.42[-4]	1.22[-4]		3885	5.37[-4]	7.44[-5]		3660	6.93[-4]	3.07[-4]
	3846	7.27[-4]	1.20[-4]		3875	5.26[-4]	7.14[-5]		3655	7.21[-4]	3.06[-4]
$(3d_{5/2}4f_{7/2})5$	3690	4.22[-4]	1.13[-4]	$(3d_{3/2}4f_{7/2})5$	3879	6.00[-4]	2.50[-4]	$(3d_{5/2}4f_{7/2})6$	3680	1.15[-3]	1.91[-4]
	3690	4.34[-4]	1.16[-4]		3879	6.17[-4]	2.57[-4]		3680	1.18[-3]	1.98[-4]
	3684	4.37[-4]	1.15[-4]		3869	5.86[-4]	2.50[-4]		3674	1.18[-3]	1.92[-4]

about like that for neonlike iron given in Table I, for which the value of Z/N is similar to that for nickel-like gadolinium. However, there is one transition (not shown in Table II) for which our FR results differ appreciably from Hagelstein's. This is excitation to the $(3s_{1/2}4p_{1/2})_1$ level, for which our FR results approach a value about 1.5 times the results of Hagelstein, for large energies. In the case of this weak optically allowed transition, it is our value for the oscillator strength that agrees approximately with that of the program by Grant et al.,[9] as seen from Table V of Ref. 6. Hence we think our results for the collision strength are the preferred ones in this case.

Similar to the situation for neonlike ions and for the same reasons, we expect that the differences between FR results, and those obtained with the programs of Ref. 4, would decrease as Z is increased. Also, in the present case involving one step higher in n values than for neonlike ions, one would expect relativistic effects to tend to be smaller. Hence the QR results should be accurate for higher Z. In order to test this and help in establishing the range of validity of the QR approach, we have compared QR and FR results for nickel-like ions with $Z=92$ in Table III. Here the three entries for each transition are calculated by the same methods as the first three entries for each transition in Table II. One does see that indeed even for $Z=92$ the QR results are mostly in very good agreement with FR values, especially the QR values obtained using the normalization of Eq. (A25).

IV. SUMMARY AND CONCLUSIONS

A very rapid, fully relativistic distorted-wave approach and corresponding computer program have been developed for the purpose of calculating collision strengths for highly charged ions and providing the cross sections needed for applications to very-high-temperature plasmas, such as those in x-ray laser research. Results by this method are compared with those by several more elaborate programs and with a few experimental values. It appears that for $Z \gtrsim 2.5N$ the approach gives results essentially as accurate as the most elaborate fully relativistic programs available. A quasirelativistic approach that is still more rapid by about a factor of 2.5 is also described. This QR approach gives results close to the FR values for neonlike ions with $Z \lesssim 74$ and nickel-like ions with $Z \lesssim 92$. A procedure is described for readily and accurately obtaining collision strengths for a large portion of an isoelectronic sequence, when detailed calculations have been made for only a few members by making use of fits of the radial part of the collision strength to a power series in Z.

ACKNOWLEDGMENTS

APPENDIX

The appropriate normalization for the free electron radial functions is

$$\int_0^\infty [P_{\epsilon'\kappa}(r)P_{\epsilon\kappa}(r)+Q_{\epsilon'\kappa}(r)Q_{\epsilon\kappa}(r)]dr =\pi\delta(\epsilon-\epsilon') . \quad (A1)$$

In order to determine what this implies for the asymptotic form of the functions we follow a procedure that is essentially the relativistic analog of that given in Sec. 18-3 of Ref. 23. Specifically, we multiply Eq. (7) from the left by $Q_{\epsilon'\kappa}$ and subtract from this the analogous equation with ϵ and ϵ' everywhere interchanged. Then we solve for $Q_{\epsilon'\kappa}Q_{\epsilon\kappa}$ to obtain

$$Q_{\epsilon'\kappa}Q_{\epsilon\kappa}=\frac{2}{\alpha}\frac{1}{(\epsilon-\epsilon')}\left[\left[Q_{\epsilon'\kappa}\frac{d}{dr}P_{\epsilon\kappa}-Q_{\epsilon\kappa}\frac{d}{dr}P_{\epsilon'\kappa}\right]\right.$$
$$\left.+\frac{\kappa}{r}(Q_{\epsilon'\kappa}P_{\epsilon\kappa}-Q_{\epsilon\kappa}P_{\epsilon'\kappa})\right] . \quad (A2)$$

By applying analogous procedures to Eq. (8) we get

$$P_{\epsilon'\kappa}P_{\epsilon\kappa}=\frac{2}{\alpha}\frac{1}{(\epsilon-\epsilon')}\left[\left[P_{\epsilon\kappa}\frac{d}{dr}Q_{\epsilon'\kappa}-P_{\epsilon'\kappa}\frac{d}{dr}Q_{\epsilon\kappa}\right]\right.$$
$$\left.-\frac{\kappa}{r}(P_{\epsilon\kappa}Q_{\epsilon'\kappa}-P_{\epsilon'\kappa}Q_{\epsilon\kappa})\right] . \quad (A3)$$

Thus adding Eq. (A2) to Eq. (A3) we obtain a perfect differential, which we integrate from 0 to any value of r to obtain

$$\int_0^r [P_{\epsilon'\kappa}(r')P_{\epsilon\kappa}(r')+Q_{\epsilon'\kappa}(r')Q_{\epsilon\kappa}(r')]dr'$$
$$=\frac{2}{\alpha}\frac{1}{(\epsilon-\epsilon')}[P_{\epsilon\kappa}(r)Q_{\epsilon'\kappa}(r)-Q_{\epsilon\kappa}(r)P_{\epsilon'\kappa}(r)] . \quad (A4)$$

In the limit of $r\to\infty$, Eqs. (7) and (8) reduce to

$$\frac{d}{dr}P_{\epsilon\kappa}=\frac{\alpha}{2}\left[\epsilon+\frac{4}{\alpha^2}\right]Q_{\epsilon\kappa}, \quad \frac{d}{dr}Q_{\epsilon\kappa}=-\frac{\alpha}{2}\epsilon P_{\epsilon\kappa} . \quad (A5)$$

Hence, in this limit,

$$\frac{d^2P_{\epsilon\kappa}}{dr^2}=-\left[\epsilon+\frac{\alpha^2\epsilon^2}{4}\right]P_{\epsilon\kappa}=-k^2P_{\epsilon\kappa} , \quad (A6)$$

which has the solution

$$P_{\epsilon\kappa}=C_P(\epsilon)\sin(kr+\delta_\kappa) . \quad (A7)$$

Then from Eqs. (A5),

$$Q_{\epsilon\kappa}=C_Q(\epsilon)\cos(kr+\delta_\kappa)=\frac{\alpha}{2}\frac{\epsilon}{k}C_P(\epsilon)\cos(kr+\delta_\kappa) . \quad (A8)$$

Applying this to Eq. (A4),

$$\lim_{r\to\infty}\int_0^r [P_{\varepsilon'\kappa}(r')P_{\varepsilon\kappa}(r')+Q_{\varepsilon'\kappa}(r')Q_{\varepsilon\kappa}(r')]dr'$$

$$=\frac{C_P(\varepsilon)C_P(\varepsilon')}{(\varepsilon-\varepsilon')}\left[\frac{\varepsilon'}{k'}\sin(kr+\delta_\kappa)\cos(k'r+\delta_\kappa)\right.$$

$$\left.-\frac{\varepsilon}{k}\cos(kr+\delta_\kappa)\sin(k'r+\delta_\kappa)\right].$$

$$(A9)$$

The part in parentheses can be expressed as $(\varepsilon/k)\sin[(k-k')r]$ plus a part that oscillates infinitely rapidly as $r\to\infty$ and contributes nothing. Thus using

$$\lim_{r\to\infty}\frac{1}{k-k'}\sin(k-k')r=\pi\delta(k-k'),\qquad (A10)$$

we have[24]

$$\int_0^\infty [P_{\varepsilon'\kappa}(r)P_{\varepsilon\kappa}(r)+Q_{\varepsilon'\kappa}(r)Q_{\varepsilon\kappa}(r)]dr$$

$$=\pi C_P(\varepsilon)C_P(\varepsilon')\frac{\varepsilon}{k}\left|\frac{k-k'}{\varepsilon-\varepsilon'}\right|\delta(k-k')$$

$$=\pi C_P(\varepsilon)^2\frac{\varepsilon}{k}\delta(\varepsilon-\varepsilon').\qquad (A11)$$

Hence, comparing this with Eq. (A1), one sees that

$$C_P(\varepsilon)=\left[\frac{k}{\varepsilon}\right]^{1/2}=\frac{1}{\varepsilon^{1/4}}\left[1+\frac{\alpha^2\varepsilon}{4}\right]^{1/4}.\qquad (A12)$$

In practice one does not evaluate $P_{\varepsilon\kappa}$ to such large r that Eq. (A7) applies. Instead, one simply goes out to some large value r_0, somewhat greater than that for which the bound functions have significant values, and where, following Hagelstein and Jung,[4] the Wentzel-Kramers-Brillouin solution

$$P_{\varepsilon\kappa}(r)=C\left[\frac{a_P(r)}{\eta(r)}\right]^{1/2}\sin\phi(r),\quad \phi(r)=\int_0^r\eta(s)ds\qquad (A13)$$

should apply. Using Eq. (A13) in Eq. (11), and then substituting into Eq. (13), gives

$$\eta^{1/2}\frac{d^2}{dr^2}\eta^{-1/2}+\omega(r)=\eta^2(r).\qquad (A14)$$

Since η should be a slowly varying function of r for large r, one would expect the zeroth-order approximation $\eta(r)=\omega(r)^{1/2}$ would be quite a good approximation. In fact, we found no improvement by going to a higher-order approximation as in Ref. 4. Thus we use

$$P_{\varepsilon\kappa}(r)=C\left[\frac{a_P(r)}{\omega(r)^{1/2}}\right]^{1/2}\sin\phi(r),\quad r>r_0\qquad (A15)$$

with $\omega(s)^{1/2}$ replacing $\eta(s)$ in the second of Eqs. (A13) for this region. In the limit $r\to\infty$, one sees from Eqs. (12), (14), and (15) that

$$\omega(r)=a_Pa_Q=\frac{\alpha^2}{4}\left[\varepsilon+\frac{4}{\alpha^2}\right]\varepsilon=k^2,\qquad (A16)$$

and

$$\left[\frac{a_P(r)}{\omega(r)^{1/2}}\right]^{1/2}=\left[\frac{2}{\alpha}\right]^{1/2}\left[1+\frac{\alpha^2\varepsilon}{4}\right]^{1/4}\varepsilon^{-1/4}$$

$$=\left[\frac{2}{\alpha}\right]^{1/2}C_P.\qquad (A17)$$

Thus $C=(\alpha/2)^{1/2}$. Now for large r in the vicinity of r_0, the unnormalized large-component radial function will be

$$P_{\varepsilon\kappa}^u(r)=B\sin\phi(r),\qquad (A18)$$

where B is the amplitude of $P_{\varepsilon\kappa}^u$ at $r=r_0$. Hence, collecting results, the properly normalized large-component continuum radial function is

$$P_{\varepsilon\kappa}=\left[\frac{\alpha a_P(r_0)}{2\omega(r_0)^{1/2}}\right]^{1/2}\frac{P_{\varepsilon\kappa}^u(r)}{B}.\qquad (A19)$$

Actually it is Eq. (13) for $F_{\varepsilon\kappa}$ that we solve numerically. If the amplitude of $F_{\varepsilon\kappa}^u$, the unnormalized solution of Eq. (13), is B' at $r=r_0$, then from Eq. (11), $B=B'a_P(r_0)^{1/2}$ and $P_{\varepsilon\kappa}^u(r)=a_P(r)^{1/2}F_{\varepsilon\kappa}^u(r)$. Hence, in place of Eq. (A19), we can write

$$P_{\varepsilon\kappa}(r)=\left[\frac{\alpha a_P(r)}{2\omega(r_0)^{1/2}}\right]^{1/2}\frac{F_{\varepsilon\kappa}^u(r)}{B'}.\qquad (A20)$$

When the QR approach described in Sec. II D is used, one cannot obtain the analog of Eq. (A20), rigorously. However, one would expect the appropriate replacement for the coefficient C_P in the analog of Eq. (A7) to be

$$C_P^{QR}(\varepsilon)=[C_P^2(\varepsilon)+C_Q^2(\varepsilon)]^{1/2}=C_P(\varepsilon)\left[\frac{1+\frac{\alpha^2}{2}\varepsilon}{1+\frac{\alpha^2}{4}\varepsilon}\right]^{1/2},$$

$$(A21)$$

where use was made of Eqs. (2) and (A8). Then $P_{\varepsilon\kappa}^{QR}$ for $r>r_0$ is given by Eq. (A15) with C replaced by C^{QR} given by

$$C^{QR}=\left[\frac{\alpha}{2}\right]^{1/2}\left[\frac{1+\frac{\alpha^2}{2}\varepsilon}{1+\frac{\alpha^2}{4}\varepsilon}\right]^{1/2}.\qquad (A22)$$

Hence, in the QR approach, Eq. (A20) is replaced with

$$P_{\varepsilon\kappa}^{QR1}(r)=\left[\frac{\alpha}{2}\frac{\left[1+\frac{\alpha^2}{2}\varepsilon\right]}{\left[1+\frac{\alpha^2}{4}\varepsilon\right]}\frac{a_P(r)}{\omega(r_0)^{1/2}}\right]^{1/2}\frac{F_{\varepsilon\kappa}^u(r)}{B'}.$$

$$(A23)$$

When the additional approximation $\kappa=-1$ is made in Eq. (14), so that the radial functions for the free electron become independent of j, Eq. (A23) is replaced with

$$P_{\varepsilon l}^{QR2}(r)= \left[\frac{\alpha}{2} \frac{\left[1+\dfrac{\alpha^2}{2}\varepsilon\right]}{\left[1+\dfrac{\alpha^2}{4}\varepsilon\right]} \frac{a_P(r)}{\omega'(r_0)^{1/2}} \right]^{1/2} \frac{F_{\varepsilon l}^{u2}(r)}{B'} ,$$

(A24)

where $\omega'(r_0)$ is given by Eq. (14) with $\kappa=-1$ and evaluated at $r=r_0$, while $F_{\varepsilon l}^{u2}(r)$ is the unnormalized solution of Eq. (13) with $\omega(r)$ replaced by $\omega'(r)$ given by Eq. (14) with $\kappa=-1$. Actually we have found empirically, by comparing results for collision strengths with the FR

values, that improved QR results with $\kappa=-1$ are obtained if Eq. (A24) is replaced by

$$P_{\varepsilon l}^{QR3}(r)= \left[\frac{\alpha}{2} \frac{\left[1+\dfrac{\alpha^2}{2}(\varepsilon-V)\right]}{\left[1+\dfrac{\alpha^2}{4}(\varepsilon-V)\right]} \frac{a_P(r)}{\omega'(r_0)^{1/2}} \right]^{1/2} \frac{F_{\varepsilon l}^{u2}(r)}{B'} ,$$

(A25)

which reduces to the same value as that given by Eq. (A24) in the limit $r\to\infty$.

---

*Present address: Department 48B/428, IBM, Neighborhood Road, Kingston, NY 12401.

[1] P. L. Hagelstein and S. Dalhed, Phys. Rev. A 37, 1357 (1988).

[2] M. S. Pindzola and S. L. Carter, Phys. Rev. A 22, 898 (1980).

[3] Y.-K. Kim and J. P. Desclaux, Phys. Scr. 36, 796 (1987).

[4] P. L. Hagelstein and R. K. Jung, At. Data Nucl. Data Tables 37, 121 (1987).

[5] A. Bar-Shalom, M. Klapisch, and J. Oreg, Phys. Rev. A 38, 1773 (1988).

[6] D. H. Sampson, H. L. Zhang, A. K. Mohanty, and R. E. H. Clark, preceding paper, Phys. Rev. A 40, 604 (1989).

[7] H. L. Zhang, D. H. Sampson, and A. K. Mohanty, in Abstracts from the Sixth Topical Conference of the American Physical Society on Atomic Processes in High Temperature Plasmas, Sante Fe, NM, 1987, Los Alamos National Library Publication No. LALP-87-30.

[8] Actually in the present case the wave function of the core, which is really the target ion, contains mixing as in Eq. (I.4). Hence, more precisely, the matrix elements of Eq. (3) are analogous to linear sums of the matrix elements occurring in the diagonalization of the Hamiltonian for an $(N+1)$-electron ion.

[9] I. P. Grant, B. J. McKenzie, P. H. Norrington, D. F. Mayers, and N. C. Pyper, Comput. Phys. Commun. 21, 207 (1980).

[10] C. Bottcher (private communication); C. Bottcher, D. C. Griffin, and M. S. Pindzola, J. Phys. B 16, L65 (1983).

[11] A. Burgess and V. B. Sheorey, J. Phys. B 7, 2403 (1974).

[12] D. H. Sampson and R. E. H. Clark, Astrophys. J. Suppl. 44, 169 (1980).

[13] Y.-K. Kim (private communication).

[14] L. B. Golden, R. E. H. Clark, S. J. Goett, and D. H. Sampson, Astrophys. J. Suppl. 45, 603 (1981).

[15] D. H. Sampson, G. M. Weaver, S. J. Goett, and H. L. Zhang, At. Data Nucl. Data Tables 35, 223 (1986).

[16] H. L. Zhang and D. H. Sampson, At. Data Nucl. Data Tables (to be published).

[17] J. P. Desclaux, Comput. Phys. Commun. 9, 31 (1975).

[18] K. J. Reed, Phys. Rev. A 37, 1791 (1988); and (private communication).

[19] R. E. Marrs, M. A. Levine, D. A. Knapp, and J. R. Henderson, Phys. Rev. Lett. 60, 1715 (1988).

[20] H. L. Zhang, D. H. Sampson, R. E. H. Clark, and J. B. Mann, At. Data Nucl. Data Tables 37, 17 (1987).

[21] P. L. Hagelstein, Phys. Rev. A 34, 874 (1986).

[22] W. H. Goldstein, J. Oreg, A. Zigler, A. Bar-Shalom, and M. Klapisch, Phys. Rev. A 38, 1797 (1988).

[23] R. D. Cowan, Theory of Atomic Structure and Spectra (University of California Press, Berkeley, 1981).

[24] This result is not altered by the fact that the δ_κ in Eqs. (A7)–(A9) actually depend on k (or k') and r through a logarithmic term.