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Continuum orbital approximations in weak-coupling theories for inelastic electron scattering*

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Two approximations, motivated by heavy-particle scattering theory, are tested for weak-coupling electron-atom (ion) inelastic scattering theory. They consist of replacing the one-electron scattering orbitals by their Langer uniform approximations and the use of an average trajectory approximation which entirely avoids the necessity for generating continuum orbitals. Numerical tests for a dipole-allowed and a dipole-forbidden event, based on Coulomb-Born theory with exchange neglected, reveal the error trends. It is concluded that the uniform approximation gives a satisfactory prediction for traditional weak-coupling theories while the average approximation should be limited to collision energies exceeding at least twice the threshold energy. The accuracy for both approximations is higher for positive ions than for neutral targets. Partial-wave collision-strength data indicate that greater care should be exercised in using these approximations to predict quantities differential in the scattering angle. An application to the $2s\,^2S$-$2p\,^2P$ transition in Ne VIII is presented.

I. INTRODUCTION

The application of weak-coupling theories to electron-atom (ion) inelastic collisions has, in principle, certain advantages over higher-order theories. There are reasons to expect[1,2] that weak-coupling theories become more accurate over a broader range of collision energies (E') for ionic than for neutral targets, at least for cases of multipole-allowed transitions. Weak-coupling methods also require less computer execution time and programming effort. These attributes become important if one wishes to survey a large number of systems and transitions over E' extending from threshold to the high-energy asymptotic region. Such surveys are motivated by attempts to model detailed aspects of high-temperature plasmas. A specific example is the line radiation observed from tenuous high-temperature Tokamak plasmas.[3] Also the ability to extend the various weak-coupling theories into the large E' asymptotic region provides useful insights such as those discussed in Sec. III.

The practical problems encountered in evaluating the partial-wave treatment of weak-coupling theory leads one to search for methods to treat highly oscillatory integrands and to further reduce computer costs. These are motivations for this study of the Langer uniform approximation (U)[4] and the average approximation (A) developed by Riley.[5] The U approximation to continuum orbitals is anticipated to be reliably accurate for all E' and to provide one program capable of evaluating all the weak-coupling theories. A useful numerical check based on comparisons with traditional non-partial-wave Born (B) data will thereby be available. This program should be a computational method competitive with the standard Coulomb-Born (CB) method[6] and be a less time-consuming technique for evaluating the distorted-wave (DW) predictions. The U approximation also has programming advantages when applied to the DW method and it avoids the necessity for a good Coulomb function generator when evaluating the CB cross section. The range of E' for which the A approximation is useful is restricted to E' larger than several times threshold, but it does solve the oscillatory integrand problem and provides considerable savings of computer time. It should also be noted that weak-coupling theories are the most advanced to be applied routinely to the ionization problem[7] and considerable exploration remains to be done. The ionization problem is beyond the scope of this work, but the techniques being considered here appear well adapted to such a study.

Section II of this paper defines the basic weak-coupling equations being used and the specific nature of the U and A approximations. To better focus attention on these techniques, only direct scattering will be considered. Section III presents the results from a number of calculations on simple systems. These data will display the precision inherent in these techniques as a function of excess charge on the target, q, the collision energy, E', and the partial-wave collision strengths for two basic types of transitions. Cross-section data for the $2s\,^2S$-$2p\,^2P$ transition in Ne VIII are also presented. These data are used to amplify some of the above discussion where special attention is

given to the approach of the different weak-coupling theories to their high-energy limiting behavior. This example is chosen because one expects exchange effects to be relatively unimportant. Although exchange for weak-coupling theories should in general be included in a consistent way, the study of the U and A approximations in this context is deferred.[8]

II. THEORY

The generic character of weak-coupling theory for electron-atom scattering is discussed in many places.[6,9,10] Perhaps the best development starts with the weak-coupling limit of the appropriate strong-coupling theory, such as that given in Ref. 1 or in Ref. 11 for one-electron targets. Ignoring exchange effects and treating certain couplings associated with reorientation of the target as a perturbation, the continuum electron orbital must satisfy an equation having the form

$$\left[\frac{d^2}{dr^2}+p(r)\right]F_{kl}(r)=0\,, \tag{1}$$

where

$$p(r)=k^2+(2\mu/\hbar^2)[(Ze^2/r)-V(r;\nu,\nu)]-l(l+1)r^{-2} \tag{2}$$

and

$$\lim_{r\to 0}F_{kl}(r)\sim O(r^{l+1})\,, \tag{3}$$

$$\lim_{r\to\infty}F_{kl}(r)\sim k^{-1/2}\sin[kr+\alpha\ln(2kr)-(\tfrac{1}{2}l\pi)+\sigma_l]\,, \tag{4}$$

$$\sigma_l=\arg\Gamma(l+1-i\alpha)+\delta_l,\quad \alpha=qe^2/\hbar v\,. \tag{5}$$

Here, Ze is the nuclear charge of the target, v is the center-of-mass collision velocity, l is the angular momentum of the scattering electron and $\hbar^2k^2/2\mu=E$, where E is the center of mass collision energy and μ is the reduced mass of the projectile plus target. The usual radial variable is r and δ_l is the residual phase shift. The abbreviation ν has been used for the target quantum numbers and q is defined below.

In general, $V(r;\nu,\nu)$ of Eq. (2) will depend on the total angular momentum of target plus scattering electron, but it is often replaced by its spherical average in weak-coupling calculations.[10,12] The coupling to form the total angular momentum can be ignored as a consequence of this approximation and the potential becomes

$$\begin{aligned}V(r_{N+1},\nu,\nu)&\cong(2L+1)^{-1}\sum_{M_L}\sum_{i=1}^{N}\int d\Omega(\hat{r}_{N+1})\,|Y_{lm}(\hat{r}_{N+1})|^2\int d\tau_1\cdots d\tau_N\,|\Psi(LM_LSM_S)|^2(e^2/r_{i,N+1})\\&\cong(2L+1)^{-1}\sum_{M_L}\sum_{i=1}^{N}\int d\tau_1\cdots d\tau_N\,|\Psi(LM_LSM_S)|^2(e^2/r_{i,>})\,.\end{aligned} \tag{6}$$

Here Ψ describes an N-electron target with angular momentum quantum numbers LM_L and SM_S for the space and spin degrees of freedom. The abbreviation ν represents LM_LSM_S for this choice of target description. The element of solid angle for the unit vector $\hat{r}$ is $d\Omega(\hat{r})$ and Y_{lm} is a spherical harmonic. The ith electron's volume element for all degrees of freedom, including spin, is $d\tau_i$. The distance between the scattering electron and the ith target electron is $r_{i,N+1}=|\vec{r}_{i,N+1}|$ and $r_{i,>}$ is the greater of r_i and r_{N+1}. Obviously,

$$\lim_{r\to\infty}V(r;\nu,\nu)\sim Ne^2/r \tag{7}$$

results from Eq. (6). The quantity q,

$$q=Z-N\,, \tag{8}$$

defines the net charge of the target nucleus plus bound electrons.

An element of the S matrix in the weak-coupling limit is defined[11] as

$$S(kl\nu,k'l'\nu')=(4i\mu/\hbar^2)\times\int_0^\infty dr\,F_{kl}(r)V(r;\nu,\nu')F_{k'l'}(r),\quad \nu\neq\nu'\,. \tag{9}$$

The primed and unprimed quantum numbers define the quantum numbers before and after the inelastic collision, respectively. The transition potential for the inelastic event is

$$\begin{aligned}V(r_{N+1};\nu,\nu')=\sum_i\int d\Omega(\hat{r}_{N+1})Y^*_{lm}(\hat{r}_{N+1})Y_{l'm'}(\hat{r}_{N+1})\\\times\int d\tau_1\cdots d\tau_N\,\Psi^*(\nu)\\\times(e^2/r_{i,N+1})\Psi(\nu'),\quad \nu\neq\nu'\,,\end{aligned} \tag{10}$$

where, as in Eq. (6) and for reasons discussed below, the coupling to form the total angular momentum of target plus scattering electrons has been omitted.

The use of the uncoupled representation, Eq. (6), for the potential appearing in Eq. (2) obviously produces a F_{kl} independent of the total angular momentum for the scattering system.[10] Consequently, the total cross section for the uncoupled theory, when appropriately summed and averaged over space and spin degeneracies, is equal to that found by recoupling Eq. (10) to form the total angular momentum. This circumstance can be seen in the CB formulas given, for example, in Ref. 6

and noting that the total angular momentum sum in the total cross section can be done analytically. Equation (6) is an approximation only in the context of DW theory and one that should be carefully checked for transitions dominated by a few partial waves, such as spin-forbidden processes.

To finish the definition of the cross section, Ψ is taken to be a *single* determinant of one-electron orbitals having the form

$$r^{-1}R_{nl}(r)Y_{lm}(\hat{r})\delta(m_s|\sigma)\,, \tag{11}$$

where R_{nl} is an appropriately normalized radial function and the Kronecker delta function δ describes the electron spin. Both $\Psi(\nu)$ and $\Psi(\nu')$ are constructed from different subsets of the same list of orthonormal orbitals having this form. This form for Ψ will not in general be an eigenfunction with the eigenparameters implied by ν, ν', but one can always be constructed from linear combinations of such determinants. This approach is applicable either to the usual Hartree-Fock method or to configuration interaction approximations to Ψ. The appropriate changes in the following equations can be constructed once the linear combination is defined. Designating the orbital excited during the collision event by a, Eq. (10) becomes

$$V(r;\nu,\nu') = \sum_{\lambda=|l_a-l'_a|}^{l_a+l'_a} \int d\Omega(\hat{r}')d\Omega(\hat{r})Y^*_{lm}(\hat{r})Y^*_{l_am_a}(\hat{r}')P_\lambda(\cos\theta)Y_{l'm'}(\hat{r})Y_{l'_am'_a}(\hat{r}')$$
$$\times \int_0^\infty dr'\, R_{n_al_a}(r')(e^2r_<^\lambda/r_>^{\lambda+1})R_{n'_al'_a}(r'), \quad \nu \neq \nu'\,. \tag{12}$$

Here θ is the angle between $\hat{r}$ and $\hat{r}'$ and the $<,>$ subscripts indicate the lesser or greater of $|\vec{r}|$ and $|\vec{r}'|$, respectively. A few manipulations of the standard cross section formulas, given in Ref. 6 for example, show that the desired inelastic total cross section is

$$\sigma(LS, L'S') = (2L'+1)^{-1}\sum_{M_LM'_L}\sigma(\nu,\nu')$$
$$= \pi k'^{-2}(2L'+1)^{-1}(2S'+1)^{-1}\Omega(n_al_a, n'_al'_a)\,, \tag{13}$$

where

$$\Omega(n_al_a, n'_al'_a) = \sum_{l'}\Omega_{l'}(n_al_a, n'_al'_a)\,, \tag{14}$$

$$\Omega_{l'}(n_al_a, n'_al'_a) = [16e^4\mu^2(2L'+1)(2S'+1)\hbar^{-4}]$$
$$\times\sum_{l,\lambda}(2l+1)(2\lambda+1)^{-1}\left|C(l\lambda l', 00)C(l_a\lambda l'_a, 00)\int_0^\infty\int_0^\infty dr\,dr'\,F_{kl}(r)R_{n_al_a}(r')(r_<^\lambda/r_>^{\lambda+1})F_{k'l'}(r)R_{n'_al'_a}(r')\right|^2, \tag{15}$$

and C is a Clebsch-Gordan coefficient.[13] Equations (14) and (15) define the dimensionless collision strength with the normalization used in Ref. 11.

The substitution of Eq. (6) for $V(r;\nu,\nu)$ of Eq. (2) defines our DW theory. The use of Eq. (7) to define $V(r;\nu,\nu)$ for all r produces the CB cross section, and the neglect of $V(r;\nu,\nu)$ plus taking $Z=0$ in Eq. (2) defines the B cross section.

The uniform approximation[4] consists of replacing the solutions of Eq. (1)–(5) with

$$F_{kl}(r) \cong \sqrt{\pi}[d\phi(r)/dr]^{-1/2}\mathrm{Ai}[-\phi(r)]\,, \tag{16}$$

where

$$\tfrac{2}{3}[\phi(r)]^{3/2} = \int_{r_0}^{r} dt\,[p(t)]^{1/2}, \quad r \geq r_0\,,$$

$$\tfrac{2}{3}[-\phi(r)]^{3/2} = \int_{r}^{r_0} dt\,[-p(t)]^{1/2}, \quad r \leq r_0\,,$$

and it is assumed that $p(r)$, see Eq. (2), has a simple and unique zero at $r=r_0$. The regular Airy function is $\mathrm{Ai}(x)$. Also, $l(l+1)$ appearing in Eq. (2) is replaced by $(l+\frac{1}{2})^2$. This is required by Eq. (3). Equation (3) is a somewhat stronger requirement than is strictly necessary but it is a desirable quality and it has the added feature of producing the usual WKB phase-shift approximation to δ_l of Eq. (5). The use of Eq. (16) in the evaluation of Eq. (15) will result in cross sections designated by DWU, CBU, or BU, depending on the choice of $V(r;\nu,\nu)$ discussed in the preceding paragraph.

Riley's average approximation and several similar approximations have been developed in the study of heavy-particle scattering. Reference 5 cites a rather complete list of this literature. Some aspects of the heavy-particle scattering problem seem quite different from those encountered in electron scattering. However, the

evaluation of integrals of the type defined by Eq. (9) is common to the two problems and the error analysis provided in Ref. 5 leads one to expect reasonable accuracy in the electron scattering problem once the initial scattering energy E' becomes sufficiently large. Such an approximation is studied here as an alternative to developing special integration techniques for cases in which the integrand of Eqs. (9) or (15) becomes highly oscillatory.

The average approximation developed by Riley is presented in Sec. III of Ref. 5. These procedures must be followed to produce the average approximation appropriate to the present problem. The differences are mainly ones of redefinition after recognizing that the derivation in Ref. 5 implicitly assumes $l=l'$. The result, in the notation of this section, is

$$S(kl\nu,k'l'\nu') \cong (4i\mu/\hbar^2)\int_{r_s}^{\infty} dr\, V(r;\nu,\nu')2^{-1}P(r)^{-1/2}\cos[\psi(r)], \tag{17}$$

where

$$P(r)=\tfrac{1}{2}[p(r)+p'(r)],$$

$$\psi(r)=\tfrac{1}{2}\int_{r_s}^{r} dx[p'(x)-p(x)]P(x)^{-1/2},$$

and the assumed existence of a simple and unique zero of $P(r)$ defines r_s. Here, $p(r)$ is defined by Eq. (2) and the usual substitution of $(l+\frac{1}{2})^2$ for $l(l+1)$ has been made. Remember that the primed and unprimed quantities indicate use of the initial and final parameters for the scattering electron. In the CB case $\psi(r)$ is easily shown to be

$$\begin{aligned}\psi(r)=\mu\Delta E\hbar^{-2}\{&a^{-1}[X(r)]^{1/2}-(0.5ba^{-3/2})\\ &\times\ln(\{2[aX(r)]^{1/2}+2ar+b\}d)\}\\ &-[(l'+0.5)^2-(l+0.5)^2](-4c)^{-1/2}\\ &\times\{\tfrac{1}{2}\pi+\sin^{-1}[d(br+2c)r^{-1}]\},\end{aligned} \tag{18}$$

where

$$X(r)=ar^2+br+c,\quad X(r_s)=0,$$

$$a=\mu\hbar^{-2}(E+E'),\quad b=2\mu qe^2\hbar^{-2},$$

$$c=-0.5[(l'+0.5)^2+(l+0.5)^2],$$

$$d=(b^2-4ac)^{-1/2}.$$

The excitation energy is symbolized by ΔE. The quantities r_s, $P(r)$, and $\psi(r)$ are not simple algebraic expressions in the distorted-wave case but the tabular manipulations required for a given numerical $V(r;\nu,\nu)$ and $V(r;\nu',\nu')$ are relatively easy and efficient to program for a digital computer.

Study of Eqs. (17) and (18) shows that this approximation is easily evaluated if one is careful of the integrable singularities and, in fact, becomes easier as E' increases. Hence, if sufficient accuracy for this approximation can be established, the problems encountered in evaluating Eq. (9) for large E' can be avoided by use of Eq. (17).

III. NUMERICAL RESULTS

Since the object is to test the uniform approximation, Eq. (16), and the average approximation, Eq. (17), when evaluating the cross section, Eqs. (13)–(15), simple targets will be used. This will avoid any questions concerning the target orbitals used to evaluate Eqs. (6) and (12). Also most of these tests will be made using the Coulomb-Born approximation since this provides the exact solutions to Eq. (1) in the well-studied form of Coulomb functions. The inference that similar results apply to the distorted-wave case seems natural.

The first test results are shown in Figs. 1 and 2. They show the ratio

$$R(\mathrm{CBU})=\Omega_{\mathrm{CBU}}(n_al_a,n'_al'_a)/\Omega_{\mathrm{CB}}(n_al_a,n'_al'_a), \tag{19}$$

and the obvious analog R(CBA) for the reaction,

$$e^-+T^{+q}(1s)\rightarrow e^-+T^{+q}(2s). \tag{20}$$

By $T^{+q}(nl)$ we mean a one-electron target with a nuclear charge $Z=q+1$, see Eq. (8), in the indicated quantum state. A percentage error is defined by $100\,[R(\mathrm{CBU})-1]$. The variable

$$x=E'/\Delta E$$

is chosen to represent the collision energy because of Born scaling laws. [The plot of R(B)

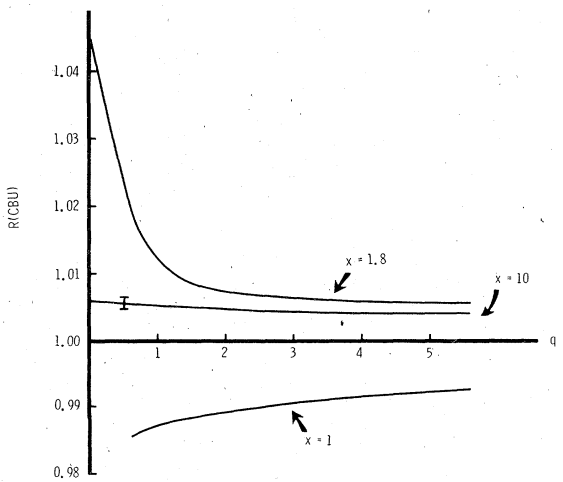

FIG. 1. R(CBU) shown as a function of x and q for the reaction defined by Eq. (20). The vertical mark indicates the precision to which these values of R are known.

versus x is independent of q.] Since data were generated only for integer q, some artistic license was exercised in the $0 \leq q \leq 1$ range where R is rapidly varying in some cases. These plots of R versus q for a few chosen values of x should give a reasonable picture of the error of the U and A approximations as a function of these parameters.

The evaluation of the U and A cross sections was carried out with an overall precision of ±1 in 10^4 while Ω_{CB} was evaluated with a greater precision. This precision limit is reflected in Figs. 1 and 2 by the vertical marks.

From Fig. 1, it can be seen that R(CBU), for $q>0$, is negative for $x=1$ and positive for $x=1.8$. These x values roughly represent the maximum deviations found for each q studied. Hence it is safe to infer that $|R-1|$ essentially is a monotonically decreasing function for increasing $x(>1.8)$ in this range of q. The behavior of R(CBU) for $q=0$ and $x=1$ is indeterminate and was not calculated by limiting procedures. Consequently, the $x=1$ curve is not well known for $q<1$.

Figure 2 shows similar data for R(CBA). The x, q surface appears more complicated for $x<2$ and $q<3$ but otherwise differing from the R(CBU) surface only by exhibiting slightly larger errors. The character of R(CBA) for $x=1$ was not established but, as pointed out in Sec. III, this approximation is not intended for use in the threshold region.

The decrease of $|R-1|$ as q increases shown in Figs. 1 and 2 is especially significant since the treatment of highly charged ions is one of the motivations for this work. This cross section for fixed x decreases roughly as Z^{-2} as q increases. Hence, the interplay of the various factors associated with the use of Eqs. (16) and (17) results in an error decreasing with increasing q even though the cross section, i.e., range of $V(r;\nu,\nu')$, is rapidly decreasing.

The study of a $1s$-$2s$ transition was chosen because it represents a "worst case" situation. The large-r behavior of $V(r;\nu,\nu')$, Eq. (12), is an exponentially decreasing function of r for this case. Hence the value of $S(kl\nu,k'l'\nu')$ will depend strongly on the behavior of the solutions to Eq. (1) for $r\sim r_0$ and the small l' terms in Eq. (14) will tend to dominate the total collision strength. U-approximation errors[1] in the transition region, $r\sim r_0$, and for small l' are therefore emphasized. Also, this should be a relatively severe test of the A approximation because of its approximate treatment of the classically forbidden regions of motion.[5]

Obviously, one could find a $V(r;\nu,\nu')$ that would produce errors larger than shown in Figs. 1 and 2. The lack of a general error analysis must be replaced by examples, such as those given here, and intuition. An example of intuition would be to suspect larger errors for extremely small cross sections for cases with oscillatory $V(r;\nu,\nu')$ because of the implied cancellations in the evaluation of Eq. (9).

To substantiate the implication that Eq. (20) does not represent the most favorable case for the U and A approximations, data for

$$e^- + C^{+5}(1s) \rightarrow e^- + C^{+5}(2p) \tag{21}$$

are presented in Fig. 3. The parameter λ in Eqs. (12) and (15) is restricted to unity for this dipole-allowed case and the longest possible interaction range is found; $V(r;\nu,\nu')=O(r^{-2})$ for r large. For example, it can be seen from Figs. 1, 2, and 3 that $|R-1|$ for $x=10$ is decreased by a factor of about 3 for the U theory and between 2 to 3 for the A theory. The situation is quite similar for the neutral analog to Eq. (21). To summarize the neutral case which is not shown, R(BU) shows an error of about 0.5% near the cross section maxi-

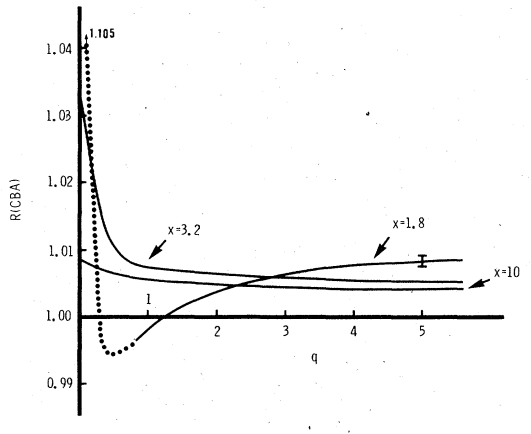

FIG. 2. R(CBA) shown as a function of x and q for the reaction defined by Eq. (20). The vertical mark indicates the precision to which these values of R are known.

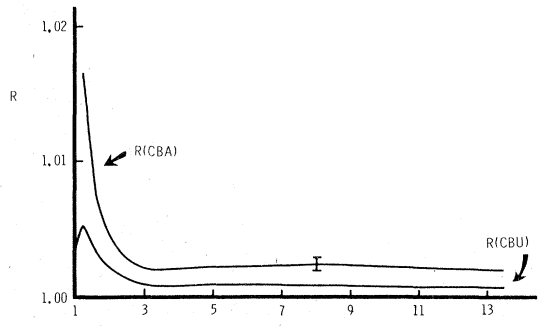

FIG. 3. R(CBU) and R(CBA) shown as a function of x for the reaction defined by Eq. (21). The vertical mark indicates the precision to which these values of R are known.

TABLE I. Values of R computed for the indicated reactions, see Eq. (19), are shown for the partial collision strengths, Eqs. (14) and (15). The column labeled "exp" gives the order of magnitude of the individual partial-collision strengths.

	Eq. (20) for $q=5$ and $x=1.835$			Eq. (21) for $x=1.835$		
l'	R (CBU)	exp	R (CBA)	R (CBU)	exp	R (CBA)
0	0.9802	−3	0.8745	1.0465	−3	0.7053
1	1.0132	−2	1.0092	0.9447	−3	1.6643
2	1.0138	−2	1.1421	0.9990	−2	0.9514
3	1.0116	−4	1.1596	1.0054	−2	0.9559
4	1.0100	−4	1.1105	1.0055	−2	0.9924
5	1.0085	−5	1.0298	1.0047	−3	1.0281
6	1.0134	−6	0.9384	1.0039	−3	1.0637
7	1.0304	−7	0.8518	1.0033	−3	1.1013
8	1.0132	−8	0.7875	1.0027	−4	1.1418
9	0.8697	−9	0.7260	1.0024	−4	1.1851
10				1.0022	−4	1.2309
11				1.0017	−5	1.2794
12				1.0012	−5	1.3291
13				1.0011	−5	1.3811
14				0.9997	−6	1.4354
15				1.0017	−6	1.4919
Total[a]	1.0051		1.0077	1.0025		1.0056

[a] These are the R values for the total collision strengths, Eq. (15).

mum, $x \cong 2$, with the error increasing as x decreases, and with an error decreasing to near the values shown in Fig. 3 as x becomes large. The R(BA) error is less than −3% for $x=2$, changes sign at $x \cong 5.5$, and never exceeds 0.3% for $x > 5.5$.

Insight into the origin of the U and A errors is provided by Table I where the partial collision strength, Eqs. (14) and (15), is shown for two cases from the above study. In general, the trends with changing l remain the same as x changes, with the errors increasing (decreasing) as x decreases (increases). The error for the total collision strength is less than that observed for a typical partial contribution in both the dipole-allowed and dipole-forbidden cases. This observation may not prove to be a rule but the general tendency for errors to cancel in the l' sum is observed here as it has been in the heavy-particle scattering studies.[5] (The lengthy sums over l' encountered in dipole-allowed cases for large x and q are avoided by the use of well-known sum rules.[14,15] This is also a useful option for DW theory if one suitably restricts the range of l' for which it is used.)

The collision strengths for the reaction

$$e^- + \mathrm{Ne}^{+7}[2s\,^2S] \rightarrow e^- + \mathrm{Ne}^{+7}[2p\,^2P]$$

are shown in Fig. 4 to provide an application of these techniques. The Ne VIII orbitals required for Eq. (11) and $\Delta E = 0.5943$ hartrees were taken from a Hartree-plus-statistical-exchange calculation.[16] These wave functions result in, from Eq. (12),

$$\lim_{r\to\infty} V(r;\,^2P,\,^2S) \sim de^2r^{-2} = (-0.6232)e^2a_0r^{-2}\,, \quad (22)$$

where d is the dipole-length matrix element. The data shown in Fig. 4 do not contain exchange contributions. These effects must ordinarily be included. However, they are unusually small for this case,[8] less than 6%, and, since the treatment of exchange in the U and A approximations is deferred to a later study, the exchange collision strengths are not presented.

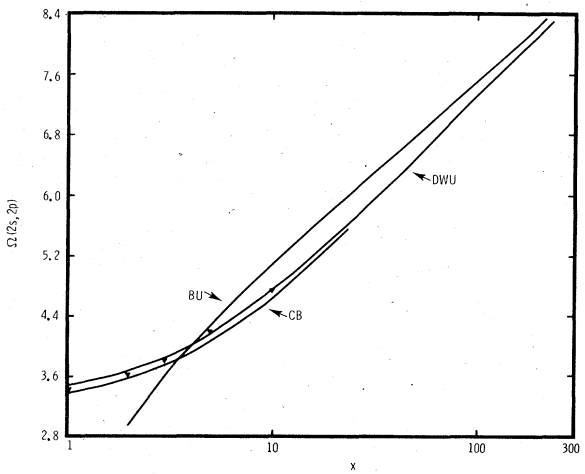

FIG. 4. Collision strength in the indicated approximations shown for Ne VIII as a function of x. The ▼ indicate CBI data taken from Ref. 12.

The CB and CBU collision strengths could not be distinguished if both were shown in Fig. 4. This is consistent with the implications of the results of the preceding examples. A similar relationship should exist for the DW and DWU collision strengths.

The A approximation is somewhat less accurate for this case than it was for the dipole-forbidden case presented above, having an error of -3.5% for $x = 1.8$ and which remains negative while decreasing in magnitude as x increases. The reason for the differences between the two dipole-allowed examples presented here is not known. Although these errors are not great, the need for some care in extrapolating the A results presented here for the one-electron targets to other cases is indicated.

Comments on the physics contained in Fig. 4 seem appropriate. Reference 17 data, which are therein labeled CBI, shown in Fig. 4 should be directly comparable to the CB data from this study. The agreement is not quantitative but certainly within the usual expectations for such comparisons. The use of different target wave functions is always a source of difficulty in these comparisons although in this case it is a relatively insensitive point.

An important and practical test based on the high-energy behavior of the cross section can be made for the case of dipole-allowed transitions. For large k', it is well known that

$$\lim_{k'\to\infty} k'^2\sigma(LS, L'S')/\pi \sim \tfrac{4}{3}\, a_0^{-2} |d|^2 \ln x \qquad (23)$$

can be established,[18] where d is defined in Eq. (22). Equation (23) determines the slope for large x that should be exhibited in curves like that shown in Fig. 4. Since d depends only on the target wave functions and is an often-studied quantity, Eq. (23) will provide at least qualitative insight into the differences between various theoretical studies. Unfortunately, Ref. 17 does not provide a value for $|d|^2$ but, since crude orbitals with Slater's scaling parameters give $|d| = 0.5938 a_0$ to be compared with that given in Eq. (22), the suspicion that the wave functions are not crucial is supported.

Equation (23) leads to another observation. The large x asymptotic slope from Fig. 4 should predict $a_0^{-2}|d|^2 = 0.3884$ while BA, CBU, and DWU(A) curves give 0.386, 0.427, and 0.420, for $100 \leq x \leq 200$. The BA prediction does not change while the others give every indication of going to the correct limiting value for x increasing beyond 400. The strong Coulomb effects contained in the CB and DW approximations, for this example, depress the cross section value compared to the B prediction. This ordering of approach to the behavior demanded by Eq. (23) is in general expected although these differences are unexpectedly large. Note that the B theory is often assumed to be quite accurate for $x \cong 100$. Since the difficult problem of extracting this slope from experimental data often leads to some discussion,[19] this Coulomb effect for positive-ion targets should not be ignored.

The differences between the slope predicted by Eqs. (22) and (23) and that found from differentiating the numerical cross section data found for this and numerous other examples[2] are typically less than 1% for sufficiently large x. This is taken as a confirmation of our numerical techniques and the precision claimed in the preceding discussion.

The only experimental test available for these data is concerned with rate coefficients. The theoretical prediction based on any of the data presented in Fig. 4, excluding the BA curve, will lie within the experimental error bars of $\pm 35\%$.[20] Rather complete theoretical studies of an isoelectronic collision event in N V are available.[21,22] The expected scaling with isoelectronic sequences leads to the following conclusions. The effects of exchange should indeed be small. Results from CB, DW, and close-coupling methods should differ only to the order of 10–20%.

The data in Fig. 4 present a reasonably accurate and complete prediction. Equation (23) provides a means to extrapolate these data up to the region of relativistic collision energy.

IV. CONCLUSIONS

The preceding material defines the uniform and average approximations as applied to weak-coupling theory for electron-atom (ion) scattering. The different examples used for error analysis are typical of results to be expected. The nature of the application will determine whether or not these approximations are considered useful. In the context of usual scattering theory, a precision of several percent is often adequate for a total cross section. The U approximation seems to meet this requirement for all x while the A approximation is not recommended for $x < 2$. A number of other systems have been treated[2] which verify these statements. All results indicate that the relative error decreases for increasing q in the range $0 \leq q \leq 7$. The cautions expressed in Sec. III should be noted if one wishes to predict differential cross sections or any quantity heavily dependent on large-angle scattering.

It is difficult to give a quantitative estimate of the savings of computer time associated with these approximations because of the large number of parameters, integration ranges, different results for different transitions, etc., that must be defined. Based on the experiences of this work, we

conclude that CB and CBU use comparable times although the CBU offers small savings in time and it makes the transition into asymptotic regions a little more easily. The DW and DWU times were not tested, but the DWU approach should offer a reasonable improvement in time as well as a savings in storage and programming requirements. The CBA and DWA approximations are 6–10 times quicker than the corresponding U approximation in the case of a dipole-allowed transition for intermediate x. The savings increase dramatically for increasing x. These savings are reduced for the dipole-forbidden case studied in Sec. III.

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