Incident-energy dependence of electron-ion collision cross sections

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It is shown that the dependence of electron-impact cross sections σ for the excitation of ions on the incident energy T can be represented by compact expressions for a wide range of T from thresholds to 10 keV. These expressions are $\sigma T = A \ln T + B + C/T + D \ln T/T$ for dipole- and spin-allowed transitions, $\sigma T = A + B/T + C/T^2 + D/T^3$ for dipole-forbidden but spin-allowed transitions, and $\sigma T = (A + BT)/(1 + CT + DT^2)$ for spin-forbidden transitions, where A, B, C, and D are constants that depend on target properties but not on T. These formulas should provide accurate cross sections in applications where many atomic cross sections are needed. Examples are presented for the excitations of Be-like Fe^{+22} ion by electron impact.

For applications in which a large number of electron-ion collision cross sections is needed, such as plasma modeling, it is convenient to represent cross sections by compact formulas so that the numerical values of the cross sections can be accurately reproduced at arbitrary incident electron energies T. The T dependence of plane-wave Born-approximation cross sections σ_{PW} for a fast (but nonrelativistic) incident electron has been known for many decades:[1,2]

$$\sigma_{PW} = (\pi a_0^2 R / T g_1) \Omega_{PW} , \quad (1)$$

with

$$\Omega_{PW} = c_1 \ln(T/T) + c_2 + c_3 R/T + \cdots , \quad (2)$$

where Ω_{PW} is the collision strength for excitation or ionization, a_0 is the Bohr radius, R is the Rydberg energy, g_i is the initial state degeneracy, and c_1, c_2, etc. are constants that depend on target properties but not on T.[3,4] Moreover, these constants represent certain physical interactions between the incident and target electrons.[1-4]

In principle, Eq. (2) can be extended further with more negative powers of T with corresponding constants. However, terms that are needed to improve the plane-wave Born-approximation cross sections affect the values of such constants, making it futile to continue such an extension. For instance, plane-wave Born-approximation cross sections for excitations of ions vanish at the threshold while Coulomb Born-approximation, distorted-wave Born-approximation, and experimental cross sections approach finite, nonvanishing values.

In this paper, a simple relationship between a plane wave and a Coulomb wave at the origin is used to infer that Coulomb Born-approximation cross section σ_{Coul} should have the form

$$\sigma_{Coul} \approx \begin{cases} \sigma_{PW}/T & \text{for low } T & (3) \\ \sigma_{PW} & \text{for high } T . & (4) \end{cases}$$

For highly charged ions, the Coulomb interaction between the incident electron and the target ion nucleus is dominant, making other details, such as electron exchange and correlation, minor corrections to the relationship (3) and (4).

Equation (2) is known as the Bethe formula; it is more reliable for high T, and $c_1 = 0$ for dipole-forbidden (but spin-allowed) transitions. The cross section for an inelastic collision in the first Born approximation is given by

$$\sigma_{if} = m^2 (2\pi\hbar)^{-4} (k'/k) \int d\Omega_{\mathbf{k}'} \, | V_{if} |^2 , \quad (5)$$

with the interaction matrix element V_{if} defined as

$$V_{if} \Big\langle \phi_{\mathbf{k}'}(\mathbf{r}_0) \Psi_f(\mathbf{r}_1, \ldots, \mathbf{r}_N) \times \left| \sum_{j=1}^{N} \frac{e^2}{| \mathbf{r}_j - \mathbf{r}_0 |} \right| \phi_{\mathbf{k}}(\mathbf{r}_0) \Psi_i(\mathbf{r}_1, \ldots, \mathbf{r}_N) \Big\rangle , \quad (6)$$

where $\hbar$ = (Planck's constant)/2π, m is the electron mass, e is the electronic charge, $\hbar\mathbf{k}$ and $\hbar\mathbf{k}'$ are the momenta of the incident and scattered electrons, Ψ_i and Ψ_f are the initial- and final-state wave functions of the target ion, $\phi_{\mathbf{k}}$ and $\phi_{\mathbf{k}'}$ are the wave functions of the incident and scattered electrons, and $\mathbf{r}_j$ are the electron coordinates.

The only difference in the plane-wave Born-approximation and the Coulomb Born-approximation cross sections is in the choice of $\phi_{\mathbf{k}}$ and $\phi_{\mathbf{k}'}$: plane waves are used in the former while Coulomb waves are used in the latter. From Eqs. (5) and (6) we see that the ratio $\sigma_{Coul}/\sigma_{PW}$ depends on the ratio of continuum wave functions at all $\mathbf{r}_0$. When the interaction with the nucleus dominates, however, the wave-function ratio at the origin will decisively influence the cross-section ratio.

The ratio of a Coulomb wave to a plane wave of the same wave vector at the origin is well known.[5] For an attractive interaction,

$$R(k)=|\phi_{\mathbf{k}}(r=0)|^2_{\mathrm{Coul}}/|\phi_{\mathbf{k}}(r=0)|^2_{\mathrm{PW}}$$
$$=2\pi Z/[k(1-e^{-2\pi Z/k})] , \quad (7)$$

where Z is the nuclear charge of the target ion. Furthermore,

$$R(k)\simeq\begin{cases}2\pi Z/k & \text{for small } k\\ 1 & \text{for large } k .\end{cases}$$

The cross-section ratio depends on $R(k)R(k')$, $T=(\hbar k)^2/2m$, and $T-E=(\hbar k')^2/2m$, where E is the excitation energy:

$$\sigma_{\mathrm{Coul}}/\sigma_{\mathrm{PW}}\simeq\begin{cases}1/\sqrt{T(T-E)} & \text{for low } T \quad (8)\\ 1 & \text{for high } T . \quad (9)\end{cases}$$

Since we are interested more in a compact expression for cross sections than an exact one, we take only the leading term in Eq. (8), i.e.,

$$\sigma_{\mathrm{Coul}}/\sigma_{\mathrm{PW}}\simeq 1/T \quad \text{for low } T . \quad (10)$$

When Eq. (10) is applied to (2), the only new T dependence is $\ln T/T$, which is expected to be important for low incident energies. By combining Eqs. (2), (9), and (10), we can conclude that the following T dependence should be sufficient to represent σ_{Coul} at a wide range of T:

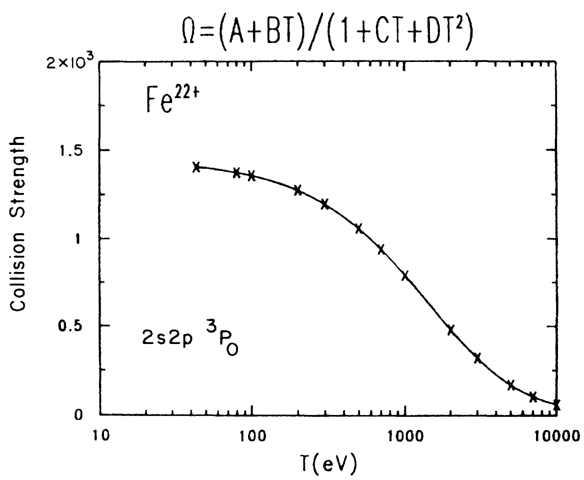

FIG. 1. Collision strength for the $2s^2\,{}^1S_0\rightarrow 2s2p\,{}^3P_0$ transition of Fe^{+22}. A multiconfiguration Dirac-Fock wave function $(2s^2+2p^2)$ was used to describe the initial target state and relativistic distorted waves were used for the incident and scattered electrons. Note that this is a spin-forbidden and optically forbidden $(J=0\rightarrow J=0)$ transition. The solid curve represents the collision strength fitted using Eq. (17) and crosses are the original theoretical values (except for the threshold value at $T=43.4$ eV, which was extrapolated from those at higher T).

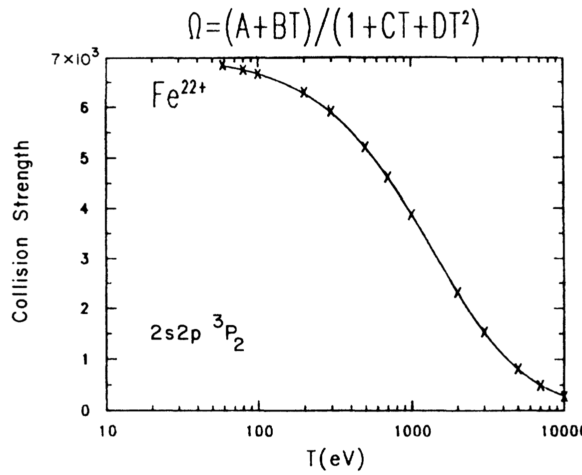

FIG. 2. Collision strength for the $2s^2\,{}^1S_0\rightarrow 2s2p\,{}^3P_2$ transition of Fe^{+22}. See Fig. 1 for legends. This is an electric quadrupole allowed but spin-forbidden transition. The solid curve represents the collision strength fitted using Eq. (17).

$$\sigma_{\mathrm{Coul}}=(\pi a_0^2 R/Tg_i)\Omega_{\mathrm{Coul}} , \quad (11)$$

with

$$\Omega_{\mathrm{Coul}}=A\ln(T/R)+B+CR/T+D\ln(T/R)/(T/R) , \quad (12)$$

where A, B, C, and D are constants that depend on the target ion properties but not on T. As in the case of σ_{PW}, $A=D=0$ for a dipole-forbidden (but spin allowed) transition. We used R as the energy unit in Eq. (12) and subsequent equations, but it could be replaced by any energy unit (as we did in Table I).

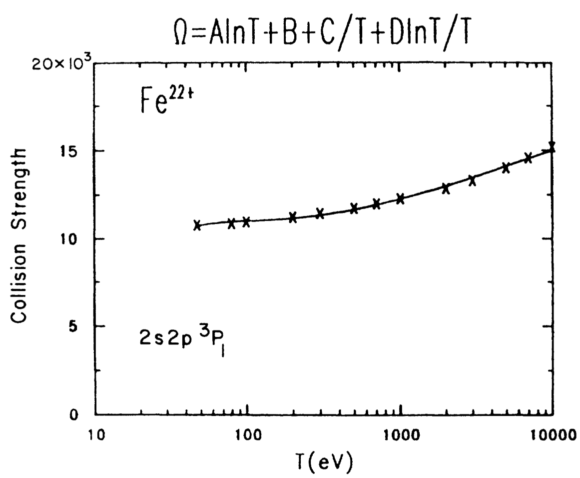

FIG. 3. Collision strength for the $2s^2\,{}^1S_0\rightarrow 2s2p\,{}^3P_1$ transition of Fe^{+22}. See Fig. 1 for legends. The final state of the ion was described by a multiconfiguration Dirac-Fock wave function to account for the intermediate coupling. This is a dipole-allowed but (nonrelativistically) spin-forbidden transition. The solid curve represents the collision strength fitted using Eq. (12).

TABLE I. Collision strength fitting parameters [Eqs. (12) and (17)] for the electron-impact excitation of Fe^{+22} from its ground state ($1s^2 2s^2$, $J=0$). Incident energy T must be given in the units indicated. 1 a.u. = 27.2114 eV. The numbers in square brackets are powers of 10.

Excited state	Fitted equation	Energy unit (a.u.)	A	B	C	D
$2s2p\ ^3P_0$	(17)	10	1.443[−3]	5.696[−6]	1.779[−1]	1.444[−2]
$2s2p\ ^3P_1$	(12)	1	1.408[−3]	6.607[−3]	3.108[−3]	4.840[−3]
$2s2p\ ^3P_2$	(17)	10	7.101[−3]	5.001[−5]	1.774[−1]	1.679[−2]
$2s2p\ ^1P_1$	(12)	1	1.164[−1]	−5.145[−2]	2.598[−1]	3.651[−1]

For a dipole-forbidden (but spin-allowed) transition, both logarithmic terms in Eq. (12) vanish, thus providing the possibility of introducing more negative powers of T in the collision strength for a better representation of the cross section. For instance, Ω_{Coul} in Eq. (11) should be replaced by

$$\Omega_{\text{forb}} = A + BR/T + C(R/T)^2 + D(R/T)^3 \ . \quad (13)$$

So far, our discussion has been nonrelativistic and hence did not mention spin. In the nonrelativistic context, a spin flipping collision can take place if the incident electron replaces one of the target electrons with opposite spin. One can show[6] that, for a spin flipping collision, the plane-wave Born-approximation cross section approaches

$$[\sigma_{\text{exch}}]_{\text{PW}} \propto T^{-3} \quad (\text{i.e., } [\Omega_{\text{exch}}]_{\text{PW}} \propto T^{-2}) \quad \text{for high } T \ . \quad (14)$$

We found, however, that our distorted-wave *cross sections* for Be-like ions [$(2s^2, J=0) \rightarrow (2s2p, J=0,2)$ transitions] behave like

$$[\sigma_{\text{exch}}]_{\text{DW}} \propto T^{-2} \quad (\text{or } [\Omega_{\text{exch}}]_{\text{DW}} \propto T^{-1}) \quad \text{for high } T \ . \quad (15)$$

Moreover, when we use partial wave expansions of plane waves, i.e., spherical Bessel functions, in lieu of distorted waves, we do indeed find expected asymptotic behavior, Eq. (14). This is an indication that distorted-wave cross sections for spin-forbidden transitions have a different asymptotic behavior from that of plane-wave cross sections. Dillon[7] noticed that electron-impact experimental data on the $1s^2\ ^1S_0 \rightarrow 1s2s\ ^3S_1$ and $1s^2\ ^1S_0 \rightarrow 1s4s\ ^3S_1$ of He exhibited $\sigma \propto T^{-2}$ asymptotic behavior. This difference in the asymptotic behavior cannot be ascribed to relativistic interactions because we used only the Coulomb repulsion as the interaction between the incident electron and the target ion [see Eq. (6)]. This difference should be studied further, perhaps by comparing theoretical and experimental angular distributions of the scattered electron.

After some trial, we found that a Padé approximant of the form

$$\sigma_{\text{exch}} = (\pi a_0^2 R / T g_i)\Omega_{\text{exch}} \ , \quad (16)$$

with

$$\Omega_{\text{exch}} = (A + BR/T)/(1 + CR/T + DR^2/T^2) \quad (17)$$

fitted calculated cross sections for spin- (and dipole-) forbidden transitions very well. As in Eqs. (12) and (13), A, B, C, and D in Eq. (17) are constants that depend on the target ion properties but not on T. Unlike in Eqs. (12) and (13), however, the fitting constants in Eq. (17) do not represent any particular physical interaction.

Since the T dependence in Eqs. (12), (13), and (17) is based on qualitative arguments rather than on an exact mathematical relationship, we expect the T dependence also to apply to distorted-wave Born-approximation cross sections. Indeed, we found that Eqs. (12), (13), and (17) can fit distorted-wave Born-approximation cross sections for both spin-allowed and spin-forbidden excitations of ions by electron impact from threshold to 10 keV. Formulas similar to Eq. (12) with the $\ln T/T$ term have been used by others,[8] but the origin of the term has never been clarified.

When the incident electron energy exceeds 10 keV, relativistic forms of these fitting formulas must be used.[9,10] For instance, T/R in the logarithmic terms must be replaced by $[\beta^2/(1-\beta^2)-\beta^2]$, where β is the speed of the incident electron in units of the speed of light c. There are other changes needed to express cross sections in terms of β^2, but such refinements (though important for $T > 10$ keV) would make these formulas far more complicated, thus defeating our original intention of getting simple and compact expressions.

We present in Figs. 1–3 applications of Eqs. (12) and (17) to electron-impact excitations of Be-like Fe^{+22} ion from its ground state $1s^2 2s^2\ ^1S_0$ to the $1s^2 2s2p\ ^3P_{0,1,2}$ levels. The theoretical cross sections were calculated in the distorted-wave Born approximation[11] using relativistic wave functions for the target, incident, and scattered electrons. The fitted results reproduce the original cross sections to better than 1% everywhere except at the thresholds and at $T = 10$ keV. Details of our relativistic distorted-wave Born-approximation calculations have been reported elsewhere.[12] Near the threshold, however, we found that the behavior of cross sections fitted to Eq. (12) is sensitive to how close the first theoretical point is to the threshold. We recommend that the cross sections at the threshold be provided (e.g., by extrapolating theoretical points as we did in Figs. 1–3) before Eq. (12) is used for fitting. The actual values of the fitted parameters are given in Table I.

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