INELASTIC ELECTRON-ION SCATTERING IN A DENSE PLASMA

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ABSTRACT

The Born approximation was used to investigate the influence of a dense plasma on the inelastic scattering of electrons by one-electron ions. Scaled collision strengths $Z^2\Omega$ for $1s + 2s$, $1s + 2p$ and $2s + 2p$ transitions in an ion of arbitrary nuclear charge Z were computed for a Debye-Hückel model of the screened Coulomb interaction. Over a wide range of screening lengths, the effect of the plasma environment is to appreciably reduce cross sections just above threshold.

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1. INTRODUCTION

The interpretation of line emission from dense, high-temperature plasmas, such as those occurring in inertial confinement fusion experiments, requires detailed knowledge of spectroscopic and collision properties of ions under extreme conditions (Bekefi *et al.*, 1976; Boiko *et al.*, 1979; and Weisheit, 1981). Some progress has been made in determining the influence of the plasma on atomic structure (Rogers *et al.*, 1970; Rozsnyai, 1972). However, very little is known about plasma effects on important collisional processes. Cross sections for electron impact excitation and ionization of isolated positive ions are finite at threshold because of the long-range Coulomb interaction between the collision partners (Massey and Burhop, 1969), but in a dense plasma partial shielding by nearby charged particles reduces this electrostatic interaction at large separations. Therefore, we expect the effects of plasma screening on collision cross sections to be most significant in the near-threshold region. Moreover, it is this energy regime to which thermal excitation rates often are most sensitive since, in many important instances, the excitation threshold exceeds the plasma electrons' mean kinetic energy.

This paper reports the first model calculations of inelastic cross sections for collisions of electrons with hydrogenic ions in dense, hot plasmas. In Sec. 2 our model is described, and in Secs. 3 and 4 our results are presented and discussed. Unless otherwise noted, quantities are expressed in atomic units.

2. THEORETICAL MODEL

The cross section for the transition $n'l_a \rightarrow n'l'_a$ in a one-electron ion, induced by an incident electron having initial kinetic energy $E = k^2/2$, is given by (cf. Seaton, 1961)

$$Q(nl_a + n'l'_a) = \left[\frac{\pi}{(2l_a + 1)k^2} \right] O(nl_a, n'l'_a), \quad (1)$$

where the collision strength O is defined in terms of the partial collisions strengths and transition (T) matrix elements,

$$\gamma_L(nl_a, n'l'_a) = \frac{\pi}{L} Q_L(nl_a, n'l'_a), \quad (2)$$

and where

$$\gamma_L(nl_a, n'l'_a) = (2L + 1) \sum_{q, q'} \{T(nl_a q, n'l'_a q'; L)\}^2. \quad (3)$$

The small spin-dependent interactions between the incident electron and the ion are ignored, so the total orbital angular momentum $\vec{L}$ is conserved in the collision. In Eqs. (2) and (3), L takes on all values consistent with the vector addition of $\vec{l}_a$ and the partial wave angular momentum $\vec{l}$, viz. $|\vec{l}_a + \vec{l}| \geq L \geq |\vec{l}_a - \vec{l}|$ and $|\vec{l}_a + \vec{l}| \geq L \geq |\vec{l}_a - \vec{l}|$.

The exchange contribution to Q is neglected and the collision problem is formulated in the first Born approximation. These simplifications permit the series of partial-wave contributions in Eqs. (2) and (3) to be summed formally to yield the familiar integral expression for the collision strength,

$$Q(nl, n'l') = 2 \int_{K_{\min}}^{K_{\max}} K dK |f_{n'l', nl}^B(\vec{k})|^2, \quad (4)$$

where the momentum change $\vec{K}$ of the scattered electron varies in magnitude from $K_{\min} = |\vec{k} - \vec{k}'|$ to $K_{\max} = |\vec{k} + \vec{k}'|$, with $\Delta E(n, n') = 1/2 (k^2 - k'^2)$ being the threshold energy for excitation. The first Born scattering amplitude f^B is related to the matrix element of the electron-ion interaction V according to the formula

$$f_{n'_a, n_a}^B(\vec{K}) = \frac{1}{2\pi} \int d\vec{r}_1 e^{i\vec{K} \cdot \vec{r}_1} \langle n'_a | V | n_a \rangle, \quad (5)$$

where $\vec{r}_1$ is the position of the projectile electron.

When the electrostatic interaction energy of particles in a plasma is much less than their mean kinetic energy, an approximate solution of Poisson's equation can be obtained for the potential of a test charge at rest in the plasma. It is well-known (Krall and Trivelpiece, 1973) that in this case the Coulomb potential is shielded, and reduced by the factor $\exp(-r/\lambda)$, where (in c.g.s. units)

$$\lambda = \left(\frac{4\pi e^2}{k_B T} \sum_j N_j Z_j^2 \right)^{-1/2} \quad (6)$$

is the Debye-Hückel screening length for a plasma of temperature T that has a density N_j of particles with charge Z_j . Here, the test charge is a hydrogenic ion possessing some thermal energy. Because of its motion, only the electrons are generally effective in providing efficient shielding (Krall and Trivelpiece, 1973), so that

$$\Lambda + \Lambda_e = (k_B T / 4\pi e^2 N_e)^{1/2} \quad (7)$$

is the screening length appropriate to the scattering process.

The Debye-Hückel approximation of the interaction is invalid in the limit of high densities and low temperatures. However, even when it is necessary to resort to a full solution of Poisson's equation, it is found (cf. Stewart and Pyatt, 1966) that far from the ion of interest the Debye-Hückel form is regained. Thus, we expect the exponentially screened electron-ion Coulomb interaction,

$$V(\vec{r}_1, \vec{r}_2) = \left(-\frac{Z}{r_1} + \frac{1}{|\vec{r}_1 - \vec{r}_2|} \right) \exp(-r_1/\Lambda) \quad (8)$$

where $\vec{r}_2$ is the position of the bound electron, to be a reasonable representation of plasma screening in the collision, especially where long-range contributions dominate. With this choice of screening, the electron-nucleus term does not contribute to the transition matrix element $\langle n' p'_a | V | n l_a \rangle$.

Measurements by Niegler and Griem (1976) of the shifts of transition wavelengths of radiating ions in plasmas suggest that the Debye-Hückel model provides a poor description of screening near the nucleus; in fact, none of the standard model potentials seems adequate in this regard. Therefore, we have chosen unscreened hydrogenic wave functions to evaluate the relevant

atomic matrix elements for most of the calculations. Besides simplicity, this choice has the added virtue of isolating the collisional effects of a screened Coulomb interaction.

The Born approximation to the scattering problem is accurate under conditions of weak coupling between target states and weak distortion of the scattered electron wave function. These conditions generally are met for the higher-order partial waves at a given impact energy, or for the total cross section in the high-energy limit. In consequence, our numerical results for the collision strengths σ probably are only qualitatively correct in the region near threshold. We have calculated partial-wave contributions σ_L as well as total collision strengths in order to get some feeling for the overall validity of the scattering calculations. These computations will be discussed in the next section.

3. NUMERICAL RESULTS

By taking advantage of the scaling properties of this collision problem with respect to nuclear charge, namely,

$$k = k(Z) = Zk(1), \quad \Lambda = \Lambda(Z) = Z^{-1}\Lambda(1), \quad \sigma = \sigma(Z) = Z^{-2}\sigma(1), \quad (9)$$

we need only to carry out the calculations for a one-electron "ion" of nuclear charge $Z = 1$. This scaling is exact for the Born (not Coulomb Born) approximation, but only approximate in general (Burgess et al., 1970). We report only the collision strength σ , since it is a convenient quantity for purposes of comparison. In the absence of strong coupling between target

states, collision strengths for unscreened ions vary smoothly with the collision energy (Burgess et al., 1970; Oh et al., 1978).

To illustrate the relative behavior of the partial-wave contributions for the $1s + 2s$ and $1s + 2p$ transitions, we show in Figs. 1 and 2 the contributions to $Z^2\Omega$ of individual L -values. Curves are plotted for several values of the (scaled) screening length $\Lambda Z = \Lambda(1)$, at the (scaled) collision energy $1/2 (k/Z)^2 = 2.25$ a.u. It is apparent in comparing Figs. 1 and 2 that the short-range (exponential) nature of the $1s + 2s$ matrix element of the screened interaction potential results in a more rapid decrease of the partial-wave contributions with increasing L than is the case for the $1s + 2p$ transition. For the latter optically allowed transition the coupling matrix element in Eq. (5) behaves asymptotically as r^{-2} (Seaton, 1961). Thus, the higher-order partial waves, which can probe only the region $r \gtrsim 1/k$, are more sensitive to the plasma screening of the long range r^{-2} coupling matrix element.

The total scaled $1s + 2s$ and $1s + 2p$ collision strengths $Z^2\Omega$ are given in Figs. 3 and 4, respectively, for the screening lengths $\Lambda Z = 10, 20, 50$, and $100 a_0$, as well as for an infinitely large screening length, $\Lambda Z = \infty$. An infinite value of ΛZ yields the plane-wave Born approximation for the unscreened one-electron ion. As expected from the behavior of the partial-wave contributions, the $1s + 2p$ transition exhibits significantly greater sensitivity to screening effects of the plasma than does the $1s + 2s$ transition. Near threshold, where distortion effects are expected to be important, the Born results, unfortunately, may be quite misleading. For the pure Coulomb case, the inelastic collision strengths and cross sections are finite at threshold. The Coulomb Born cross sections do exhibit this behavior while the plane-wave Born results do not. Coulomb Born I (CBI) results of Burgess et al., (1973) are also shown in Figs. 3 and 4 for the case $Z = 2$.

For finite screening lengths, the "correct" collision strengths and cross sections will vanish at threshold due to the distortion of the final-state continuum wave function by the long-range average electron-ion interaction. Of course, none of these calculations takes into account resonances (Massey and Burhop, 1969; Burke *et al.*, 1964) which in the weak-screening (large Λ) limit should be present in abundance. Although a more realistic representation of the plasma-ion interaction might be expected to wash out narrow resonances, they could still influence thermal reaction rate coefficients. Finally, collision strengths calculated for screened target-state energies (Rogers *et al.*, 1970) are also given in Figs. 3 and 4. The effects are seen to be relatively small.

The $2s \rightarrow 2p$ collision strength exhibits a strong sensitivity to plasma screening of the electron-ion interaction, as illustrated in Fig. 5. Plasma screening modifies atomic eigenvalues, but even at very high densities the predicted level shifts are small (Skupsky, 1980). Lifting the $2s$, $2p$ orbital angular momentum degeneracy of the hydrogenic states by using the correct eigenvalues (Rogers *et al.*, 1970) for the Debye-Hückel screened ion, we obtain the results plotted as closed circles in Fig. 5. Except just above threshold (not apparent in the figure), there is no noticeable change in $Z^2 Q(2s, 2p)$, in marked contrast to the pure Coulomb case (Burgess *et al.*, 1970).

We also investigated an alternative Debye-Hückel screening model in which the electron-electron interaction is modified by the non-spherical term $\exp(-|\vec{r}_1 - \vec{r}_2|/\Lambda)$; this represents a picture wherein the bound electron carries its own cloud of screening charge. Because the orbital speed of the bound electron is much greater than the speeds of most plasma electrons, in this alternative picture the "relevant" screening length should probably be much greater than Λ_e . However, this aside, the calculations show that by

ignoring the concentration of charge around the ion as a whole, the net effect of screening is already reduced. For example, the calculated collision strengths for spherical screening are numerically similar to the non-spherical-screening results if the screening length used in the former is about five times that used in the latter.

4. DISCUSSION

As mentioned in the introduction, collisional transition rates are needed to interpret line emission from dense plasmas. The general expression for the thermal rate coefficient (i.e., the velocity averaged cross section) for the excitation $n'l_a \rightarrow n'l'_a$ in a hydrogenic ion of nuclear charge Z is

$$Q(n'l_a \rightarrow n'l'_a) = \frac{8.01 \times 10^{-8} \bar{\sigma}(n'l_a, n'l'_a)}{(2l_a + 1)Z^2 A^{1/2}} e^{-\gamma_0} \text{ cm}^3/\text{s}, \quad (10)$$

where $Z^2 A(\text{eV}) = k_B T$ is the plasma temperature in units of electron volts, $\gamma_0 = \Delta E(n'l_a, n'l'_a)/Z^2 A$, and

$$Z^2 \bar{\sigma}(n'l_a, n'l'_a) = \int_0^\infty d\gamma Z^2 \sigma(n'l_a, n'l'_a) e^{-\gamma}, \quad (11)$$

with $\gamma = E/Z^2 A - \gamma_0$ being the integration variable.

As an illustration of the influence of plasma screening, consider the $1s \rightarrow 2s$ transition, whose unscreened hydrogenic collision strength (Burgess et al., 1970; Oh et al., 1978), $Z^2 \sigma^{(H)}(1s, 2s) = 0.45$, for large Z , is

essentially independent of energy. The screened hydrogenic collision strengths (for arbitrary Z) can be approximated by the formula

$$Z^2 \sigma_{\infty}(1s, 2s) = Z^2 \sigma_{\infty} [1 - e^{-\gamma(E/\Delta E - 1)}], \quad (12)$$

where $Z^2 \sigma_{\infty}$ is the asymptotic ($E/\Delta E \gg 1$) value and γ is an adjustable parameter. Substitution of this expression into Eq. (11) yields

$$Z^2 \sigma(1s, 2s) = Z^2 \sigma_{\infty} [\gamma / (\gamma + \gamma_0)]. \quad (13)$$

Typically, a given stage of ionization is predominant in a plasma when its ionization potential is a few times the temperature $Z^2 a_0$. Choosing $\gamma_0 = 3$, we find that plasma screening decreases the excitation rate coefficient $\sigma(1s, 2s)$ to 0.33, 0.27, and 0.23, times its unscreened value when $Z\Delta = 100a_0$, $20a_0$, and $10a_0$, respectively. It is clear from Figs. 3 and 4 that the $1s + 2p$ transition rate coefficient will be even more severely reduced at a given $Z\Delta$ -value. However, because $\gamma_0 = 0$ for the $2s + 2p$ transition, plasma screening has a somewhat smaller effect on its collisional rate coefficient.

A specific numerical example is provided by a University of Rochester experiment (Yaakobi *et al.*, 1979) in which a neon-filled glass microballoon was imploded by intense laser irradiation. Strong resonance lines of hydrogen-like and helium-like neon ions were observed, and the plasma conditions were estimated to be $N_e = 7 \times 10^{22} \text{ cm}^{-3}$ and $Z^2 a_0 = 300 \text{ eV}$. These

values yield $\nu_0 = 3.3$ and $Z\lambda_e = 92a_0$. Even though our Born calculations are only qualitatively correct, they suggest that significant reductions of collisional rate coefficients are likely to result from screening effects in the dense plasmas now being generated in many laboratories.

In the future, we intend to perform "few-state" close coupling calculations for some screened-Coulomb scattering processes. Comparison with the Born results should enable us to estimate the importance of distortion and strong-coupling effects. Some measure of the influence of exchange and correlation effects can be obtained by appropriately scaling the low-order partial-wave collision strengths from accurate bare-ion calculations (see for example review by Henry, 1980) in a manner consistent with our (plasma) close coupling studies. Other issues to be examined included possible modification of the long-range polarization interaction since plasma screening not only reduces the electric field of the incident electron, but also perturbs the ion, thereby changing its polarizability α . This could affect the threshold behavior of collision cross sections (Gaillitis and Damburg, 1963). Another problem concerns the handling of plasma screening for transitions to or from ionic states with non-zero ν_a -values, the screening factor $\exp(-r/\lambda)$ being appropriate only for spherical charge distributions. If an ion's net electrostatic potential outside the region of its ν_a bound electrons is represented by a multipole expansion, say

$$\Phi_{ion}(\vec{r}_1) = \sum_{\lambda=0,2,\dots}^{2\nu_a} \left[\frac{P_\lambda(\cos\theta_1)}{r_1^{\lambda+1}} M_\lambda(\vec{r}_2) \right], \quad (14)$$

where $M_0 = (Z - \nu_b)$, it can be shown that Debye-Hückel screening reduces each multipole term M_λ by the factor

$$e^{-r_1/\Lambda} \left[\sum_{\mu=0}^{\lambda} \binom{\lambda}{\mu} \frac{(\lambda+\mu)!}{(2\lambda)!} \left(\frac{2r_1}{\Lambda} \right)^{\lambda-\mu} \right] \quad (15)$$

(This formula is valid as long as $\Lambda \gg$ effective size of the ion.) While it is straightforward to include this change in the diagonal coupling matrix elements, it is not clear how an appropriate modification of the off-diagonal coupling matrix elements can be made.

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FIGURE CAPTIONS

- Fig. 1 Partial collision strengths $Z^2\gamma_L$ as a function of L for the $1s + 2s$ transition at energy $E/Z^2 = 2.25$ a.u. and screening lengths $\Lambda Z = 10, 20, 50$ and $100 a_0$.
- Fig. 2 Partial collision strengths $Z^2\gamma_L$ as a function of L for the $1s + 2p$ transition at energy $E/Z^2 = 2.25$ a.u. and screening lengths $\Lambda Z = 10, 20$ and $50 a_0$.
- Fig. 3 Total collision strengths $Z^2\gamma$ as a function of energy E/Z^2 (in a.u.) for the $1s + 2s$ transition for screening lengths $\Lambda Z = 10, 20, 50, 100$ and ∞a_0 (—). Results corresponding to screened target-state energies for $\Lambda Z = 10 a_0$ and $20 a_0$ (----) are above the respective unscreened-energies curves. Coulomb Born I (CBI) results for $Z = 2$ are also shown.
- Fig. 4 Total collision strengths $Z^2\gamma$ as a function of energy E/Z^2 (in a.u.) for the $1s + 2p$ transition for screening lengths $\Lambda Z = 10, 20, 50$ and ∞a_0 (—). Results corresponding to screened target-state energies for $\Lambda Z = 10 a_0$ (closed circles) are just above the unscreened-energies curve. Coulomb Born I (CBI) results for $Z = 2$ are also shown.
- Fig. 5 Total collision strengths $Z^2\gamma$ as a function of energy E/Z^2 (in a.u.) for the $2s + 2p$ transition for screening lengths $\Lambda Z = 10$ and $20 a_0$ (—). Results for screened target-state energies are also shown (closed circles).

Figure 1

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Figure 4

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