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Quantum-Mechanical Calculation for the Electron-Impact Broadening of the Resonance Lines of Singly Ionized Magnesium†

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Using close-coupling calculations of Burke and Moores for the scattering of electrons by Mg^+ ions in the $3\,^2S_{1/2}$ and $3\,^2P_{1/2,3/2}$ states, Baranger's expression for the impact approximation width of an isolated line is implemented for the components of the resonance doublet. These widths are extrapolated to below inelastic thresholds and averaged over elastic resonances according to theoretical threshold laws. In the experimental energy range, results compare reasonably with semiclassical approximations and with a semiempirical method involving effective Gaunt factors extrapolated to zero electron energy.

I. INTRODUCTION

While semiclassical calculations[1,2] of the broadening of atomic lines by electron impacts are generally in satisfactory agreement with measurements[3] (to about ±20% in terms of widths), ion lines were found to be wider than calculated (assuming straight perturber paths) by factors $\gtrsim 2$ in numerous experiments. However, measured widths were shown in a preceding paper[4] to fit (by factors ~ 1.5 on the average) a semiempirical formula containing effective Gaunt factors, which are only functions of $kT/\Delta E$, i.e., the ratio of perturber (thermal) energy and splitting between levels connected by allowed dipole transitions. These effective Gaunt factors are analogous to those used to estimate inelastic cross sections,[5] but had to be extrapolated[4] below threshold energies to obtain "optical" cross sections in satisfactory agreement with experiment. Presumably this accounted for elastic collisions which would then dominate for $kT/\Delta E \lesssim 1$, a common situation for isolated (not hydrogenic) ion lines. (For atomic lines, the opposite situation $kT/\Delta E > 1$, tends to prevail.)

The importance of elastic contributions had been realized before,[6,7] but their estimations using either a second-order impact parameter method[6,8] (which is, therefore, only first order in the phase shifts, while at least quadratic terms are needed for line widths) or an adiabatic classical-path approximation[7] (which had to be supplemented by semiquantitative criteria to separate inelastic collisions) were almost as *ad hoc* as the effective Gaunt factor method and were much more involved. More-

over, it seemed doubtful whether any semiclassical approximation would be useful for $kT/\Delta E \lesssim 1$ and small relative angular momentum quantum numbers of the perturbing electrons ($\ell \lesssim 5$ in typical cases).[4] One of the obvious shortcomings of these approximations is the appearance of discontinuities at inelastic thresholds, which were, for example, avoided in Alekseev and Yukov's work[8] by simply integrating the inelastic terms over all perturber velocities, including the below-threshold range.

When the discrepancy with (straight) classical-path calculations was first pointed out,[9] an obvious remedy was the replacement of straight by hyperbolic classical paths which, as emphasized before,[10] leads to a considerable increase in the inelastic cross sections near threshold. And indeed, some hyperbolic classical-path calculations[11,12] carried to second order in the iterated solution of the time-dependent Schrödinger equation (which, therefore, could account explicitly only for inelastic collisions) agreed reasonably well with experiments. However, one of these calculations[11] included terms that would be absent in the case of weakly interacting systems[4,13] and are difficult to evaluate quantitatively. The other calculation[12] involved the use of second-order perturbation theory also for some so-called strong collisions, thus violating unitarity.[4] Replacement of straight by hyperbolic perturber orbits in the classical-path (impact-parameter method) theory,[1] therefore, may not be sufficient to remove all the disagreements with measured widths of isolated ion lines.

Inclusion[10,12] of higher (quadrupole) terms in the multipole expansion for the interaction Hamiltonian does not affect the widths very much in most practical (i.e., $kT \ll \mathrm{Ry} = 13.6$ eV) cases, nor do superelastic collisions seem to be very important. Finally, while it is known[14] that a properly symmetrized impact-parameter (classical-path) method[15] yields inelastic cross sections for optically allowed (dipole) transitions in fair agreement with quantum-mechanical calculations, and that the (symmetrized) impact-parameter method is essentially equivalent to the semiclassical Coulomb excitation theory[16] used in one[12] of the earlier calculations not allowing explicitly for elastic collisions, this procedure still leads to discontinuities at inelastic thresholds. It is thus subject to similar doubts as the other versions of the semiclassical approximation.

In view of the uncertainties of semiclassical calculations and because of the absence of any *ab initio* calculations for the elastic contributions, we undertook the present, fully quantum-mechanical calculations, using results of the close-coupling method.[17] A disadvantage of this method is the restriction to a small number of interacting states ($3S$, P, and D in our case) because of the computational effort. This restriction, while limiting the estimated accuracy of the results presented here to $\sim \pm 20\%$, should not seriously impair comparisons with the various semiclassical or semiempirical methods, if they are also restricted to the same set of interacting states. However, in the case of Ca^+, where $4S$, $3D$, and $4P$ are allowed for in the close-coupling calculations,[17] omission, especially of $4D$, would seem to lead to large errors in the width of the resonance line ($4S$-$4P$), thus invalidating even such relative comparisons. (A similar situation prevails for heliumlike and lithiumlike ions.) The Mg^+ resonance doublet components thus appear to be the only isolated ion lines for which reasonably accurate quantum-mechanical electron broadening calculations are now possible.

Before describing our calculations, we should emphasize that some of the introductory remarks must be modified when line shifts are discussed rather than widths. Here there is no inelastic contribution, and second-order perturbation theory does give an explicit contribution by elastic collisions, making some of the semiclassical calculations[6,8] of the elastic contribution more reliable (not necessarily the other, essentially adiabatic, calculation[7]). Rather good agreement with quantum-mechanical calculations would, therefore, be expected in this case, but neither of these shift calculations could be compared directly with measurements – because of shifts induced by collisions with other ions and because of the additional (and comparable[4]) plasma polarization shift[18] caused by the average negative space charge surrounding a positive ion immersed in a plasma. (While this dielectric monopole effect certainly exists, as evidenced by the predominance of blue shifts for Stark-broadened ion lines in contrast to the usual red shifts of atomic lines, its quantitative understanding is still lacking.)

II. THEORY

According to Baranger[19–21] and Kolb and Griem,[22] widths w (from peak to half-intensity points of the Lorentz profiles) and shifts d of impact-broadened "isolated" spectral lines can be expressed in terms of S matrices describing the *elastic* scattering of single electrons on initial (i) and final (f) states of the line. The basic formula is

$$w + id = \nu \left[\langle\langle (J_i M_i')(J_f M_f') \left| \sum \langle\langle (j' m')_i (j' m')_f \right| 1 - S_f^* S_i \left| (j m)_i (j m)_f \right\rangle\right\rangle \left| (J_i M_i)(J_f M_f) \right\rangle\rangle \right]_{\mathrm{av}} , \qquad (1)$$

where ν is the frequency of collisions with an electron in a definite quantum state characterized by total angular momentum quantum number j and magnetic quantum number m. For electron wave functions normalized over all space, we have

$$\nu = (\pi/2v)\,(\hbar/m)^2\,N \tag{2}$$

in terms of electron density N and velocity v. (We assume monoenergetic electrons for the time being.) The average is over ("atomic") magnetic quantum numbers M_i, M_f, and M_i', M_f' before and after the collision, and can be expressed, as shown by Baranger,[20] in terms of Clebsch-Gordan coefficients or, equivalently, in terms of Wigner's[23] 3-j symbols as

$$(\cdots)_{\text{av}} \rightarrow \sum_{M_i M_i' M_f M_f' n = -1,0,1} (-1)^{M_i + M_i' + 2J_f} \begin{pmatrix} J_f & 1 & J_i \\ M_f' & n & -M_i' \end{pmatrix} \begin{pmatrix} J_f & 1 & J_i \\ M_f & n & -M_i \end{pmatrix}. \tag{3}$$

The sum in Eq. (1) is over all initial $(j, m)_{i,f}$ and final $(j', m')_{i,f}$ electron states (being operated on by S_i or S_f only), and the * sign denotes the complex conjugate of the matrix elements.

Introducing the transition matrix through

$$T = 1 - S \tag{4}$$

and summing over M_f, M_f' and M_i, M_i' in the terms involving only T_i or T_f^* with the help of the orthogonality relations for products of 3-j symbols summed over magnetic quantum numbers, the above relations lead to

$$\begin{aligned} w + id = \frac{\pi}{2v}\left(\frac{\hbar}{m}\right)^2 N \sum_{jmj'm'} \Bigg(& \frac{1}{2J_i+1} \sum_{M_i} \langle J_i M_i jm \,|\, T_i \,|\, J_i M_i jm \rangle + \frac{1}{2J_f+1} \sum_{M_f} \langle J_f M_f jm \,|\, T_f^* \,|\, J_f M_f jm \rangle \\ & - \sum_{n M_i M_i' M_f M_f'} (-1)^{M_i + M_i' + 2J_f} \begin{pmatrix} J_f & 1 & J_i \\ M_f' & n & -M_i' \end{pmatrix} \begin{pmatrix} J_f & 1 & J_i \\ M_f & n & -M_i \end{pmatrix} \\ & \times \langle J_f M_f' j' m' \,|\, T_f^* \,|\, J_f M_f jm \rangle \langle J_i M_i' j' m' \,|\, T_i \,|\, J_i M_i jm \rangle \Bigg). \end{aligned} \tag{5}$$

Phases in the first two terms are always even for $M_i' = M_i$, $M_f' = M_f$. Also, $j', m' = j, m$ follows in these cases from the orthogonality of the 3-j symbols in the atomic magnetic quantum numbers and from the conservation of total angular momentum $\vec{\gamma}_{i,f} = \vec{J}_{i,f} + \vec{j}$ and its Z component $\mu_{i,f} = M_{i,f} + m$. To reduce the number of independent T matrix elements, it is advantageous to make use of these conservation laws by transforming to the $JMjm, \gamma\mu$ representation. (Note that the T matrix is then not only diagonal in γ and μ but is also independent of μ because of the rotational invariance of the total Hamiltonian.) The transformation coefficients again involve 3-j symbols, e.g.,

$$\langle JMjm \,|\, \gamma\mu \rangle = (-1)^{j-J-\mu} (2\gamma+1)^{1/2} \begin{pmatrix} J & j & \gamma \\ M & m & -\mu \end{pmatrix}. \tag{6}$$

The first two terms in Eq. (5) transform with the help of the orthogonality relations mentioned above and using the independence of the new T matrix on μ to an entirely expected form, while the last term can be written in terms of 6-j symbols[23] after performing the sum over all magnetic quantum numbers (see the Appendix). The resulting expression[24] is

$$\begin{aligned} w + id = \frac{\pi}{2v}\left(\frac{\hbar}{m}\right)^2 N \sum_{jj'} \Bigg(& \frac{1}{2J_i+1} \sum_{\gamma_i} (2\gamma_i+1)\, T_{jj}^{\gamma_i} + \frac{1}{2J_f+1} \sum_{\gamma_f} (2\gamma_f+1)\, (T_{jj}^{\gamma_f})^* \\ & + (-1)^{j'+j} \sum_{\gamma_i \gamma_f} (2\gamma_i+1)(2\gamma_f+1) \begin{Bmatrix} \gamma_i & \gamma_f & 1 \\ J_f & J_i & j' \end{Bmatrix} \begin{Bmatrix} \gamma_i & \gamma_f & 1 \\ J_f & J_i & j \end{Bmatrix} (T_{j'j}^{\gamma_f})^* \, T_{j'j}^{\gamma_i} \Bigg), \end{aligned} \tag{7}$$

where we introduced a more compact notation for the T matrix elements in the new representation. (Because all T's here are for elastic collisions, we could set $J'=J$.)

In most line-broadening applications, spin-dependent forces may be neglected. Then total orbital angular momentum λ and spin σ are conserved separately, and it is easier to work in the $LS\frac{1}{2}l, \lambda\sigma M_\lambda M_\sigma$ representation; L, S, and l, $\frac{1}{2}$ being the corresponding quantum numbers for atom and electron. The corresponding transformation involves the 9-j symbols,[23] e.g.,

$$T_{j'j}^{\gamma} = \sum_{\lambda\sigma l' l} (2j'+1)^{1/2}(2j+1)^{1/2}(2J+1)(2\lambda+1)(2\sigma+1) \begin{Bmatrix} L & l' & \lambda \\ S & \frac{1}{2} & \sigma \\ J & j' & \gamma \end{Bmatrix} \begin{Bmatrix} L & l & \lambda \\ S & \frac{1}{2} & \sigma \\ J & j & \gamma \end{Bmatrix} T_{l'l}^{\lambda\sigma} . \tag{8}$$

Also, in this case, orthogonality relations lead to considerable simplifications in the linear terms (initial and final electrons being in the same state), and the resulting expression is

$$w+id = \frac{\pi}{2v}\left(\frac{\hbar}{m}\right)^2 N \sum_{ll'} \left(\sum_{\lambda_i\sigma_i} \frac{(2\lambda_i+1)(2\sigma_i+1)}{(2L_i+1)(2S_i+1)} T_{ll}^{\lambda_i\sigma_i} + \sum_{\lambda_f\sigma_f} \frac{(2\lambda_f+1)(2\sigma_f+1)}{(2L_f+1)(2S_f+1)} (T_{ll}^{\lambda_f\sigma_f})^* \right.$$

$$+ \sum (-1)^{j'+j} (j', j, J_i, J_f, \gamma_i, \gamma_f, \lambda_i, \lambda_f, \sigma_i, \sigma_f) \begin{Bmatrix} \gamma_i & \gamma_f & 1 \\ J_f & J_i & j' \end{Bmatrix} \begin{Bmatrix} \gamma_i & \gamma_f & 1 \\ J_f & J_i & j \end{Bmatrix}$$

$$\left. \times \begin{Bmatrix} L_i & l' & \lambda_i \\ S_i & \frac{1}{2} & \sigma_i \\ J_i & j' & \gamma_i \end{Bmatrix} \begin{Bmatrix} L_f & l' & \lambda_f \\ S_f & \frac{1}{2} & \sigma_f \\ J_f & j' & \gamma_f \end{Bmatrix} \begin{Bmatrix} L_i & l & \lambda_i \\ S_i & \frac{1}{2} & \sigma_i \\ J_i & j & \gamma_i \end{Bmatrix} \begin{Bmatrix} L_f & l & \lambda_f \\ S_f & \frac{1}{2} & \sigma_f \\ J_f & j & \gamma_f \end{Bmatrix} (T_{l'l}^{\lambda_f\sigma_f})^* T_{l'l}^{\lambda_i\sigma_i} \right) , \tag{9}$$

where $\sum\{j', j, \ldots\}$ stands for the weighted sum with statistical weights $(2j'+1)(2j+1)\times\ldots$, summed over all arguments of $\{\cdots\}$ except J_i and J_f.

Some simplifications of this general formula (which is the basis of our present calculations) are possible for particular transitions, e.g., for the lines considered here ($S_i=S_f=\frac{1}{2}$, $L_i=1$, $L_f=0$, $\lambda_f=l=l'$, $J_i=\frac{1}{2}, \frac{3}{2}$, and $J_f=\frac{1}{2}$) the "final" 9-j coefficients are proportional to 6-j coefficients,[25] namely,

$$\begin{Bmatrix} 0 & l & l \\ \frac{1}{2} & \frac{1}{2} & \sigma_f \\ \frac{1}{2} & j & \gamma_f \end{Bmatrix} = \begin{Bmatrix} \gamma_f & \sigma_f & l \\ j & \frac{1}{2} & l \\ \frac{1}{2} & \frac{1}{2} & 0 \end{Bmatrix} = \frac{(-1)^{\sigma_f+j+l+(1/2)}}{2^{1/2}(2l+1)^{1/2}} \begin{Bmatrix} \gamma_f & \sigma_f & l \\ \frac{1}{2} & j & \frac{1}{2} \end{Bmatrix} . \tag{10}$$

When the T matrices are independent of $\sigma_{i,f}=0,1$, we can, accordingly, for our transitions first sum over σ_f, using Eq. (10), which results in $j'=j$ on account of the orthogonality of the 6-j symbols, and then over γ_f, thus removing the 6-j symbols occurring in Eq. (9). Finally, we sum over σ_i and γ_i, utilizing the orthogonality relation[23] for the initial 9-j symbols, and $j=l\pm\frac{1}{2}$, obtaining

$$w+id = \frac{\pi}{v}\left(\frac{\hbar}{m}\right)^2 N \sum_l \left(\frac{1}{3} \sum_{\lambda_i=l, l\pm1} (2\lambda_i+1) T_{ll}^{\lambda_i} + \sum_{\lambda_f=l} (2\lambda_f+1)(T_{ll}^{\lambda_f})^* \right.$$

$$\left. - \frac{1}{3} \sum_{\lambda_i=l, l\pm1} \sum_{\lambda_f=l} (2\lambda_i+1)(T_{ll}^{\lambda_f})^* T_{ll}^{\lambda_i} \right) . \tag{11}$$

This simple result might have been anticipated, because, in this approximation, the spin could have been

ignored from the outset. Then the lower level would have been single, and the rotational average would have amounted to an average over magnetic quantum numbers ($M_L = 0, \pm 1$) of the upper level, corresponding to $\frac{1}{3}\sum_{\lambda_i}$ in Eq. (11) because of the transformation to the $LSls$, $\lambda\sigma M_\lambda M_\sigma$ representation.

Coulomb scattering can be separated by writing

$$T_{l'l} = e^{i(\eta_{l'}+\eta_l)}(\delta_{l'l} + T'_{l'l}), \tag{12}$$

with the Coulomb phase shifts

$$\eta_l = \arg\Gamma(l+1-ie^2/\hbar v) . \tag{13}$$

Substitution into Eq. (9) now shows that the latter, or Eq. (11), remains valid for the shift if one makes the replacement

$$T_{ll}^{\lambda\sigma} \to (e^{2i\eta_l} - 1)T'^{\lambda\sigma}_{ll} \tag{14}$$

in the linear terms and uses the new T' elements in the product term. In regard to the width, one sees, with the help of the optical theorem, namely,

$$\mathrm{Re}T_{ll} = \mathrm{Re}[e^{2i\eta_l}(1+T'_{ll})] = \tfrac{1}{2}\sum_{l'}|T_{l'l}|^2 = \tfrac{1}{2}\sum_{l'}|\delta_{l'l}+T'_{l'l}|^2 = \tfrac{1}{2}+\mathrm{Re}T'_{ll}+\tfrac{1}{2}\sum_{l'}|T'_{l'l}|^2, \tag{15}$$

that the appropriate replacement is

$$T_{ll}^{\lambda\sigma} \to \tfrac{1}{2}\sum_{l'}|T'^{\lambda\sigma}_{l'l}|^2 \tag{16}$$

in the linear terms when the cross term is again calculated with the new T' elements. (Note that the sum over l' in this replacement implies a summation over elastic *and inelastic* processes, while the cross term still only involves elastic scattering contributions.) The width is, thus, seen to be given by the sum of total cross sections for initial and final states (ignoring pure Coulomb scattering) minus the cross term in

$$T'^{\lambda_i\sigma_i}_{ll} \text{ and } (T'^{\lambda_f\sigma_f}_{ll})^* ,$$

as was expected from Baranger's analysis.[19,21] As a matter of fact, his expression for the width is entirely recovered, when the nonCoulomb elastic cross sections are combined with the cross term to form an expression proportional to

$$|T'^{\lambda_i\sigma_i}_{ll} - T'^{\lambda_f\sigma_f}_{ll}|^2 ,$$

ignoring the angular average for this comparison.

Finally, the actually tabulated[17] (real and symmetric) R matrices are related to T' by

$$T' = [-2iR/(1-iR)] . \tag{17}$$

III. CALCULATIONS

The close-coupling calculations[17] were performed for some fixed energies of the total system referred to the ground state of the ion, whereas we require T' matrices as a function of the system energies relative to the $3S$ and $3P$ states, respectively. Fortunately, there is by coincidence (for initial electron energies of $k^2 = 0.67$ Ry) one such set of T' or rather R matrices, because those for $3S$ at a total energy of 0.67 Ry and those for $3P$ at 1 Ry almost correspond to the same relative energy, the $3S$-$3P$ interval being ~0.32 Ry. For an initial electron energy of ~0.67 Ry, Eq. (9), with the various replacements discussed above, could therefore be calculated directly.

For all other initial energies, some interpolation or extrapolation was necessary. This task was greatly facilitated by the observation that the first two terms in Eq. (9) essentially represent the

total (nonCoulomb elastic plus inelastic) cross sections of $3P$ and $3S$ respectively. These were thus calculated for the set of total energies used by Burke and Moores,[17] and the $3P$ cross section replotted as a function of relative energy, which for $k^2 \gtrsim 0.32$ Ry mostly involved interpolation. This caused no difficulty, because the total cross section (averaged over resonances) is continuous[26] at inelastic thresholds, i.e., at $k^2 = 0.64$ Ry (for the $3S$-$3D$ transition) in this case. (Earlier work on the threshold behavior is reviewed in Ref. 26.)

The lowest energy point available is $k^2 = 0.35$ Ry, and considerable extrapolation was therefore required below the $3S$-$3P$ and $3P$-$3D$ thresholds, both at ~0.32 Ry. Continuity of the total cross sections is hardly sufficient for extrapolation to zero energy, as there may well be a change in the derivative of this cross section at inelastic thresholds. We, therefore, extrapolated the Y matrices (as defined by Seaton[27] corresponding to Burke and Moores's R matrices), transformed back to R and T' and thus evaluated the width by summing over partial waves. Except at $k^2 = 0.67$ Ry, this procedure (now involving also interpolation) was used to calculate the third (interference) term in Eq. (9) as well. Two different fits for Y were tried; one quadratic in k^2, and another involving the ratio of two linear forms (to account for poles). None of these was entirely satisfactory, especially near zero energy. However, errors in the total width from these extrapolations and interpolations should not exceed 10% for $k^2 \gtrsim 0.32$ Ry, although they may be somewhat larger near zero energy.

The interference term, which is always negative, is never more than 25% of the sum of the first two terms in Eq. (9) for $3\,^2S_{1/2} - 3\,^2S_{1/2}$, or 30% for $3\,^2S_{1/2} - 3\,^2P_{3/2}$. (The total cross sections are the same for both components.) Furthermore, it is also generally continuous[28] at thresholds (when averaged over resonances below these energies). Only below $k^2 = 0.32$ Ry, corresponding to $3S$-$3P$ and $3P$-$3D$ thresholds, where both T matrices are oscillatory, the averaged $T_i T_f^*$ matrix product is not necessarily equal to its value just above threshold. Using quantum-defect procedures as described in Ref. 28, the product was, therefore, evaluated and averaged numerically and found to deviate from its value above threshold by $\lesssim 20\%$, corresponding to $\lesssim 5\%$ change in the linewidth.

IV. RESULTS AND DISCUSSION

Rather than giving the linewidths, it is more instructive to represent the results in terms of effective Gaunt factors g, from which the (half) half-width can be calculated according to

$$w = (4\pi^2/3v)(\hbar/m)^2 N \times 19.8 g \,. \qquad (18)$$

Here, 19.8 is the value (in atomic units) of the sum

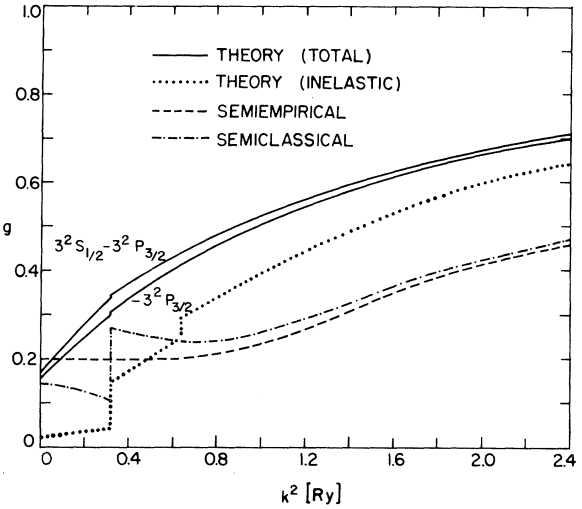

FIG. 1. Effective Gaunt factors for the electron-impact broadening of Mg^+ resonance lines as functions of initial electron energies.

of the absolute values squared of the matrix elements of $\vec{r}$ (the atomic electron position operator) for initial and final states, summed over all perturbing states ($3S$ and $3D$ in case of $3P$, and $3P$ in case of $3S$). This Gaunt factor, as obtained from the present calculations, corresponds to the solid curves on Fig. 1. (Note that the discontinuity at $k^2 = 0.32$ Ry is not quantitatively significant, nor are the changes in slopes at this energy and at $k^2 = 0.64$ Ry.) Also indicated are the inelastic (and superelastic) contributions which are almost negligible below $k^2 = 0.32$ Ry, i.e., in the most important energy range in practice. (Mg^+ is further ionized at temperatures corresponding to higher electron energies in all but extreme nonequilibrium situations.) Broadening due to elastic collisions, therefore, usually dominates the electron-impact broadening of these lines.

Also shown on Fig. 1 are the semiempirical Gaunt factors as proposed by Van Regemorter[5] but extrapolated to zero energy,[4] and representative of the simpler semiclassical approximations,[7,12] a Gaunt factor calculated according to Roberts and Davis.[7] While an effective Gaunt factor $g = 0.20$ is clearly consistent with the present results below the first threshold, the quasiclassical approximation falls short by a factor ~1.5 for most energies in this range. However, the near agreements at zero energy and above the first threshold suggest that a quasiclassical calculation[8] ignoring thresholds will give more satisfactory results. Inclusion of quadrupole interactions[10,12,29] further reduces the deficiency of the quasiclassical width in the below threshold region, and ~10% agreement with the present results is reached.[30]

At larger perturber energies, the present results exceed those of the two other methods[4,7] by a factor

~2. This is evidently due to higher multipole interactions, as the other two approximations become exact at high energies (within the framework of the dipole approximation). As a matter of fact, our results for g – for $k^2 \lesssim 0.4$ Ry within a few percent – can be fitted to

$$g = 0.165 + 0.50k^2 \,, \tag{19a}$$

$$g = 0.155 + 0.47k^2 \,, \tag{19b}$$

for $3\,^2S_{1/2} - 3\,^2P_{1/2}$ and $3\,^2S_{1/2} - 3\,^2P_{3/2}$, respectively; and the second term indeed corresponds closely in relative magnitude to quadrupole corrections as used, e.g., in calculations[31] for hydrogen lines. (Note that $\ln\rho_{max}/\rho_{min}$ in Ref. 31 corresponds to $\pi g/\sqrt{3} \approx 1.8g$.)

It still remains to discuss the influence of interacting states not included in the close-coupling calculations.[17] Most important of these is probably $4S$, whose inclusion would result in an increase in the factor 19.8 in Eq. (18) by ~10%. While the corresponding increase in width is relatively small, say ~10%, inclusion of $4S$ might half the shift (judging from estimated quadratic Stark effects). This shift, being perhaps only ~20% of the (half) half-width, therefore, cannot be calculated with any reliability from the present close-coupling results.[17] (See also the discussion of competing effects at the end of the Introduction.)

To facilitate applications and comparison with (future) experiments, we finally state our results for the (half) half-widths (in angstroms) after averaging over a Maxwellian electron velocity distribution and increasing the factor 19.8 in Eq. (18) by ~10% as

$$w_\lambda = 4.7 \times 10^{-19} N(\mathrm{Ry}/kT)^{1/2} \times [0.165 + 0.50(kT/\mathrm{Ry})] \,, \tag{20a}$$

$$w_\lambda = 4.7 \times 10^{-19} N(\mathrm{Ry}/kT)^{1/2} \times [0.155 + 0.47(kT/\mathrm{Ry})] \,, \tag{20b}$$

for the $J = \frac{1}{2} \to \frac{1}{2}$ and $\frac{1}{2} \to \frac{3}{2}$ components. It is hoped that these formulas are accurate to ~±20% for $kT/\mathrm{Ry} \lesssim 0.2$, i.e., for $T \lesssim 30\,000$ °K. (For higher temperatures, the average should be performed numerically, using the g values given on Fig. 1 with a +10% correction to allow for other interacting states.) Equations (20a) and (20b) yield widths that are larger by factors of 3–5 in the experimental temperature range than the original (straight) classical-path predictions by one of us[2] in which, moreover, perturbations of the ground state had been neglected. However, the (quasi-static) ion-broadening parameter α given in Ref. 2 remains almost unchanged, i.e., small ($\alpha \approx 0.02$ at $N = 10^{16}$ cm^{-3}). Broadening by ions will, therefore, increase the width over that from electron-impact broadening by less than ~20% for densities $N \lesssim 10^{19}$ cm^{-3}. In cases where the impact approximation applies to ions as well, the correction for ion broadening should be still smaller (~10%). It is finally worth noting that the widths of the two multiplet components do not differ by more than the estimated theoretical error.

APPENDIX

According to Eqs. (1), (3), and (4) we require

$$\begin{aligned}[\langle\langle if|1 - S_f^* S_i|if\rangle\rangle] \to \sum_{\substack{M_i M_i' M_f M_f' n = 0,\pm 1 \\ jmj'm'}} (-1)^{M_i + M_i' + 2J_f} \begin{pmatrix} J_f & 1 & J_i \\ M_f' & n- & M_f' \end{pmatrix} \begin{pmatrix} J_f & 1 & J_i \\ M_f & n- & M_i \end{pmatrix} \\ \times (\langle J_i M_i' jm|T_i|J_i M_i jm\rangle \delta_{M_f' M_f} + \langle J_f M_f' jm|T_f^*|J_f M_f jm\rangle \delta_{M_i' M_i} \\ - \langle J_f M_i' j'm'|T_f^*|J_f M_f jm\rangle \langle J_i M_i' j'm'|T_i|J_i M_i jm\rangle) \,,\end{aligned} \tag{A1}$$

using the orthogonality of the various wave functions in the linear terms. With the orthogonality relations for 3-j symbols, e.g.,

$$\sum_{M_f n} \begin{pmatrix} J_f & 1 & J_i' \\ M_f & n- & M_i' \end{pmatrix} \begin{pmatrix} J_f & 1 & J_i \\ M_f & n- & M_i \end{pmatrix} = \frac{\delta_{J_i' J_i} \delta_{M_i' M_i}}{2J_i + 1} \,, \tag{A2}$$

the first two terms reduce to the average over magnetic quantum numbers M_i and M_f, respectively, in

Eq. (5). [The phase factors here are always +1, because $2(M_i+J_f)=2(M_i+J_i)\pm 2, 0$ is always even, and because $M_i'+M_i$ is equal to $M_f'+M_f\pm 2, 0$ due to $M_f'=M_i'-n$, $M_f=M_i-n$, $n=0, \pm 1$.]

In the $JMj\,m$, $\gamma\mu$ representation the linear terms then become, with Eq. (6),

$$\frac{1}{2J+1}\sum_{Mjm}\langle JMjm\,|\,T\,|\,JMjm\rangle=\frac{1}{2J+1}\sum_{Mjm\gamma\mu}(2\gamma+1)\begin{pmatrix}J & j & \gamma\\ M & m & -\mu\end{pmatrix}^2\langle Jj\gamma\mu\,|\,T\,|\,Jj\gamma\mu\rangle$$

$$=\frac{1}{2J+1}\sum_{jj\gamma\mu}T_{jj}{}^{\gamma}=\frac{1}{2J+1}\sum_{jj\gamma}(2\gamma+1)\,T_{jj}{}^{\gamma}\ , \tag{A3}$$

using the analog of Eq. (A2) summed over M and m and finally the fact that $\langle Jj\gamma\mu\,|\,T\,|\,Jj\gamma\mu\rangle\equiv T_{jj}{}^{\gamma}$ is independent of μ. The phases combine to $2(j-J-\mu)$ in this case. Either J or μ are half-integer, as is j, making $j-J-\mu$ always integer, and thus the combined phase factor +1.

The cross term is in the new representation from Eqs. (A1) and (6):

$$\langle\langle\langle if\,|\,T_f^{*}T_i\,|\,if\rangle\rangle\rangle=\sum_{\substack{M_iM_i'M_fM_f'n\\ jj'mm'\gamma_i\gamma_f\mu_i\mu_f}}(-1)^{M_i'+M_i+2J_f}\begin{pmatrix}J_f & 1 & J_i\\ M_f' & n & -M_i'\end{pmatrix}\begin{pmatrix}J_f & 1 & J_i\\ M_f & n & -M_i\end{pmatrix}$$

$$\times(-1)^{j'+j-2J_f-2\mu_f}(2\gamma_f+1)\begin{pmatrix}J_f & j' & \gamma_f\\ M_f' & m' & -\mu_f\end{pmatrix}\begin{pmatrix}J_f & j & \gamma_f\\ M_f & m & -\mu_f\end{pmatrix}$$

$$\times(-1)^{j'+j-2J_i-2\mu_i}(2\gamma_i+1)\begin{pmatrix}J_i & j' & \gamma_i\\ M_i' & m' & -\mu_i\end{pmatrix}\begin{pmatrix}J_i & j & \gamma_i\\ M_i & m & -\mu_i\end{pmatrix}(T_{j'j}{}^{\gamma_f})^{*}T_{j'j}{}^{\gamma_i}\ . \tag{A4}$$

[Actually, the phases can be combined to $M_i'+M_i+2(j'+j)-2J_i$, because $2\mu_i+2\mu_f$ is always even.] With the help of the symmetry relations for 3-j symbols, Eq. (A4) may be rearranged to allow the double application of Eq. (2.20) in Ref. 23. Alternatively, the latter[32] can be manipulated into a form resembling, e.g., the product of "unprimed" factors in Eq. (A4), namely,

$$\begin{pmatrix}\gamma_i & \gamma_f & 1\\ \mu_i & \mu_f & n\end{pmatrix}\begin{Bmatrix}\gamma_i & \gamma_f & 1\\ J_f & J_i & j\end{Bmatrix}=\sum_{M_iM_fm}(-1)^{J_f+J_i+j+M_f+M_i-m}\begin{pmatrix}\gamma_i & J_i & j\\ -\mu_i & M_i & m\end{pmatrix}\begin{pmatrix}J_f & \gamma_f & j\\ -M_f & \mu_f & -m\end{pmatrix}\begin{pmatrix}J_f & J_i & 1\\ M_f & -M_i & n\end{pmatrix}$$

$$=\sum_{M_iM_fm}(-1)^{2J_f+2J_i+j+1+M_f+M_i-m}\begin{pmatrix}J_i & j & \gamma_i\\ M_i & m & -\mu_i\end{pmatrix}\begin{pmatrix}J_f & j & \gamma_f\\ M_f & m & -\mu_f\end{pmatrix}\begin{pmatrix}J_f & 1 & J_i\\ M_f & n & -M_i\end{pmatrix}\ . \tag{A5}$$

The terms $2J_f+2J_i$ can of course be omitted in the phase. The phase resulting from multiplying Eq. (A5) by its "primed" equivalent is, therefore, $j'+j+M_f'+M_f+M_i'+M_i-m'-m$, which differs from the phase in Eq. (A4) by $j'+j-2J_i-2\mu_f+2(m'+m)$. Since $2(m'+m)$ and $2(J_i+\mu_f)$ are always even or odd, respectively, the difference in phases can be written as $j'+j+1$, and Eq. (A4) therefore can be written as

$$\langle\langle\langle if\,|\,T_f^{*}T_i\,|\,if\rangle\rangle\rangle=-\sum_{jj'n\gamma_i\gamma_f\mu_i\mu_f}(2\gamma_i+1)(2\gamma_f+1)\begin{pmatrix}\gamma_i & \gamma_f & 1\\ \mu_i & \mu_f & n\end{pmatrix}^2(-1)^{j'+j}$$

$$\times \begin{Bmatrix} \gamma_i & \gamma_f & 1 \\ J_f & J_i & j' \end{Bmatrix} \begin{Bmatrix} \gamma_i & \gamma_f & 1 \\ J_f & J_i & j \end{Bmatrix} (T_{j'j}^{\gamma_f})^* T_{j'j}^{\gamma_i} \,. \tag{A6}$$

This finally reduces to the corresponding terms in Eq. (7) on account of the normalization of 3-j symbols when summed over μ_i and μ_f, yielding $\sum'(\cdots)^2 = \frac{1}{3}$, and then over $n = 0, \pm 1$, resulting in $\sum(\cdots)^2 = 1$.

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