BULL. AUSTRAL. MATH. SOC. 70F35, 78A45
VOL. 9 (1973), 465-468.

# Abstracts of Australasian PhD theses

## An investigation of the collision broadening of spectral lines

**Robert John Dyne**

A theoretical investigation was carried out into various aspects of the broadening of spectral lines as the result of collisions between the radiating atom and charged or neutral particles. The general theory of line broadening was considered, the usual approximations, the classical path assumption and the impact and quasi-static approximations, discussed, and criteria for the applicability of these approximations were presented. Isolated spectral lines, under conditions which satisfy the impact approximation, have a lorentzian profile for which the width and shift are expressible in terms of the diagonal elements of the scattering matrix for the collision.

An exponential form was chosen to represent the diagonal elements of the $S$-matrix,

$$S_{nn}(\rho, v) = \exp\left[-i\alpha_n(\rho, v)\right] ,$$

instead of the usual perturbation expansion. Such a representation has the advantages that the $S$-matrix remains unitary to all orders of approximation of the complex phase shift, $\alpha_n(\rho, v)$, the width and shift satisfy directly a dispersion relation, and the expressions for the width and shift reduce to the correct form in the limits of high and low temperatures without the introduction of an impact parameter cutoff and *ad hoc* correction factors.

Calculations of electron impact broadening in the *two-level* approximation (where only one atomic level is considered to perturb the

Received 8 August 1972. Thesis submitted to the University of Queensland, August 1972. Degree approved, July 1973. Supervisor: Dr B.J. O'Mara.

upper level of the transition) provide insight into the adiabatic and non-adiabatic processes which occur during the collision. However, whereas the two-level approximation may provide an order-of-magnitude estimate of the line width and shift, it was shown that the effect of other perturbing levels is usually significant. For both the exponential representation of the $S$-matrix and the perturbation expansion of Griem *et al.* [4], there occur maximum differences of fifteen percent in the width and shift. However, the errors in the experimental observations are usually of this magnitude.

Comparisons between theoretical and experimental widths and shifts have been carried out for a number of spectral lines of neutral helium under different experimental conditions as well as for various lines of other elements. In general, there was an overall improvement in the agreement between theory and observation if the exponential form of the $S$-matrix is chosen, although, in many cases, the improvement was not significant. For these cases, the complex phase shift, $\alpha_n(\rho, v)$, was small and a truncated expansion of the exponential form is valid. For the inert gases, there was significant improvement in the theoretical results as the result of calculating the dipole matrix elements in $jK$ coupling rather than $LS$ coupling. It is suggested from this investigation that errors may exist in other regions of line-broadening theory, for example, the treatment of ion collisions, Debye shielding effects, and the calculation of multipole matrix elements for complex atoms. (Sections of this work have been published in [3].)

The proposition of several authors that an empirical interaction potential between two neutral atoms, containing at most two unknown parameters, can be determined by inversion of the observed line width and shift, has also been investigated. Although these authors have noted large discrepancies between theoretical and experimental values of the van der Waals' constant if a Lennard-Jones $(12, 6)$ form of the interaction is chosen, it was shown that inversion was possible using the theoretical value of the van der Waals' constant provided a more realistic form of the repulsive component of the interaction (containing two unknown parameters) was chosen. However, since the potential function determined by these methods was not unique, the suitability of such a procedure must be

questioned.

In view of the importance of the broadening by hydrogen and helium in the atmospheres of cooler stars (spectral type $F$ and later), various methods of calculation of the interaction potential between two neutral atoms were considered in order to establish which, if any, is the most suitable for the estimation of spectral line widths and shifts for astrophysical application. For interactions with hydrogen, a method suggested by Brueckner [2] provides reasonably accurate line widths from a simple formula for spectral lines other than resonance lines. For resonance lines, where interactions with the ground state are important, this method fails as the ground state interaction is not included. The molecular orbital calculations of Lewis *et al.* [5] provide a more accurate representation of the interatomic potential, incorporating the mutual interactions of the atomic levels, for alkali-hydrogen collisions, although such a method requires a large computational effort. In none of the cases considered is the method proposed by Roueff [6] satisfactory for the calculation of line widths due to hydrogen collisions.

Collisions with inert gases, in particular with helium are also important in the broadening of spectral lines in stellar spectra. For such interactions, Roueff's method and a method suggested by Baylis [1] provide similar estimates of the line width. The latter method is at present only applicable to the broadening of alkali resonance lines, while Roueff's method may be applied to all radiating atoms and to any perturbing atom for which the dipole polarizability and electron scattering length are known. As a result of the inclusion of the atomic states important in the formation of the resonance lines in the set of basis states, Baylis's method must be preferred over the method of Roueff for the resonance lines of alkalis. However, for spectral lines of other atoms, Roueff's procedure provides line widths in reasonable agreement with experimental observations.

At present, no theory is adequately capable of explaining the observed line shifts produced by collisions with neutral atoms, with the exception of the van der Waals' theory for collisions with argon.

## References

[1] W.E. Baylis, "Semiempirical, pseudopotential calculation of alkali-noble-gas interatomic potentials", *J. Chem. Phys.* 51 (1969), 2665-2679.

[2] Keith A. Brueckner, "Collision broadening by neutral hydrogen", *Astrophys. J.* 169 (1971), 621-632.

[3] R.J. Dyne and B.J. O'Mara, "A convergent theory of spectral line broadening in the impact approximation", *Astronom. and Astrophys.* 18 (1972), 363-372.

[4] H.R. Griem, M. Baranger, A.C. Kolb and G. Oertel, "Stark broadening of neutral helium lines in a plasma", *Phys. Rev.* 125 (1962), 177-195.

[5] E.L. Lewis, L.F. McNamara and H.H. Michels, "Broadening of the sodium *D* lines by atomic hydrogen. An analysis in terms of the NaH molecular potentials", *Phys. Rev. A* (3) 3 (1971), 1939-1948.

[6] E. Roueff, "A theoretical model for the interaction between excited and ground state atoms. Application to pressure broadening", *Astronom. and Astrophys.* 7 (1970), 4-9.