



Interatomic potentials and applications to spectral line broadening

G. Peach

Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, United Kingdom; e-mail: g.peach@ucl.ac.uk

Abstract. The use of three-body models to construct a Hamiltonian and hence obtain interatomic potentials is discussed and the accuracy of the model assessed. Extensive tests of this approach have been carried out for the NaH molecule, since this system is particularly important for applications to the solar spectrum where the broadening of alkali lines is mainly due to perturbation by neutral hydrogen. The broadening of spectral lines by neutral atoms is considered and calculations of the pressure broadening of alkali resonance lines by helium are presented. This data is important for the interpretation of the observed spectra of cool dwarf stars. Finally, the validity of the simple Van der Waals formula for the line width is tested against detailed quantum mechanical calculations.

Key words. Interatomic potentials: Na-H system – Spectral line broadening: calculations – Cool stars: alkali resonance doublets

1. Introduction

Accurate pressure broadened profiles of alkali resonance doublets are needed for modelling of the atmospheres of cool stars and for generating their synthetic spectra in the region 400 - 900 nm. When the usual impact theory of line broadening is used, see Baranger (1958), the profile is simply Lorentzian and the widths and shifts of the lines can be calculated, provided that interaction potentials for the emitter-perturber system are available. However when the lines utterly dominate their region of the spectrum, it becomes important to also accurately represent the profile in the line wings, where the impact theory is no longer valid. The non-Lorentzian profiles of the strongly broadened Na I and K I doublets have been

studied by Burrows & Volobuyev (2003) and Allard et al. (2003), with the emphasis on approximate or unified semiclassical models that can describe the far wings of the profiles. Also Zhu et al. (2005) have carried out quantum mechanical calculations of the emission and absorption spectra for the wings of the lithium resonance line. However highly accurate calculations of the central Lorentzian cores are still needed and in this paper we present calculations of the widths for alkali lines broadened by helium.

Accurate calculations of line widths are impossible unless interatomic potentials for the emitter-perturber system are well known. The calculation of these potentials for both ground and excited electronic states, valid over a wide range of interatomic separations, represents a big challenge in itself and in this paper, three-body models of atom-atom systems are dis-

Send offprint requests to: G. Peach

cussed and their accuracy assessed by comparison with data obtained using approaches developed in quantum chemistry.

The original impact theory of spectral line broadening that Baranger developed is purely quantum mechanical, but further approximations to this theory are often made. They are of two types, firstly the quantum-mechanical treatment is replaced by a semi-classical one and secondly the interatomic potential used is replaced by the asymptotic Van der Waals interaction. To test the validity of these approximations, results for Lorentzian line widths are presented for lithium and sodium lines broadened by helium for $70.0 \text{ K} \leq T \leq 3000 \text{ K}$.

2. Interatomic potentials

Large quantum chemistry calculations can provide very accurate potentials for electronic states of atom-atom systems at short and intermediate separations, but are limited to the study of electronic states of relatively low excitation. However spectral line broadening problems often involve low-energy scattering by interaction potentials for the more highly excited states and so methods must be developed to obtain an accurate representation of these potentials at medium and large interatomic separations. If a valence electron of the emitter is in an excited state and the perturber is assumed to be always in its ground state, a three-body model of the system is intuitively appealing and is also practicable.

The adiabatic molecular potentials for the $A^{m+} + B^{n+} + e^-$ system can be obtained by using a three-body model in which the ions A^{m+} and B^{n+} are represented by polarisable atomic cores. This model is most accurate if these two cores are tightly bound so that the excitation of core states need only be accounted for by second-order perturbation theory through the inclusion of their polarizabilities. Model potentials which may be l -independent or l -dependent, are used to represent the electron-atom and electron-atomic ion interactions and the basic methods adopted for obtaining these model potentials are discussed by Peach (1982). For example if $m \neq 0$, potentials for the system $A^{m+} + e^-$ are determined

by fitting the spectrum of the ion $A^{m+ - 1}$, but if $m = 0$, the potentials are adjusted so as to reproduce the elastic scattering phase shifts for electrons scattered by the neutral atom A^0 . In either case, these potentials generate wave functions that contain the correct number of nodes and this means that the model potentials also support unphysical bound states corresponding to the presence of closed shells in the A^{m+} and B^{n+} ions. This effect is taken into account in the calculation of the molecular potentials by including the unphysical states in the atomic basis used in the diagonalization of the Hamiltonian for the three-body model.

Molecular potentials for the Li-He, Na-He and K-He systems have been obtained using the three-body model and are discussed by Leo et al. (2000). Subsequently they have been used in line broadening calculations by Mullanphy et al. (2007).

2.1. Modelling of atom-atom system

The electron-core interactions are modelled using the following form:

$$V_{a,b}(r) = -\frac{Z}{r}(1 + \delta + \delta' r) \exp(-\alpha r) - \frac{z}{r} - \frac{\alpha_d}{2r^4} F_1(r) - \frac{\alpha_q}{2r^6} F_2(r) + 3\frac{\beta_d}{r^6} F_3(r) + \text{small energy term (optional)}, \quad (1)$$

where $Z + z = \text{nuclear charge}$, $z = m, n$ and α_d and α_q are the static dipole and quadrupole polarizabilities. The coefficient β_d is a dynamical correction to the dipole polarizability and the functions $F_1(r)$, $F_2(r)$ and $F_3(r)$ are cut-off factors that ensure that the long-range contributions to the potential vanish at the origin. Parameters α , δ and δ' are then varied so as to reproduce as closely as possible the known atomic data.

The core-core interaction is specified by

$$V_c(R) \approx -z_a^2 \frac{\alpha_d^b}{2R^4} - z_b^2 \frac{\alpha_q^a}{2R^6} + \text{short - range terms}, \quad (2)$$

where R is the interatomic separation. The possible options for the choice of the short-range term are:

- (a) use the three-body model itself to generate the potential;
- (b) use a simple analytic form based on perturbation theory.

Choices (a) and (b) differ only for separations of the order of $R \approx R_A + R_B$ where R_A and R_B are the mean radii of the cores A^{m+} and B^{n+} .

Finally the three-body interaction is given by

$$V_3(\mathbf{r}, \mathbf{R}) \approx \frac{\alpha_d}{r^2 R^2} P_1(\hat{r} \cdot \hat{R}) + \frac{\alpha_q}{r^3 R^3} P_2(\hat{r} \cdot \hat{R}) \\ + \text{small energy term (optional)}, \quad (3)$$

for large values of R where $P_1(\hat{r} \cdot \hat{R})$ and $P_2(\hat{r} \cdot \hat{R})$ are Legendre polynomials.

The model Hamiltonian is then given by

$$H = -\frac{1}{2} \nabla^2 + V_a(r_a) + V_b(r_b) + V_c(R) \\ + V_3(\mathbf{r}_a, \mathbf{R}) + V_3(\mathbf{r}_b, \mathbf{R}), \quad (4)$$

where r_a and r_b are the position vectors of the electron relative to cores A^{m+} and B^{n+} . A set of atomic basis states on one or both centres is used and the Hamiltonian matrix is then diagonalized to obtain the electronic energies.

2.2. Principles and problems

In equation (1) the form of the long-range interactions produced by polarization are based on well-known second-order perturbation theory. The three-body term in equation (3) must be included in order to ensure that the correct behaviour of the adiabatic potentials is obtained for large separations. For example if $m = 1$ and $n = 0$, potentials for the system $A^0 + B^0$ tend to the Van der Waals form, $-C_6/R^6$ as $R \rightarrow \infty$. No circular procedures are adopted so that the variable parameters that appear in the model Hamiltonian (4) are determined using data that is totally independent of any existing data for the molecule concerned.

Some problems arise in constructing the model Hamiltonian. The positions of virtual states in electron-core model potentials are

sensitive to the precise fit to the atomic data. This applies particularly in the case of the electron-neutral atom potentials. Also, a different potential may have to be used for ground states; for example it is not possible to find a central potential that reproduces the positions of all the excited singlet states of helium *and* predicts the binding energy of $\text{He}(1s^2)$ correctly. This is not surprising, since in this case the core electron and the valence electron are in fact equivalent. Therefore it is necessary to use a separate model potential which is chosen to reproduce the energy of the state and to give its correct polarizability.

2.3. The Na^*-H system

Extensive tests have been carried out to see how accurate a three-body model proves to be when applied to the system Na^*-H . This has been chosen as a test case because $\text{H}(1s)$ is not a very tightly bound atom and in addition, $\text{H}^-(1s^2)$ is bound and so a state which asymptotically separates to the configuration $\text{Na}^+ + \text{H}^-$ interacts strongly with the other states of the type $\text{Na}(nl) + \text{H}(1s)$. The core-core potential is generated by initially using a simple analytic form for the $\text{Na}^{2+}(2p^5)-\text{H}^+$ interaction which is fed into the three-body model to obtain a potential for $\text{Na}^+(2p^6)-\text{H}^+$. This in turn is then fed back into the model to obtain a potential for $\text{Na}^+(2p^6)-\text{H}$. Finally this provides the input core-core potential for the Na^*-H system.

3. Spectral line broadening

An early version of impact theory was published by Lindholm (1941). The relative motion of the two atoms in the collision is treated semi-classically and is assumed to follow a straight-line path. The half-half width w and shift d are given by

$$w + id = 2\pi N \left\{ \int_0^\infty v f(v) dv \right. \\ \left. \times \int_0^\infty [1 - \exp(i\eta)] \rho d\rho \right\}_{\text{Av}}, \quad (5)$$

where 'Av' denotes an average over degenerate components of the line and N is the perturber

number density. The impact parameter is denoted by ρ and the relative velocity is v . The function $f(v)$ is the Maxwell velocity distribution normalized so that

$$\int_0^\infty f(v)dv = 1. \quad (6)$$

The phase shift η is obtained from

$$\eta(\rho, v) = -\frac{1}{\hbar} \int_{-\infty}^\infty V(t) dt \quad (7)$$

and for Van der Waals broadening $V(t)$ is replaced by $-C_6/R^6(t)$ and then the integrals can be evaluated analytically, see Peach (1981).

The quantum-mechanical impact theory of Baranger (1958) in its simplest form can be established simply by making the transition

$$(Mv\rho)^2 \rightarrow \hbar^2 l(l+1) \quad (8)$$

and then

$$2\rho d\rho \rightarrow \frac{\hbar^2}{(Mv)^2} (2l+1)\Delta l, \quad (9)$$

and the integral over ρ is replaced by a sum over l . The phase shift $\eta(\rho, v)$ is replaced so that

$$\eta(\rho, v) \rightarrow 2[\eta_i(l, v) - \eta_f(l, v)], \quad (10)$$

where $\eta_i(l, v)$ and $\eta_f(l, v)$ are elastic scattering phase shifts for scattering in the adiabatic potentials that describe the initial and final states of the system.

The approximation to the quantum-mechanical theory that corresponds most closely to the semi-classical assumption of a straight-line path is to use first-order perturbation theory for the phase shifts η_i and η_f in equation (10), in which the scattering wavefunctions are replaced by plane waves. This is commonly referred to as the Born approximation. The scattering theory required is discussed by Geltman (1969) and its application to the spectral line broadening problem by Peach & Whittingham (2009).

4. Results

The $X^1\Sigma$ and $A^1\Sigma$ states have been very accurately determined by Olson & Liu (1980) and

Table 1. Interaction potential energies, $V(R)$, for $X^1\Sigma$ states of NaH in a.u.

| $R(a_0)$ | $V(R)^1$ | $V(R)^2$ |
|----------|------------|------------|
| 2.550802 | -0.0222056 | 0.0173076 |
| 2.576990 | -0.0257018 | 0.0127261 |
| 2.606257 | -0.0293679 | 0.0077912 |
| 2.639061 | -0.0332010 | 0.0024712 |
| 2.676012 | -0.0371990 | -0.0032134 |
| 2.717955 | -0.0413606 | -0.0092307 |
| 2.766100 | -0.0456853 | -0.0155804 |
| 2.822284 | -0.0501734 | -0.0224013 |
| 2.889504 | -0.0548261 | -0.0297956 |
| 2.973243 | -0.0596454 | -0.0376331 |
| 3.085685 | -0.0646341 | -0.0462748 |
| 3.269457 | -0.0697958 | -0.0561524 |
| 3.566044 | -0.0724457 | -0.0637470 |
| 3.926517 | -0.0697958 | -0.0641757 |
| 4.239926 | -0.0646341 | -0.0603022 |
| 4.484732 | -0.0596454 | -0.0559067 |
| 4.703898 | -0.0548261 | -0.0514642 |
| 4.910000 | -0.0501734 | -0.0470963 |
| 5.108979 | -0.0456853 | -0.0428457 |
| 5.304375 | -0.0413606 | -0.0387301 |
| 5.498659 | -0.0371990 | -0.0347577 |
| 5.693791 | -0.0332010 | -0.0309332 |
| 5.891502 | -0.0293679 | -0.0272634 |
| 6.093461 | -0.0257018 | -0.0237557 |
| 6.301393 | -0.0222056 | -0.0204220 |
| 7.0 | -0.0124200 | -0.0114645 |
| 8.0 | -0.0047285 | -0.0043448 |
| 10.0 | -0.0005987 | -0.0005714 |
| 11.75 | -0.0001111 | -0.0001159 |
| 12.0 | -0.0000889 | -0.0000942 |
| 13.5 | -0.0000275 | -0.0000310 |
| 15.0 | -0.0000116 | -0.0000126 |
| 17.0 | -0.0000037 | -0.0000049 |

¹ Olson & Liu (1980), Zemke et al. (1984)

² present work

Zemke et al. (1984) using a combination of *ab initio* quantum chemistry techniques and an RKR analysis of observed spectra. Very similar results have been obtained by Leininger et al. (2000) who use very large Gaussian basis sets and carry out a full CI calculation. In tables 1 and 2 the present work based on the three-body model is compared with that of Olson & Liu (1980) and Zemke et al. (1984). For the $X^1\Sigma$ state the three-body model predicts the position of the minimum to be at $R \approx 3.8a_0$, which

Table 2. Interaction potential energies, $V(R)$, for the $A^1\Sigma$ states of NaH in a.u.

| $R(a_0)$ | $V(R)^1$ | $V(R)^2$ |
|----------|------------|------------|
| 3.18532 | -0.0139258 | -0.0140319 |
| 3.21537 | -0.0154006 | -0.0155388 |
| 3.24769 | -0.0169040 | -0.0170848 |
| 3.28265 | -0.0184318 | -0.0186636 |
| 3.32025 | -0.0199810 | -0.0202466 |
| 3.36126 | -0.0215497 | -0.0218462 |
| 3.40567 | -0.0231363 | -0.0234554 |
| 3.45367 | -0.0247389 | -0.0250770 |
| 3.50582 | -0.0263556 | -0.0266930 |
| 3.56289 | -0.0279841 | -0.0282868 |
| 3.62563 | -0.0296213 | -0.0298757 |
| 3.69536 | -0.0312632 | -0.0314701 |
| 3.77322 | -0.0329057 | -0.0330282 |
| 3.86185 | -0.0345434 | -0.0345929 |
| 3.96408 | -0.0361712 | -0.0361413 |
| 4.08427 | -0.0377834 | -0.0376901 |
| 4.22751 | -0.0393748 | -0.0392079 |
| 4.40363 | -0.0409405 | -0.0407241 |
| 4.62681 | -0.0424770 | -0.0422317 |
| 4.92652 | -0.0439824 | -0.0437476 |
| 5.39253 | -0.0454570 | -0.0453076 |
| 6.03466 | -0.0461876 | -0.0461498 |
| 6.64126 | -0.0454570 | -0.0454093 |
| 7.07136 | -0.0439824 | -0.0438514 |
| 7.37201 | -0.0424770 | -0.0422590 |
| 7.62429 | -0.0409405 | -0.0406401 |
| 7.85125 | -0.0393748 | -0.0389998 |
| 8.06309 | -0.0377834 | -0.0373436 |
| 8.26529 | -0.0361712 | -0.0356773 |
| 8.46163 | -0.0345434 | -0.0340024 |
| 8.65457 | -0.0329057 | -0.0323211 |
| 8.84544 | -0.0312632 | -0.0306394 |
| 9.03554 | -0.0296213 | -0.0289597 |
| 9.22565 | -0.0279841 | -0.0272864 |
| 9.41613 | -0.0263556 | -0.0256256 |
| 9.60737 | -0.0247389 | -0.0239820 |
| 9.79956 | -0.0231363 | -0.0223606 |
| 9.99307 | -0.0215497 | -0.0207645 |
| 10.18790 | -0.0199810 | -0.0191989 |
| 10.38481 | -0.0184318 | -0.0176630 |
| 10.58493 | -0.0169040 | -0.0161537 |
| 10.78959 | -0.0154006 | -0.0146677 |
| 11.00124 | -0.0139258 | -0.0131960 |
| 11.75 | -0.0090740 | -0.0085823 |
| 12.0 | -0.0077220 | -0.0072714 |
| 13.5 | -0.0023670 | -0.0021438 |
| 15.0 | -0.0006230 | -0.0005462 |
| 20.0 | -0.0000047 | -0.0000129 |

¹ Olson & Liu (1980), Zemke et al. (1984)² present work**Table 3.** Interaction potential energies, $V(R)$, for $a^3\Sigma$ states of NaH in a.u.

| $R(a_0)$ | $V(R)^1$ | $V(R)^2$ |
|----------|-----------|-----------|
| 1.5 | 0.457088 | 0.538711 |
| 1.75 | 0.308218 | 0.365211 |
| 2.0 | 0.209415 | 0.243135 |
| 2.5 | 0.099873 | 0.107539 |
| 3.0 | 0.051073 | 0.051465 |
| 3.5 | 0.028792 | 0.028141 |
| 4.0 | 0.017934 | 0.017616 |
| 4.5 | 0.011974 | 0.011953 |
| 5.0 | 0.008224 | 0.008311 |
| 6.0 | 0.003792 | 0.003822 |
| 8.0 | 0.000593 | 0.000507 |
| 10.0 | 0.000041 | -0.000008 |
| 12.0 | -0.000015 | -0.000032 |
| 15.0 | -0.000008 | -0.000010 |
| 20.0 | -0.000002 | -0.000002 |
| 30.0 | -0.000000 | -0.000000 |

¹ Olson & Liu (1980)² present work

is slightly shifted from the accurate value of $R \simeq 3.57a_0$, and the well depth is reduced by about 10.6%. It is clear that the three-body model should be more accurate for excited electronic states, but even so for the case of the $A^1\Sigma$ state the agreement is particularly good. In table 3 the present results for the $a^3\Sigma$ potential are compared with the results of Olson & Liu (1980). The agreement is very good for $R > 2.5a_0$. In all cases, the present potentials should be the most accurate for large values of R , because atomic basis states are used which give essentially exact results for the energies at infinite separation.

In tables 4, 5 and 6 results obtained using impact theory are shown for the half-half widths of lines of lithium and sodium broadened by helium. In each case the full quantum-mechanical result is compared with the results from the Born and Van der Waals approximations. It is clear that typically the Born approximation predicts widths that are about 20% too small. For the lowest temperatures the Van der Waals approximation is close to the Born results indicating that the asymptotic part of the potential is the dominant influence and demonstrates the equivalence of the Born and

Table 4. Transition Li $2p^2P-2s^2S$ at 670.97 nm. Half half-widths w/N (in units of $10^{-21}\text{MHz m}^3/\text{atom} = (2\pi)^{-1} \times 10^{-9}\text{rad s}^{-1}\text{cm}^3/\text{atom}$)

| $T(\text{K})$ | Born | | Van der |
|---------------|----------------------------|----------------------------|---------------------------|
| | Impact Theory ¹ | Impact Theory ² | Waals Theory ² |
| 70.0 | 0.1476 | 0.1015 | 0.0847 |
| 80.0 | 0.1546 | 0.1074 | 0.0882 |
| 100.0 | 0.1674 | 0.1180 | 0.0943 |
| 200.0 | 0.2184 | 0.1584 | 0.1161 |
| 300.0 | 0.2567 | 0.1883 | 0.1311 |
| 500.0 | 0.3147 | 0.2342 | 0.1528 |
| 700.0 | 0.3599 | 0.2702 | 0.1690 |
| 1000.0 | 0.4151 | 0.3145 | 0.1881 |
| 1500.0 | 0.4882 | 0.3734 | 0.2124 |
| 2000.0 | 0.5477 | 0.4217 | 0.2316 |
| 2500.0 | 0.5985 | 0.4634 | 0.2476 |
| 3000.0 | 0.6433 | 0.5004 | 0.2615 |

¹ Peach & Whittingham (2009)² present work**Table 5.** Transition Na $3p^2P-3s^2S$ at 589.36 nm. Half half-widths w/N (in units of $10^{-21}\text{MHz m}^3/\text{atom} = (2\pi)^{-1} \times 10^{-9}\text{rad s}^{-1}\text{cm}^3/\text{atom}$)

| $T(\text{K})$ | Born | | Van der |
|---------------|----------------------------|----------------------------|---------------------------|
| | Impact Theory ¹ | Impact Theory ² | Waals Theory ² |
| 70.0 | 0.1504 | 0.1174 | 0.1097 |
| 80.0 | 0.1590 | 0.1242 | 0.1142 |
| 100.0 | 0.1745 | 0.1367 | 0.1221 |
| 200.0 | 0.2312 | 0.1839 | 0.1504 |
| 300.0 | 0.2714 | 0.2188 | 0.1698 |
| 500.0 | 0.3320 | 0.2723 | 0.1979 |
| 700.0 | 0.3793 | 0.3144 | 0.2190 |
| 1000.0 | 0.4374 | 0.3662 | 0.2437 |
| 1500.0 | 0.5149 | 0.4354 | 0.2752 |
| 2000.0 | 0.5779 | 0.4922 | 0.3000 |
| 2500.0 | 0.6319 | 0.5411 | 0.3208 |
| 3000.0 | 0.6795 | 0.5846 | 0.3388 |

¹ Peach & Whittingham (2009)² present work

the semi-classical straight-line path approximations. However at the higher temperatures, the shorter range part of the potentials become important and the Van der Waals approximation consistently underestimates the width by about a factor of two. This effect was originally found by Dimitrijević & Peach (1990) in their analysis of regularities in the widths of spectral lines broadened by neutral atoms. It is concluded that the Van der Waals approximation is inadequate for use in the analysis of astronomical spectra.

5. Conclusions

The present calculations have demonstrated that the use of the three-body model can yield accurate interatomic potentials at medium and large separations, particularly for excited electronic states which are the most important for applications to the spectral line broadening problem. Detailed calculations of the potentials for the Na–H system have been carried out which are important for applications to solar spectra. Results for the broadening of lithium and sodium lines by helium perturbers at temperatures relevant to the analysis of the atmo-

Table 6. Transition Na $3d^2D-3p^2P$ at 819.32 nm. Half half-widths w/N (in units of $10^{-21}\text{MHz m}^3/\text{atom} = (2\pi)^{-1} \times 10^{-9}\text{rad s}^{-1}\text{cm}^3/\text{atom}$)

| $T(\text{K})$ | Born | | Van der |
|---------------|----------------------------|----------------------------|---------------------------|
| | Impact Theory ¹ | Impact Theory ² | Waals Theory ² |
| 70.0 | 0.2528 | 0.2018 | 0.2035 |
| 80.0 | 0.2663 | 0.2125 | 0.2118 |
| 100.0 | 0.2908 | 0.2317 | 0.2265 |
| 200.0 | 0.3860 | 0.3028 | 0.2789 |
| 300.0 | 0.4563 | 0.3539 | 0.3149 |
| 500.0 | 0.5609 | 0.4305 | 0.3671 |
| 700.0 | 0.6413 | 0.4893 | 0.4061 |
| 1000.0 | 0.7383 | 0.5600 | 0.4519 |
| 1500.0 | 0.8641 | 0.6518 | 0.5104 |
| 2000.0 | 0.9617 | 0.7251 | 0.5564 |
| 2500.0 | 1.0410 | 0.7870 | 0.5949 |
| 3000.0 | 1.1175 | 0.8411 | 0.6284 |

¹ Peach & Whittingham (2009)² present work

spheres of cool stars show that significant errors arise if the widely used Van der Waals approximation is adopted.

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