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RECENT RESULTS FOR WIDTHS OF LINES IMPORTANT IN THE SPECTRA OF COOL STARS

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Abstract. The broadening of spectral lines by neutral perturbers is an important factor in the interpretation of the observed spectra of cool stars and is often included in the analysis by using a simple van der Waals formula. Detailed calculations are carried out for selected lines and are used to examine the validity of this formula for a range of temperatures.

Key words: atomic processes – line: profiles – Sun: photosphere – stars: white dwarfs, brown dwarfs

1. INTRODUCTION

Accurate pressure broadened profiles of alkali resonance doublets are required for modelling of the atmospheres of cool stars and for generating their synthetic spectra in the region 400–900 nm. When the theory of line broadening developed by Baranger (1958a,b,c) is used, the profile is simply Lorentzian and the widths and shifts of the lines can be calculated.

Accurate calculations of line widths and shifts 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. The use of three-body models of atom-atom systems to calculate interatomic potentials is discussed by Peach (1982, 2010b) and comparisons with *ab initio* calculations for the Na*-H system are presented in Section 3.

The general quantum-mechanical theory of Baranger is applied to lines of lithium and sodium broadened by hydrogen and helium and to a self-broadened line of argon for temperatures in the range 70 K $\leq T \leq$ 10000 K. Comparisons are made with the corresponding van der Waals formula to test its validity.

2. 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

$$w + \mathrm{i}d = 2\pi N \{ \int_0^\infty v f(v) \mathrm{d}v \int_0^\infty [1 - \exp(\mathrm{i}\eta)] \, \rho \, \mathrm{d}\rho \, \}_{\mathrm{Av}} \, . \tag{1}$$

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

$$\int_0^\infty f(v) \mathrm{d}v = 1 \, . \tag{2}$$

The phase shift η is obtained from

$$\eta(\rho, v) = -\frac{1}{\hbar} \int_{-\infty}^{\infty} V(t) \, \mathrm{d}t \tag{3}$$

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

The impact approximation to the general theory of Baranger in its simplest form can be established simply by making the transition

$$(Mv\rho)^2 \to \hbar^2 \, l(l+1) \tag{4}$$

and then

$$2\rho \mathrm{d}\rho \to \frac{\hbar^2}{(Mv)^2} \, (2l+1) \Delta l \, , \tag{5}$$

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

$$\eta(\rho, v) \to 2 \, [\eta_i(l, v) - \eta_f(l, v)] \, , \tag{6}$$

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 general theory, see Baranger (1958a), is discussed in detail by Peach & Whittingham (2009) and Peach (2010a). Essentially the effects of the complete scattering wave functions are included in the expression for the width and shift instead of just their asymptotic forms.

Table 1. Interaction potential energies, $V(R)$, for the $X^1\Sigma$ states of NaH in a.u. [a]Leininger et al. (2000), Olson & Liu (1980), Zemke et al. (1984); [b]present work

$R(a_0)$	$V(R)^a$	$V(R)^b$
2.550802	−0.0222056	0.0173076
2.606257	−0.0293679	0.0077912
2.676012	−0.0371990	−0.0032134
2.766100	−0.0456853	−0.0155804
2.889504	−0.0548261	−0.0297956
3.085685	−0.0646341	−0.0462748
3.566044	−0.0724457	−0.0637470
4.239926	−0.0646341	−0.0603022
4.703898	−0.0548261	−0.0514642
5.108979	−0.0456853	−0.0428457
5.498659	−0.0371990	−0.0347577
5.891502	−0.0293679	−0.0272634
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

Table 2. Interaction potential energies, $V(R)$, for the $A^1\Sigma$ states of NaH in a.u. [a]Leininger et al. (2000), Olson & Liu (1980), Zemke et al. (1984); [b]present work

$R(a_0)$	$V(R)^a$	$V(R)^b$
3.18532	−0.0139258	−0.0140319
3.24769	−0.0169040	−0.0170848
3.32025	−0.0199810	−0.0202466
3.40567	−0.0231363	−0.0234554
3.50582	−0.0263556	−0.0266930
3.62563	−0.0296213	−0.0298757
3.77322	−0.0329057	−0.0330282
3.96408	−0.0361712	−0.0361413
4.62681	−0.0424770	−0.0422317
6.64126	−0.0454570	−0.0454093
7.37201	−0.0424770	−0.0422590
8.26529	−0.0361712	−0.0356773
9.03554	−0.0296213	−0.0289597
9.79956	−0.0231363	−0.0223606
10.58493	−0.0169040	−0.0161537
11.00124	−0.0139258	−0.0131960
11.75	−0.0090740	−0.0085823
12.0	−0.0077220	−0.0072714

Table 3. Interaction potential energies, $V(R)$, for the $a^3\Sigma$ states of NaH in a.u. [a]Leininger et al. (2000), Olson & Liu (1980); [b]present work.

$R(a_0)$	$V(R)^a$	$V(R)^b$
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

Table 4. Transition Li $2p^2P$–$2s^2S$ at 670.97 nm broadened by helium. Half half-widths w/N and shifts d/N (in units of 10^{-21}MHz m^3/atom = $(2\pi)^{-1}\times 10^{-9}$rad s^{-1} cm^3/atom) [a]Peach & Whittingham (2009); [b]present work

T(K)	Impact Theory[a]		Baranger Theory[b]	
	width	shift	width	shift
70.0	0.1476	−0.0155	0.1450	−0.0170
80.0	0.1546	−0.0159	0.1522	−0.0173
100.0	0.1674	−0.0169	0.1654	−0.0181
200.0	0.2184	−0.0210	0.2173	−0.0216
300.0	0.2567	−0.0235	0.2560	−0.0238
500.0	0.3147	−0.0266	0.3144	−0.0267
700.0	0.3599	−0.0289	0.3597	−0.0289
1000.0	0.4151	−0.0316	0.4149	−0.0315
1500.0	0.4882	−0.0356	0.4881	−0.0349
2000.0	0.5476	−0.0401	0.5475	−0.0376
2500.0	0.5984	−0.0456	0.5982	−0.0398
3000.0	0.6432	−0.0523	0.6429	−0.0418

Table 5. Transition Na $3p^2P$–$3s^2S$ at 589.36 nm broadened by hydrogen. Half half-widths w/N and shifts d/N (in units of 10^{-9} rad s^{-1} cm^3/atom) [a]Kršljanin & Peach (1993); [b]present work [c]Kerkeni, et al. (1993); [d]Monteiro et al. (1985); they obtain 10.6 from their approximation (iii)

T(K)	w/N^a	w/N^b	w/N^c	d/N^a	d/N^b
5000.0	9.72	10.57[d]	11.4/11.3	−1.12	−1.165
7000.0	11.0	12.07		−1.30	−1.227
10000.0	12.5	13.90		−1.41	−1.302

Table 6. Transition Na $3p^2P$–$3s^2S$ at 589.36 nm broadened by hydrogen. Half half-widths w/N and shifts d/N (in units of 10^{-21}MHz m^3/atom = $(2\pi)^{-1} \times 10^{-9}$rad s^{-1} cm^3/atom) [a]present work; [b]Peach (1981)

T(K)	Impact Theory[a]		Baranger Theory[b]	
	width	shift	width	shift
70.0	0.3021	−0.0646	0.2546	−0.1850
80.0	0.3183	−0.0685	0.2650	−0.1926
100.0	0.3475	−0.0754	0.2834	−0.2059
200.0	0.4576	−0.0988	0.3489	−0.2535
300.0	0.5387	−0.1128	0.3940	−0.2863
500.0	0.6628	−0.1297	0.4593	−0.3337
700.0	0.7597	−0.1400	0.5081	−0.3691
1000.0	0.8777	−0.1494	0.5655	−0.4108
1500.0	1.0346	−0.1582	0.6386	−0.4640
2000.0	1.1630	−0.1640	0.6962	−0.5058
3000.0	1.3706	−0.1729	0.7862	−0.5712
4000.0	1.5386	−0.1798	0.8571	−0.6227
5000.0	1.6822	−0.1855	0.9164	−0.6658
6000.0	1.8088	−0.1906	0.9679	−0.7032
8000.0	2.0266	−0.1996	1.0552	−0.7666
10000.0	2.2118	−0.2073	1.1282	−0.8197

Table 7. Transition Na $3p^2P$–$3s^2S$ at 589.36 nm broadened by helium. Half half-widths w/N and shifts d/N (in units of 10^{-21}MHz m^3/atom = $(2\pi)^{-1} \times 10^{-9}$rad s^{-1} cm^3/atom) [a]present work; [b]Peach (1981)

T(K)	Impact Theory[a]		Baranger Theory[b]	
	width	shift	width	shift
70.0	0.1486	−0.0275	0.1097	−0.0797
80.0	0.1575	−0.0287	0.1142	−0.0830
100.0	0.1733	−0.0303	0.1221	−0.0887
200.0	0.2306	−0.0343	0.1504	−0.1092
300.0	0.2711	−0.0368	0.1698	−0.1234
500.0	0.3318	−0.0407	0.1979	−0.1438
700.0	0.3791	−0.0433	0.2190	−0.1591
1000.0	0.4372	−0.0457	0.2437	−0.1770
1500.0	0.5146	−0.0483	0.2752	−0.1999
2000.0	0.5775	−0.0502	0.3000	−0.2180
2500.0	0.6314	−0.0517	0.3208	−0.2331
3000.0	0.6789	−0.0529	0.3388	−0.2462

Table 8. Transition Na $3d^2D$–$3p^2P$ at 819.32 nm broadened by helium. Half half-widths w/N and shifts d/N (in units of 10^{-21}MHz m^3/atom = $(2\pi)^{-1} \times 10^{-9}$rad s^{-1} cm^3/atom) [a]present work; [b]Peach (1981)

T(K)	Impact Theory[a]		Baranger Theory[b]	
	width	shift	width	shift
70.0	0.2505	−0.0750	0.2035	−0.1479
80.0	0.2642	−0.0772	0.2118	−0.1539
100.0	0.2891	−0.0814	0.2265	−0.1647
200.0	0.3853	−0.0967	0.2789	−0.2026
300.0	0.4559	−0.1040	0.3149	−0.2288
500.0	0.5607	−0.1048	0.3671	−0.2667
700.0	0.6411	−0.0983	0.4061	−0.2950
1000.0	0.7384	−0.0870	0.4519	−0.3284
1500.0	0.8649	−0.0731	0.5104	−0.3708
2000.0	0.9639	−0.0656	0.5564	−0.4042
2500.0	1.0450	−0.0622	0.5949	−0.4322
3000.0	1.1137	−0.0610	0.6284	−0.4565

Table 9. Transition Ar 4s'($J = 1$)–5p'($J = 0$) at 426.06 nm broadened by argon. Half half-widths w/N and shifts d/N (in units of 10^{-21}MHz m^3/atom = $(2\pi)^{-1} \times 10^{-9}$rad s^{-1} cm^3/atom) [a]present work; [b]Peach (1981)

T(K)	Impact Theory[a]		Baranger Theory[b]	
	width	shift	width	shift
70.0	0.4938	−0.3213	0.4069	−0.2956
80.0	0.5149	−0.3386	0.4235	−0.3077
100.0	0.5515	−0.3694	0.4529	−0.3290
200.0	0.6720	−0.4810	0.5575	−0.4051
300.0	0.7406	−0.5544	0.6297	−0.4575
500.0	0.8188	−0.6475	0.7339	−0.5332
700.0	0.8665	−0.7056	0.8119	−0.5899
1000.0	0.9172	−0.7618	0.9036	−0.6565
1500.0	0.9806	−0.8173	1.0205	−0.7414
2000.0	1.0311	−0.8495	1.1125	−0.8082
3000.0	1.0964	−0.8748	1.2563	−0.9128
4000.0	1.1116	−0.8632	1.3696	−0.9951
5000.0	1.0888	−0.8288	1.4644	−1.0640
6000.0	1.0436	−0.7830	1.5467	−1.1238
8000.0	0.9287	−0.6837	1.6862	−1.2251
10000.0	0.8142	−0.5924	1.8029	−1.3099

3. RESULTS

Molecular potentials for the Li–He and Na–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 Mullamphy et al. (2007) in which the scattering was treated using a close-coupling formulation.

Extensive tests have been carried out to see how accurate a three-body model proves to be when applied to the system Na*–H. The X$^1\Sigma$, A$^1\Sigma$ and a$^3\Sigma$ states have been accurately determined by Olson & Liu (1980), Zemke et al. (1984) and Leininger et al. (2000). In Tables 1–3 their results are compared with the present work based on the three-body model. The agreement for the A$^1\sigma$ and a$^3\Sigma$ states is very good for $R > 2.5a_0$ and for the X$^1\Sigma$ state when $R > 4.5a_0$. 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. Extended tabulations are given by Peach (2010b).

In Table 4, results are shown for the resonance line of lithium broadened by helium. The general Baranger theory is compared with its corresponding impact approximation. The agreement is very good and the results become essentially identical as temperature increases.

In Tables 5 and 6 results are shown for the resonance line of sodium broadened by hydrogen. There is good agreement with other theoretical results and van der Waals theory predicts widths that are consistently less than the accurate results so that for $T = 10000$ K they are wrong by a factor of two. This effect was originally studied by Dimitrijević & Peach (1990). In Tables 7 and 8 similar comparisons are made between the Baranger and van der Waals results for two lines of sodium broadened by helium and they illustrate similar trends.

In Table 9, results for an argon line broadened by neutral argon in its ground state are shown. To obtain these proved to be particularly challenging from the point of view of building a sufficiently good model for the calculation of the Ar*–Ar interatomic potentials. The results show that in this case the Baranger theory and the van der Waals theory actually cross over at about $T = 1120$ K, but differ by over a factor of two at $T = 10000$ K.

4. CONCLUSIONS

The general Baranger theory has been used in which the scattering of perturbers by the emitting atoms is described by accurate interatomic potentials. An analysis of the widths of several lines shows that the van der Waals approximation which is widely used in the analysis of stellar spectra, can be in error by a factor of two.

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