Eur. Phys. J. D **44**, 507–514 (2007)
DOI: 10.1140/epjd/e2007-00230-6

THE EUROPEAN PHYSICAL JOURNAL D

Impact broadening of alkali lines in brown dwarfs

N.F. Allard[1,2,a], J.F. Kielkopf[3,b], and F. Allard[4,1,c]

[1] Institut d'Astrophysique de Paris, UMR 7095, CNRS, Université Pierre et Marie Curie, 98bis boulevard Arago, 75014 Paris, France
[2] Observatoire de Paris-Meudon, LERMA, UMR 8112, CNRS, 92195 Meudon Principal Cedex, France
[3] Department of Physics and Astronomy, University of Louisville, Louisville, KY 40292, USA
[4] Centre de Recherche Astronomique de Lyon, UMR 5574, CNRS, Université de Lyon, École Normale Supérieure de Lyon, 46 allée d'Italie, 69634 Lyon, France

Received 1st April 2007 / Received in final form 8 June 2007

Abstract. Spectral line widths of the light alkalies are presented for conditions prevailing in brown dwarf atmospheres. A unified line shape theory and a set of pseudopotentials are used to compute widths of Li, Na, and K resonance lines perturbed by He and H_2. While limited available experimental data confirm the trends found in the theoretical values reported here, they suggest that improved potentials are needed.

PACS. 32.70.Jz Line shapes, widths, and shifts

1 Introduction

As brown dwarfs cool off with time from spectral type M through L to T, their uppermost atmospheric layers sink below the temperature of silicate and metal crystal grain formation (1800 K). The photosphere, which emits the spectrum, is depleted of refractory elements (Ca, Ni, Si, Ti, V, Fe, Cu). In the optical part of their spectrum, between 0.4 and 1.2 μm, the strong molecular bands of TiO and VO vanish, while the alkali lines (Na, Li, K, Rb, Cs), with some weak bands of CrH, remain the only important background opacity source. The T type brown dwarf optical spectra are totally controlled by the wings of the most abundant Na I D and K I resonance doublets perturbed by H_2, the most abundant form of hydrogen in these deepest, hottest, photospheric layers. The importance of the far wings of the K I resonance doublets, centered at 0.77 μm in spectra of brown dwarfs, has been demonstrated [1–4]. These wings define a pseudo-continuum extending over more than 400 nm from the line center.

The cores, on the other hand, are formed in the uppermost, lowest density atmospheric layers still dominated by H_2 collisions. Since in a model atmosphere calculation, the resulting line profile is the integration of the flux in all layers from the deepest to the uppermost, it is important that the centers be adequately represented, i.e., they can be non-Lorentzian at the high densities of the innermost layers, while Lorentzian in the upper atmosphere but with different widths than predicted by the hydrogenic van der Waals approximation usually used for the cores [5].

In our previous papers, Allard et al. [4,6], we were interested in the far, even very far, line wings of light alkalis perturbed by helium and molecular hydrogen. These wings contribute significantly to the continuum opacity, and their strength depends critically on the details of the atom-atom interactions and their treatment in the line shape theory. Line profile calculations in our work have been done in a unified line shape semi-classical theory [7]. Moreover, the impact approximation determines the asymptotic behavior of the unified line shape correlation function. In this way the results described here are applicable to a more general line profile and opacity evaluation for the same perturbers at any given layer in the photosphere. This approach to calculating the spectral line profile requires the knowledge of molecular potentials, that is, the binary interaction between an alkali atom and a perturbing atom as a function of their separation. Additionally, the dependence of the radiative dipole moment on separation for each molecular state may significantly alter the far wing profiles from those computed with the usual assumption that the transition probability is invariant with separation. We used the molecular-structure calculations performed by Pascale [8] for the adiabatic potentials of alkali-metal–He systems, and by Rossi and Pascale [9] for the molecular potentials of alkali–H_2 systems. Model atmospheres and synthetic spectra for brown dwarf stars were computed using the atmosphere program PHOENIX [10]. The model atmospheres are described by Allard et al. [3]. The comparison with previous models shows a better modeling of the observed spectrum of SDSS 1624 when including special profiles for Na I and K I as a source of opacity [4], with the new models providing an increased opacity in the optical spectra, while a

---

[a] e-mail: `allard@iap.fr`
[b] e-mail: `kielkopf@louisville.edu`
[c] e-mail: `fallard@ens-lyon.fr`

decreased opacity in the near infrared as needed. Allard et al. [4] focused on the light alkalis Li, Na, and K, used Hund's case *a* or *b* for determining the shape of the spectral line [6], and neglected the fine structure which was insignificant in the far wing for these alkalis.

Let us note as well other recent relevant work, stimulated by the need to develop accurate models that explain brown dwarf spectra. A quantum calculation of line width and shift of light alkalis perturbed by He has been done from 70 to 3000 K by Peach et al. [11–13]. Zhu, Babb, and Dalgarno [14] and Alioua and Bouledroua [15] have made a theoretical study of the Li resonance line broadening by He from 200 to 3000 K in the far wings at wavelengths from 500 nm to 1000 nm. Their fully quantum mechanical calculation in the binary approximation of the Na and K resonance lines broadened by He would be useful in the far wing at low density [16]. Santra and Kirby [17] have made an ab initio study of K resonance lines broadened by He and H_2 using new potentials computed for the purpose with a large Gaussian basis set.

In this paper we will focus on the main line and the variation of its width with temperature. We will be concerned with the pressure broadening by He and by H_2 of the resonance lines of light alkalis in the binary collision impact regime. The fine structure has been included in the potentials of Pascale and Rossi [8,9] within the atom-in-molecule-like scheme introduced by Cohen and Schneider [18], as it was done by Allard and Spielgelman [19] for the specific application to heavy alkalis. The impact theories of pressure broadening [20–22] are based on the assumption of sudden collisions (impacts) between the radiator and perturbing atoms, and are valid when frequency displacements $\Delta\omega = \omega - \omega_0$ and gas densities are sufficiently small. In impact broadening the duration of the collision is assumed to be small compared to the interval between collisions, and the results describe the line center broadening, but not the line wing.

The usefulness of the impact approximation lies in its simplicity and especially in the fact that its characteristic shift, width and asymmetry have a dependence on density and temperature that may be calculated easily for sufficiently low density when the atomic potentials are known. Since we are considering the low pressure involved in the upper atmosphere of brown dwarfs, we might expect that the impact approximation will be a good starting point for synthetic spectra, with the understanding that it will not give a correct line wing. After a rapid account of the theory in Section 2, in Section 3 we present the specific case of lithium. We summarize the results we obtained for the case of sodium and potassium in Section 4, making a comparison of impact widths with existing experimental spectra of alkalis perturbed by helium in Section 5.

2 Unified theory

This study takes place in a dipole autocorrelation formulation of the atomic line shape in a classical path trajectory approximation. The profile is obtained as the Fourier transform (FT) of the autocorrelation function.

A detailed description of our unified theory of the shape of the Lyman lines has been given by Allard et al. [7]. Here we will only review it briefly. The spectrum is given by

$$I(\Delta\omega) = \frac{1}{\pi} \operatorname{Re} \int_0^{+\infty} \Phi(s) e^{-i\Delta\omega s} ds. \qquad (1)$$

We obtain for a perturber density n_p

$$\Phi(s) = e^{-n_p g(s)}, \qquad (2)$$

where decay of the autocorrelation function with time leads to atomic line broadening. For a transition $\alpha = (i, f)$ from an initial state i to a final state f, we have

$$\begin{aligned} g_\alpha(s) = & \frac{1}{\sum_{e,e'}{}^{(\alpha)} |d_{ee'}|^2} \\ & \times \sum_{e,e'}{}^{(\alpha)} \int_0^{+\infty} 2\pi\rho d\rho \int_{-\infty}^{+\infty} dx \tilde{d}_{ee'}[R(0)] \\ & \times [e^{\frac{i}{\hbar}\int_0^s dt V_{e'e}[R(t)]} \tilde{d}^*{}_{ee'}[R(s)] - \tilde{d}_{ee'}[R(0)]]. \qquad (3) \end{aligned}$$

We define $\tilde{d}_{ee'}(R(t))$ as a *modulated* dipole [7]

$$D(R) \equiv \tilde{d}_{ee'}[R(t)] = d_{ee'}[R(t)] e^{-\frac{\beta}{2} V_e[R(t)]}, \qquad (4)$$

where β is the inverse temperature $(1/kT)$. Here V_e is the ground state potential when we consider absorption profiles, or an excited state for the calculation of a profile in emission.

In the present context, the perturbation of the frequency of the atomic transition during the collision results in a phase shift, $\eta(s)$, calculated along a classical path $R(t)$ that is assumed to be rectilinear. The phase shift

$$\eta(s) = \frac{i}{\hbar} \int_0^s dt V_{e'e}[\,R(t)\,] \qquad (5)$$

where $\Delta V(R)$, the difference potential, is given by

$$\Delta V(R) \equiv V_{e'e}[R(t)] = V_{e'}[R(t)] - V_e[R(t)], \qquad (6)$$

and represents the difference between the electronic energies of the quasimolecular transition.

The potential energy for a state e is

$$V_e[R(t)] = E_e[R(t)] - E_e^\infty. \qquad (7)$$

At time t from the point of closest approach

$$R(t) = \left[\rho^2 + (x + \bar{v}t)^2\right]^{1/2}, \qquad (8)$$

with ρ the impact parameter of the perturber trajectory and x the position of the perturber along its trajectory at time $t = 0$.

An atomic line broadened by collisions in a low density gas has a Lorentzian profile near the line center which can be related to the FT of a radiative wave in which short duration collisions produce sudden phase changes. In the theory of impact broadened line shape the phase shifts are given by equation (5) with the integral taken between $s = 0$ and ∞. At sufficiently low densities of perturbers the symmetric center of a spectral line is Lorentzian and can be defined by two line parameters, the width and the shift of the main line. These quantities can be obtained in the impact limit ($s \rightarrow \infty$) of the general calculation of the autocorrelation function (Eq. (3)).

3 Case of lithium

3.1 Importance of lithium

Long before the discovery of young, hot, and still bright brown dwarfs [23] the presence of lithium and beryllium in the upper atmospheric layers was identified as an ideal tracer for substellarity [24,25]. Indeed, these elements burn at low temperature and are destroyed in fully convective very low mass stars. Most brown dwarfs of less than $0.6\ M_{\odot}$ would be cooled down enough not to deplete those elements significantly, and therefore show these transitions in their spectra. In particular, the λ 681 nm doublet is located in a part of an otherwise busy optical spectrum where it can emerge from the molecular pseudo-continuum despite its shallow strength (compared to potassium or sodium doublets).

The profile (core + wings) of an atomic line is normalized to unity in the computation of its contribution to the opacities. Due to the weakness of the Li lines, it is important to be able to model precisely both the core width and the wing profiles of the lines. This allows an adequate prediction of the mass at which Li lines reappear in the spectra of brown dwarfs for a given age, or reversely an accurate determination of the age of a cluster.

3.2 Adiabatic molecular potentials

We consider the system composed of a radiating alkali atom A in collision with an atom or molecule B, separated from A by distance R. In the case of an alkali-H_2 collision, B is situated at the center of mass of H_2. In equation (3) e and e' label the energy surfaces on which the interacting atoms approach the initial and final atomic states of the transition as $R \rightarrow \infty$. The sum $\sum_{e,e'}^{(\alpha)}$ is over all pairs (e, e') such that $\omega_{e',e}(R) \rightarrow \omega_{\alpha}$ as $R \rightarrow \infty$.

3.2.1 Li-He diatomic potentials

Molecular-structure calculations have been performed by Pascale [8] to obtain the adiabatic potentials for ground states and numerous excited states of alkali-metal-He systems. He used l-dependent pseudopotentials defined from spectroscopic and scattering data.

As the spin-orbit interaction is not included in these calculations, there are only two electronic states connecting to the alkali + He limit. In the case of light alkalis the fine structure is small and the system may be described by Hund's case *a* or *b* in the molecular region, where the wing is formed. For determining the line core parameters the fine structure has to be included. Spin-orbit (SO) coupling was included within the atom-in-molecule-like scheme introduced by Cohen and Schneider [18], allowing us to distinguish the D1 ($^2S_{1/2}$–$^2P_{1/2}$) and D2 ($^2S_{1/2}$–$^2P_{3/2}$) lines.

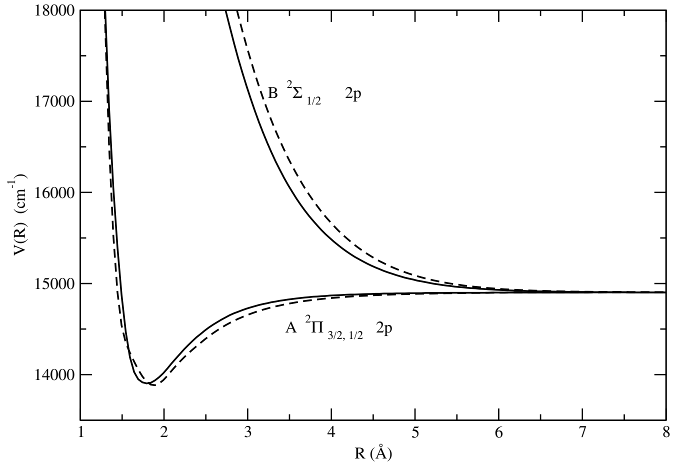

Fig. 1. Potential curves for the A and B states of the Li-He molecule with spin-orbit coupling included. The pseudopotentials [8] are called P1 (full line). Alternative ab initio potentials [14,15] are called P2 (dashed line).

Potential energy curves for the Li-He molecules in the $A^2\Pi_{1,3/2}$ and $B^2\Sigma_{1/2}$ states are shown in Figure 1 (P1 full line). Subtly different Li-He potentials, a composite of carefully chosen ab initio calculations used by Zhu et al. [14] and by Alioua and Bouledroua [15], include the SO coupling and are overplotted (P2 dashed line).

3.2.2 Li-H_2 diatomic potentials

The alkali-H_2 molecular potentials were evaluated by Rossi and Pascale [9] for the two symmetries C_{2v} ($\theta = 90°$) and $C_{\infty v}$ ($\theta = 0°$), where θ is the angle between the direction of the molecular axis and the internuclear axis. The molecule H_2 is assumed to be in its electronic ground state and its bond length fixed to the $v = 0$ equilibrium value $r_e = 1.4$ atomic units. For $\theta = 90°$, the excited states are of $^2A_1$, $^2B_1$, and $^2B_2$ symmetry. We neglect the additional effects that could occur in radiative collisions due to ro-vibrational excitation of H_2.

The R dependence of the electronic energies $V(R, r_e, \theta)$ of the first excited states for $\theta = 0°$ and $90°$ are reproduced in Figure 2 for Li, including the spin-orbit coupling as above for Li-He potentials.

3.3 Variation of the half-width of the systems Li-He/H_2 with temperature

Calculations have been done for the D1 and D2 lines of Li perturbed by He and H_2 from 500 K to 3000 K.

We have plotted in Figures 3 and 4 the results obtained in the semi-classical unified theory using the potentials P1

Table 1. Half-width (10^{-20} cm^{-1}/cm^{-3}) of alkali resonance lines perturbed by He collisions.

Alkali	Transition	Potential	500 K	1000 K	1500 K	2000 K	2500 K	3000 K
Li	$2s\ ^2S_{1/2}$–$2p\ ^2P_{1/2}$	P1	0.95	1.25	1.46	1.63	1.78	1.91
		P2	0.82	1.1	1.28	1.44	1.63	1.72
		cc	1.01	1.34	1.57	1.76	1.93	2.07
	$2s\ ^2S_{1/2}$–$2p\ ^2P_{3/2}$	P1	1.22	1.62	1.93	2.16	2.36	2.49
		P2	1.1	1.47	1.72	1.94	2.13	2.28
		cc	1.01	1.34	1.58	1.77	1.94	2.09
		v d W	1.08	1.33	1.50	1.64	1.75	1.85
Na	$3s\ ^2S_{1/2}$–$3p\ ^2P_{1/2}$	sc	0.85	1.13	1.33	1.50	1.65	1.77
		cc	0.95	1.3	1.53	1.72	1.91	2.05
	$3s\ ^2S_{1/2}$–$3p\ ^2P_{3/2}$	sc	1.31	1.72	2.05	2.27	2.54	2.74
		cc	1.07	1.42	1.64	1.84	2.02	2.17
		v d W	1.10	1.35	1.53	1.67	1.78	1.88
K	$4s\ ^2S_{1/2}$–$4p\ ^2P_{1/2}$	sc	0.94	1.22	1.44	1.62	1.77	1.9
		cc	0.99	1.35	1.64	1.9	2.15	2.37
	$4s\ ^2S_{1/2}$–$4p\ ^2P_{3/2}$	sc	1.52	2.03	2.31	2.69	2.95	3.07
		cc	1.37	1.86	2.18	2.46	2.73	2.95
		v d W	1.12	1.38	1.56	1.70	1.82	1.92

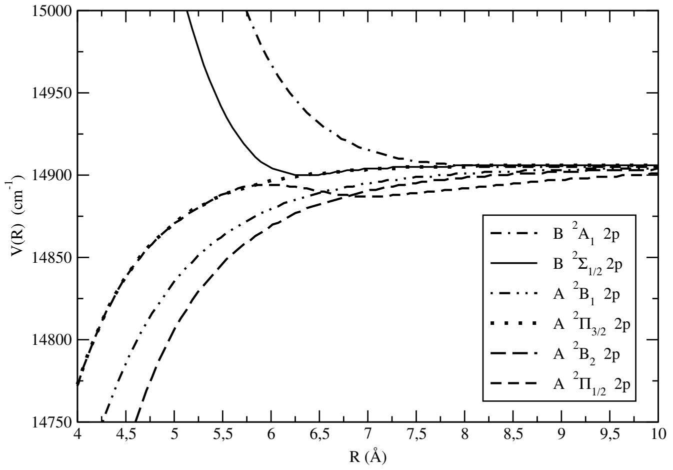

Fig. 2. Li-H_2 potentials for the resonance lines for the C_{2v} and $C_{\infty v}$ symmetries with spin-orbit coupling.

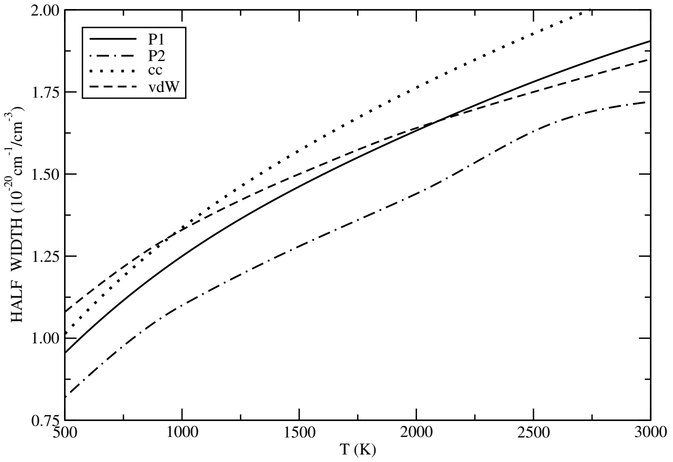

Fig. 3. Variation with temperature of the half-width of the D1 line of lithium perturbed by He collisions.

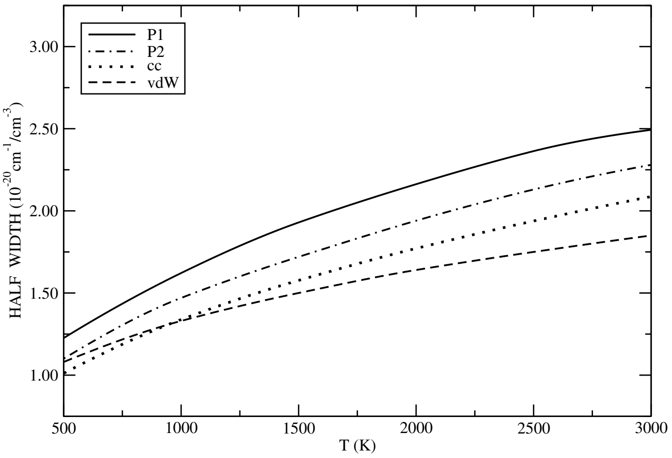

Fig. 4. Variation with temperature of the half-width of the D2 line of the D2 line of lithium perturbed by He collisions.

and P2 presented in Figure 1. It shows the sensitivity of the half-width to the potentials. We also have plotted the half-widths obtained when using van der Waals potentials (vdW). When it is assumed that the main interaction between two atoms is the long range van der Waals interaction of two dipoles, the Lindholm-Foley theory gives the usual formulae for the width and for the shift. The van der Waals damping constant is calculated according to the impact theory of the collision broadening. Despite the fact that even at thermal energies in laboratory experiments on broadening with neutral helium the van der Waals theory does not fit the observations [26,27], these formulae are still currently used in astrophysical applications.

We also have plotted the close coupled (cc) calculations of Peach et al. [12,13], based on the power law form

$$w(T) = aT^b \tag{9}$$

where the fit parameters a and b are given in Table 1 of their paper. In their work line parameters of the light alkalis perturbed by helium have been obtained from

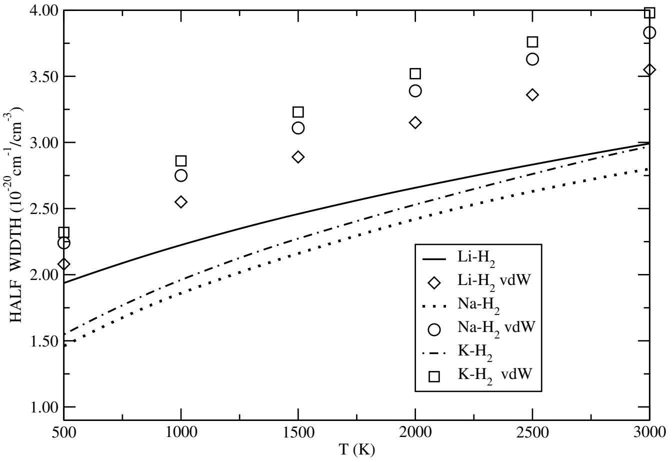

Fig. 5. Variation with temperature of the half-width of the D1 line of light alkalis perturbed by H_2 collisions.

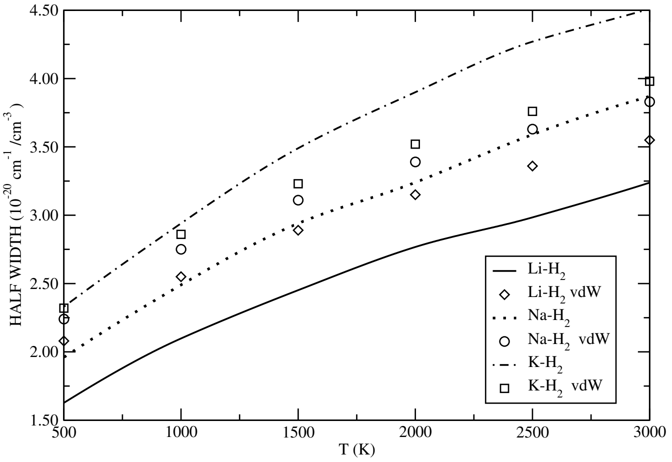

Fig. 6. Variation with temperature of the half-width of the D2 line of light alkalis perturbed by H_2 collisions.

a close-coupling description of the colliding atoms, the Baranger theory for collision broadening, and ab initio potentials described by Mullamphy et al. [13].

H_2 collisions are preponderant in brown dwarf atmospheres and the broadening due to H_2 is larger than that due to He. We are not aware of other calculations of half-widths due to alkali-H_2 collisions, and we could only compare in Figures 5 and 6 the accurate theory here with the broadening which is obtained from a van der Waals potential.

4 Case of sodium and potassium

As in the specific case of lithium we show the potential curves of Na-He and K-He in Figures 7 and 8 and of Na-H_2 and K-H_2 in Figures 9 and 10 obtained from [8,9].

Calculations have been done for the D1 and D2 lines of Na, and K perturbed by He and H_2 from 500 K to 3000 K. In Tables 1 and 2 we have reported our computed half-widths obtained in the semi-classical (sc) theory. We

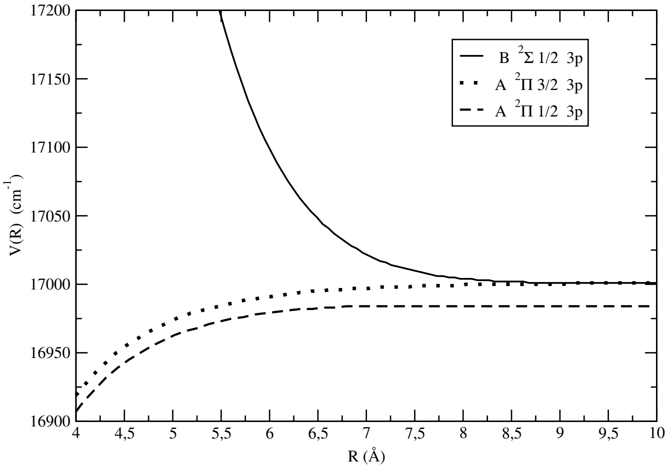

Fig. 7. Potential curves for the A and B states of the Na-He molecule with spin-orbit coupling.

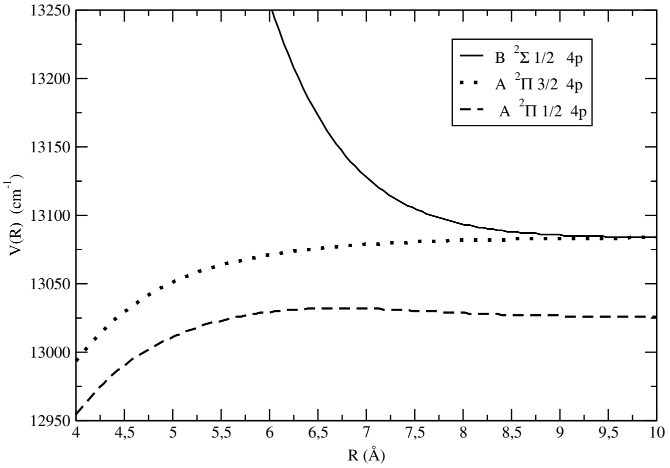

Fig. 8. Potential curves for the A and B states of the K-He molecule with spin-orbit coupling.

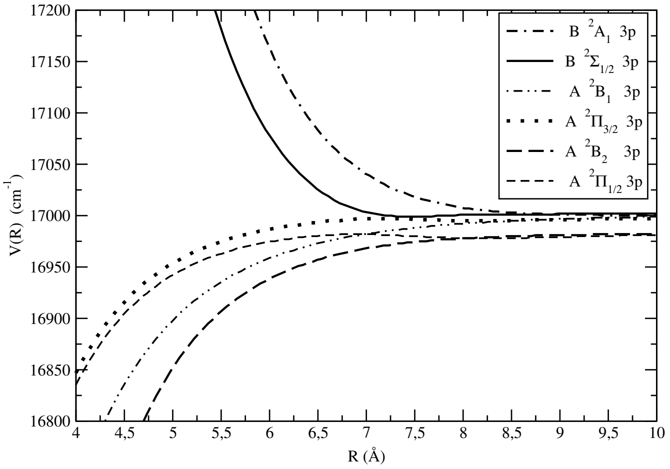

Fig. 9. Na-H_2 potentials for the resonance lines for the C_{2v} and $C_{\infty v}$ symmetries with spin-orbit coupling.

Table 2. Half width (10^{-20}cm^{-1}/cm^{-3}) of alkali resonance lines perturbed by H_2 collisions.

Alkali-H_2	Transition	500 K	1000 K	1500 K	2000 K	2500 K	3000 K
Li	$2s\ ^2S_{1/2}$–$2p\ ^2P_{1/2}$	1.94	2.22	2.46	2.66	2.83	2.99
	$2s\ ^2S_{1/2}$–$2p\ ^2P_{3/2}$	1.63	2.1	2.45	2.77	2.98	3.24
	v d W	2.08	2.55	2.89	3.15	3.36	3.55
Na	$3s\ ^2S_{1/2}$–$3p\ ^2P_{1/2}$	1.46	1.86	2.16	2.42	2.63	2.8
	$3s\ ^2S_{1/2}$–$3p\ ^2P_{3/2}$	1.96	2.49	2.94	3.24	3.59	3.87
	v d W	2.24	2.75	3.11	3.39	3.63	3.83
K	$4s\ ^2S_{1/2}$–$4p\ ^2P_{1/2}$	1.55	1.96	2.48	2.53	2.76	2.97
	$4s\ ^2S_{1/2}$–$4p\ ^2P_{3/2}$	2.33	2.94	3.49	3.90	4.27	4.51
	v d W	2.32	2.86	3.23	3.52	3.76	3.98

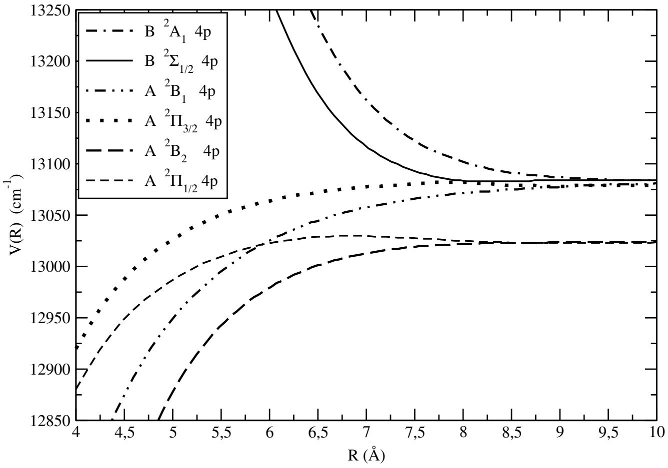

Fig. 10. K-H_2 potentials for the resonance lines for the C_{2v} and $C_{\infty v}$ symmetries with spin-orbit coupling.

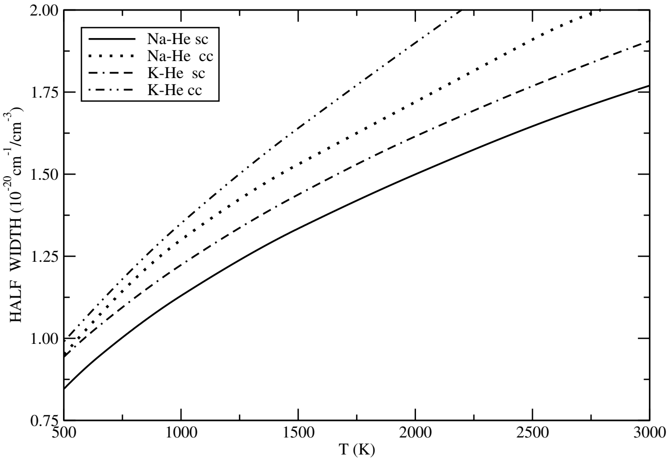

Fig. 11. Variation with temperature of the half-width of the D1 line of light alkalis perturbed by He collisions.

also have reported those derived from the power law form (cc) equation (9). Figures 11, 12, 5, and 6 show their dependence on temperature.

The $P_{1/2}$ line is due to a simple isolated A $\Pi_{1/2}$ state, whereas the $P_{3/2}$ line comes from the A $\Pi_{3/2}$ and B $\Sigma_{1/2}$ adiabatic states arising from the np $P_{3/2}$ atomic state. The broadening of the B $\Sigma_{1/2}$ state is most sensitive to potential at intermediate separations, where the potential starts to deviate from the long range part. This result confirms the study by Roueff and Regemorter [28] and Lortet and Roueff [29] of the collisions with light atoms whose polarisability is small. It was shown by them that the width of spectral lines due to collisions with hydrogen atoms does not rise from the van der Waals dispersion forces but from a shorter range interaction.

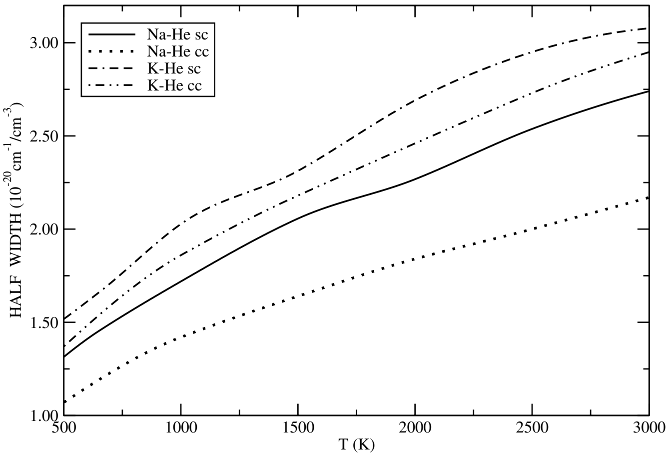

Fig. 12. Variation with temperature of the half-width of the D2 line of light alkalis perturbed by He collisions.

The combined contribution of the two last states, as illustrated in Figures 7 and 8, leads to a larger width for the D2 line. Nevertheless the ratio of half-widths D2/D1 calculated with pseudopotentials seems to be too large compared to available experiments as described below. It seems possible that this discrepancy arises from the sensitivity to the details of the potentials as noted, although the semiclassical treatment of binary collisions used here could be a factor as well. A resolution awaits new experimental results, improved potentials, and a comparison of quantal and semiclassical line shapes from the same potentials.

5 Comparison with experiments

A few laboratory experiments have measured the width, shift, and asymmetry of the light alkalis broadened by

Table 3. Comparison of experimental and theoretical half-widths (10^{-20} cm^{-1}/cm^{-3}) of the Na resonance lines perturbed by He collisions.

Na-He Reference	$3s\ ^2S_{1/2}$–$3p\ ^2P_{1/2}$ D1	$3s\ ^2S_{1/2}$–$3p\ ^2P_{3/2}$ D2	T (K)	*Notes*
Pseudopotential	0.85	1.31	500	This paper
van der Waals	1.10	1.10	500	This paper
Kielkopf (1980) [34]	1.02 ± 0.01	1.06 ± 0.02	450 ± 50	
Chatham et al. (1980) [35]	0.942 ± 0.024	1.14 ± 0.01		
McCartan and Farr (1976) [36]	1.01 ± 0.05	1.16 ± 0.10	475 ± 15	
Deleage et al. (1973) [37]	0.849 ± 0.027	0.902 ± 0.027	465 ± 55	

Table 4. Comparison of experimental and theoretical half-widths (10^{-20} cm^{-1}/cm^{-3}) of the K resonance lines perturbed by He collisions.

K-He Reference	$4s\ ^2S_{1/2}$–$4p\ ^2P_{1/2}$ D1	$4s\ ^2S_{1/2}$–$4p\ ^2P_{3/2}$ D2	T (K)	*Notes*
Pseudopotential	0.94	1.52	500	This paper
van der Waals	1.12	1.12	500	This paper
Lwin and McCartan (1978) [30]	0.82 ± 0.02	1.09 ± 0.02	410 ± 10	

He at low density. No published experimental measurements for broadening by H_2 are known to the authors. For the most part, the alkali resonance lines are so narrow under laboratory conditions that a measurement of their widths requires extremely high spectral resolution, and careful allowance for instrumental effects. The measurements must be made in absorption spectra to avoid the possibility of spectral reversal common in emission and fluorescence sources. Furthermore, because the shifts are also small, extremely good stability is required to make an accurate measurement of the dependence of shift on broadening, a process that requires measuring the wavelength of the line over a range of gas densities.

In spite of these difficulties, there are several independent measurements of the broadening of the Na resonance lines by He summarized in Table 3. All of these measurements excluded instrumental broadening and found the rate of increase of the Lorentzian component of the deconvolved line as a function of gas density over a range of densities up to about 1 atmosphere (2.7×10^{19} cm^{-3}). They are also all nearly at the same low 500 K temperature because at higher temperatures in equilibrium with metallic sodium in a cell, the absorption over pathlengths of centimeters in the laboratory is large enough to prohibit an accurate determination of the line center. At lower temperatures the absorption is too weak to measure with precision using conventional spectroscopic technology. Thus, unfortunately, these measurements cannot distinguish the effects of temperature, or verify the calculation at temperatures of astrophysical interest. They can, however, establish a benchmark for comparison under conditions for which the theories are valid. As such, they are good reference points for testing the validity of potentials suitable for computing the shift and broadening of the center of a line.

That the measurements differ from one another by more than the experimental error is an indication that systematic errors are still present in at least some of the work. Nevertheless, the average values are for D1 0.955 ± 0.079 and for D2 $1.066 \pm 0.117 \times 10^{-20}$ cm^2. Within experimental error there is no clear difference in the broadening of the D1 and D2 components of the Na resonance line by He when considering all of the experiments as a group. However, taken individually each report a broader D2 line than D1, with the average D2/D1 ratio 1.11 ± 0.075. This is much smaller than predicted by the pseudopotential calculations in this paper (1.54). On the other hand, the simple van der Waals estimate would have a ratio of 1.0, which is probably too low. Both the exact line shape computed from pseudpotential theory and the Lorentzian width computed from the van der Waals model agree with the Na-He experiments within roughly 10%.

A similar situation occurs with K-He. Lwin and McCartan [30] made a precise determination of the broadening of the K resonance lines and presented data on the width and shift of the line core, as well as the near line wings, for He and other noble gases. Their results for the core broadened by He are compared in Table 4 with our calculations. The same patterns occur in both K and Na: the recent pseudopotential calculations overestimate the core broadening and the D2/D1 ratio. Lwin and McCartan [30] commented that their measurements agreed better with the pseudopotentials available at that time [31] for the $P_{3/2}$ than for the $P_{1/2}$ component. It is interesting that they also noted that both widths and shifts for the $P_{1/2}$ component computed from potentials based on theoretical dipole–induced-dipole and dipole–induced quadrupole interactions (Kielkopf [32,33]) agreed very well with a wide range of experimental line shape measurements.

6 Conclusions

The recent discovery that the light alkali resonance lines are significant sources of opacity for brown dwarf atmospheres has created a renewed interest in their broadening by He and H_2. We have used pseudopotentials in a semiclassical unified theory of the spectral line broadening to compute line core parameters. For He the results are similar to those recently reported based on close coupling calculations and ab initio potentials, yet the differences are greater than experimental error in comparable laboratory data. For H_2 this is the first theoretical value reported, and there are no experimental tests as yet. The noted discrepancies with He suggest that there may be a need for new calculations of the potentials for alkali-He and alkali-H_2 interactions. The accuracy of such potentials could be tested by new laboratory measurements of the line core and far wing broadening. In the meantime, these results provide a reliable first estimate of broadening of alkali lines by He and H_2.

One of us (NFA) would like to thank Dr M. Bouledroua for making available the Li-He potentials used in [14,15].

References

1. J.D. Kirkpatrick, I.N. Reid, J. Liebert, R.N. Cutri, B. Nelson, C.A. Beichman, C.C. Dahn, D.G. Monet, J.E. Gizia, M.F. Skrutskie, Astrophys. J. **519**, 802 (1999)
2. A. Burrows, M.S. Marley, C.M. Sharp, Astrophys. J. **531**, 438 (2000)
3. F. Allard, P.H. Hauschildt, D.R. Alexander, A. Tamanai, A. Schweitzer, Astrophys. J. **556**, 357 (2001)
4. N.F. Allard, F. Allard, P.H. Hauschildt, J.F. Kielkopf, L. Machin, Astron. Astrophys. **411**, L473 (2003)
5. A. Schweitzer, P.H. Hauschildt, F. Allard, G. Basri, M.N.R.A.S. **283**, 821 (1996)
6. N.F. Allard, F. Allard, J.F. Kielkopf, Astron. Astrophys. **440**, 1195 (2005)
7. N. Allard, A. Royer, J. Kielkopf, N. Feautrier, Phys. Rev. A **60**, 1021 (1999)
8. J. Pascale, Phys. Rev. A **28**, 632 (1983)
9. F. Rossi, J. Pascale, Phys. Rev. A **32**, 2657 (1985)
10. P.H. Hauschildt, E. Baron, JCAM **109**, 41 (1999)
11. G. Peach, D.F.T. Mullamphy, V. Venturi, I.B. Whittingham, Mem. S.A.It **7**, 147 (2005)
12. G. Peach, S.J. Gibson, D.F.T. Mullamphy, V. Venturi, I.B. Whittingham, Spectral Line Shapes, *18th International Conference on Spectral Line Shapes*, AIP Conf. Proc. **874**, 322 (2006)
13. D.F.T. Mullamphy, G. Peach, V. Venturi, B. Whittingham, S.J. Gibson, J. Phys. B **40**, 1141 (2007)
14. C. Zhu, J.F. Babb, A. Dalgarno, Phys. Rev. A **71**, 052710 (2005)
15. K. Alioua, M. Bouledroua, Phys. Rev. A **74**, 032711 (2006)
16. C. Zhu, J.F. Babb, A. Dalgarno, Phys. Rev. A **73**, 012506 (2006)
17. R. Santra, K. Kirby, J. Chem. Phys. **123**, 214309 (2005)
18. J.S. Cohen, B. Schneider, J. Chem. Phys. **61**, 3230 (1974)
19. N.F. Allard, F. Spiegelman, Astron. Astrophys. **452**, 351 (2006)
20. M. Baranger, Phys. Rev. **111**, 481 (1958)
21. M. Baranger, Phys. Rev. **111**, 494 (1958)
22. A.C. Kolb, H. Griem, Phys. Rev. **111**, 514 (1958)
23. R. Rebolo, M.R. Zapatero-Osorio, E.L. Martin, Nature **377**, 129 (1995)
24. R. Rebolo, E.L. Martin, Magazzu, A. Astrophys. J. **389**, L83 (1992)
25. Magazzu et al., Astrophys. J. **404**, L17 (1993)
26. W.R. Hindmarsh, A.D. Petford, G. Smith, Proc. Roy. Soc. A **207**, 296 (1967)
27. N. Allard, J. Kielkopf, Rev. Mod. Phys. **54**, 3304 (1974)
28. E. Roueff, H. Van Regemorter, Astron. Astrophys. **1**, 69 (1969)
29. M.C. Lortet, E. Roueff, Astron. Astrophys. **3**, 462 (1969)
30. N. Lwin, D.G. McCartan, J. Phys. B **1**, 3841 (1978)
31. J. Pascale, J. Vandeplanque, J. Chem. Phys. **64**, 2278 (1974)
32. J. Kielkopf, J. Chem. Phys. **61**, 4733 (1974)
33. J. Kielkopf, J. Phys. B: At. Mol. Phys. **9**, L547 (1976)
34. J.F. Kielkopf, J. Phys. B **13**, 3813 (1980)
35. R.H. Chatham, A. Gallagher, E.L. Lewis, J. Phys. B **13**, L7 (1980)
36. D.G. McCartan, J.M. Farr, J. Phys. B **9**, 985 (1976)
37. J.P. Deleage, D. Kunth, G. Testor, F. Rostas, E. Roueff, J. Phys. B **6**, 1892 (1973)
38. J.F. Kielkopf, J. Phys. B **9**, L547 (1976)
39. N. Lwin, D.G. McCartan, E.L. Lewis, J. Phys. B **9**, L161 (1976)