The resonance lines of sodium and potassium in brown dwarf spectra

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- Interatomic Potentials
- Spectral Line Broadening; Baranger Theory, Impact and one-perturber approximations
- Results: comparisons and validity

Interatomic potentials

• Large quantum chemistry calculations provide very accurate potentials for electronic states of atom-atom systems at short and intermediate separations.

Limited to low excited electronic states.

• Present problems involve low-energy scattering processes for excited electronic states.

Requirement: Accurate representation of potentials at medium and large interatomic separations.

Modelling of atom-atom system

- Three-body model used; two atomic cores and one active electron, i.e. $Na^+ + He + e^-$ and $K^+ + He + e^-$.

- Electron-core interaction.

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

where $Z + z$=nuclear charge, $z = m, n$ and $F_1(r)$ and $F_2(r)$ are cutoff factors.
Parameters α, δ and δ' are varied to reproduce the positions of known energy levels for $z \neq 0$, and phase shifts for scattering for $z = 0$. The fits also predict the correct number of nodes in the wave functions.

- Core-core interaction.

$$V_c(R) \simeq -z_a^2 \frac{\alpha_d^b}{2R^4} - z_b^2 \frac{\alpha_q^a}{2R^6}$$

$$+\text{short} - \text{range terms}\,.$$

Options for short-range term.

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

Choices (a) and (b) differ only for $R \leq R_A + R_B$ where R_A and R_B are the mean radii of Na^+ and K^+.

- Three-body interaction.

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

for R large, where R is the internuclear separation. $P_1(\hat{r}\cdot\hat{R})$ and $P_2(\hat{r}\cdot\hat{R})$ are Legendre polynomials.

- The model Hamiltonian.

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

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

Principles and problems

(a) The long-range interactions are based on well-known perturbation theory.
(b) No existing data for the molecules NaHe and KHe are used to fix any variable parameters.

(c) Positions of virtual states in electron-core model potentials are sensitive to precise fit.
(d) Model potentials can be l-dependent or l-independent.
(e) A different potential may have to be used for ground states, e.g. He($1s^2$).

Theory of spectral line broadening

The main references are:

G. Peach and I.B. Whittingham,
New Astronomy Reviews, **53**, 227-30 (2009).
M. Baranger, *Phys. Rev. A*, **111**, 481-93 (1958).

- Baranger's quantum-mechanical theory.

The impact theory has been widely used, but is actually only an approximation to the general theory developed in this first important paper.

The line profile $I(\omega)$ is defined in terms of a correlation function $C(s)$ by

$$I(\omega) = \mathcal{R}\frac{1}{\pi}\int_0^\infty C(s)\exp(\mathrm{i}\Delta\omega s)\,\mathrm{d}s\,,$$

where ω is the angular frequency, $\Delta\omega$ is the angular frequency separation from the line centre and s is a time variable. $\mathcal{R}$ denotes 'real part of'. In his first paper Baranger showed that $C(s)$ can be written as

$$C(s) = \exp[-N\,g(s)]\,,$$

where N is the perturber density and $g(s)$ is split into two parts, i.e.

$$g(s) = g_1(s) + g_2(s).$$

Only the first term $g_1(s)$ is used here as in many circumstances the second term, $g_2(s)$, can be neglected.

We consider the transition $n_i L_i \rightarrow n_f L_f$ between states $n_i L_i M_i$ and $n_f L_f M_f$ of the alkali atom. The wave function describing the scattering by a potential $V_\Lambda(r)$ is given by

$$\psi_\Lambda(\mathbf{r}) = \sum_{l=0}^{\infty} (2l+1)\, \mathrm{i}^l \exp(\mathrm{i}\eta_{\Lambda l}) \frac{1}{k^{\frac{1}{2}} r} F_{\Lambda l}(k,r)\, P_l(\hat{k}\cdot\hat{r})\,,$$

where $P_l(\hat{k}\cdot\hat{r})$ is a Legendre polynomial and the radial functions $F_{\Lambda l}(k,r)$ are solutions of the equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} - 2MV_\Lambda(r) + k^2\right] F_{\Lambda l}(k,r) = 0\,.$$

The potential $V_\Lambda(r)$ and the atom-atom separation r are in atomic units and M is the reduced mass of the emitter-perturber pair in units of the electron mass m. The momentum k in atomic units is given by

$$k = \frac{Mmva_0}{\hbar},$$

where v is the relative velocity of the emitter and perturber The asymptotic form of $F_{\Lambda l}(k, r)$ is specified by

$$F_{\Lambda l}(k, r) \simeq k^{-\frac{1}{2}} \sin(kr - \frac{1}{2} l\pi + \eta_{\Lambda l}),$$

where $\eta_{\Lambda l} \equiv \eta_{\Lambda l}(k)$ is the elastic scattering phase shift, and as $r \to 0$

$$F_{\Lambda l}(k, r) \propto r^{l+1}.$$

For the cases considered here, the scattering matrix elements S_i and S_f are given by

$$S_i \equiv \langle l\Lambda_i|S|l\Lambda_i\rangle = \exp(2\mathrm{i}\eta_{\Lambda_i l})\,; \quad \Lambda_i = |M_i|\,;$$
$$S_f \equiv \langle l\Lambda_f|S|l\Lambda_f\rangle = \exp(2\mathrm{i}\eta_{\Lambda_f l})\,; \quad \Lambda_f = |M_f|\,.$$

Then we obtain

$$N\, g_1(s) = (w + \mathrm{i}d)\, s\,,$$

where

$$w + \mathrm{i}d = \mathcal{C}\,\frac{\lambda^{1/2}}{M^{3/2}} \sum_{M_i M_f \mu} \begin{pmatrix} L_i & 1 & L_f \\ M_i & \mu & M_f \end{pmatrix}^2 \times \int_0^\infty \exp(-u)\,\mathrm{d}u$$
$$\times \sum_{l=0}^{\infty} (2l+1)\,\left\{\mathrm{i}\,\exp[\mathrm{i}(\eta_{\Lambda i} - \eta_{\Lambda f})]\right\}$$
$$\times\,[\,2M \int_0^\infty F_{\Lambda_i l}(k,r)\,\Delta V\, F_{\Lambda_f l}(k,r)\,\mathrm{d}r]$$

and $\begin{pmatrix} a & b & c \\ d & e & f \end{pmatrix}$ is a 3-j coefficient.

The quantities introduced here are defined by

$$\Delta V = V_{\Lambda_i} - V_{\Lambda_f}$$

and

$$\mathcal{C} = N\, 4\sqrt{\pi}\, \frac{\hbar a_0}{m}\,;\;\; u = \frac{E}{\kappa T} = \frac{\lambda k^2}{M}\,;\;\; \lambda = \frac{\hbar^2}{2 m a_0^2 \kappa T}\,,$$

where κ is the Boltzmann constant, T is the temperature and E refers to the energy of the relative motion. All the dimensional information is contained in the factor $\mathcal{C}$ where a_0 is the Bohr radius. It then follows from that w and d are the half-half width and shift of the Lorentz profile given by

$$I(\omega) = \frac{1}{\pi}\, \frac{w}{(\Delta\omega - d)^2 + w^2}\,.$$

The well-known impact theory is obtained directly by replacing the wave functions $F_{\Lambda_i l}(k,r)$ and $F_{\Lambda_f l}(k,r)$ by their asymptotic forms so that

$$w + \mathrm{i}d = \mathcal{C}\,\frac{\lambda^{1/2}}{M^{3/2}} \sum_{M_i M_f \mu} \begin{pmatrix} L_i & 1 & L_f \\ M_i & \mu & M_f \end{pmatrix}^2 \times \int_0^\infty \exp(-u)\,\mathrm{d}u \times \sum_{l=0}^{\infty} (2l+1)\,\frac{1}{2}[1 - S_i S_f^*]\,.$$

If the Born approximation is made, the phase shifts are calculated from the expression

$$\tan(\eta_{\Lambda l}) = -2Mk \int_0^\infty r^2 V_\Lambda(r)\,[j_l(kr)]^2\,\mathrm{d}r$$

for all values of l. $j_l(kr)$ is a spherical Bessel function where

$$kr\,j_l(kr) \simeq \sin(kr - \frac{1}{2}l\pi)$$

as $r \to \infty$. The Born impact theory then follows directly.

Finally we consider the one-perturber approximation. We define the quantity

$$P(\omega) = \int_0^\infty F_{\Lambda_i l}(k_i, r)\mathcal{D}(r)F_{\Lambda_f l}(k_f, r)\,\mathrm{d}r\,;$$

$$\mathcal{D}(r) \equiv \frac{D(r)}{D(\infty)}\,,$$

where in general, $k_i \neq k_f$. The dipole moment for the transition $\Lambda_i \to \Lambda_f$ is $D(r)$, which tends to a constant, $D(\infty)$, as $r \to \infty$. Then $P(\omega)$ is given by

$$(k_i^2 - k_f^2)\,P(\omega) = 2M \int_0^\infty F_{\Lambda_i l}\,\Delta V\,\mathcal{D}\,F_{\Lambda_f l}\,\mathrm{d}r$$
$$- \int_0^\infty \frac{\mathrm{d}\mathcal{D}}{\mathrm{d}r}\left(F_{\Lambda_i l}\frac{\mathrm{d}F_{\Lambda_f l}}{\mathrm{d}r} - F_{\Lambda_f l}\frac{\mathrm{d}F_{\Lambda_i l}}{\mathrm{d}r}\right)\mathrm{d}r\,,$$

where

$$(k_i^2 - k_f^2) = \frac{2mMa_0^2}{\hbar}\,\Delta\omega\,.$$

We neglect $g_2(s)$ as experience shows that it is negligible compared with the first term. The profile in the line wings is then given by

$$L(\omega) = [P(\omega)]^2$$

and we obtain

$$I(\omega) \simeq \frac{1}{\pi} \frac{w}{\Delta\omega^2}\,; \qquad |\Delta\omega| \gg w\,, \quad |\Delta\omega| \gg |d|\,.$$

If the range of validity of the Baranger theory and the one-perturber approximations overlap, then the correlation function $C(s)$ can be replaced by

$$C(s) = 1 - N\, g_1(s)$$

and we can use these equations to obtain a unification of the two profiles $L(\omega)$ and $I(\omega)$.

Then the Lorentz profile is replaced by

$$I(\omega) = \frac{1}{\pi} \frac{w(0)}{(\Delta\omega - d)^2 + w(0)^2} \frac{w(\Delta\omega)}{w(0)},$$

where

$$w(\Delta\omega) = \mathcal{C} \frac{\lambda^{1/2}}{M^{3/2}} \sum_{M_i M_f \mu} \begin{pmatrix} L_i & 1 & L_f \\ M_i & \mu & M_f \end{pmatrix}^2$$

$$\times \int_0^\infty \exp(-u)\, \mathrm{d}u \sum_{l=0}^{\infty} (2l+1)$$

$$\times [\, 2M \int_0^\infty F_{\Lambda_i l}(k_i, r)\, \Delta V\, F_{\Lambda_f l}(k_f, r)\, \mathrm{d}r]^2 \,,$$

and

$$u = \frac{\lambda k_i^2}{M} \,.$$

Results and discussion

Calculations have been completed for the widths of the sodium and potassium resonance lines broadened by helium using the interaction potentials described in earlier work. The extensive temperature range chosen, 100 K $\leq T \leq$ 10000 K, serves two purposes. It provides the data required for the analysis of the spectra of cool stars, but also tests the range of validity of the various theoretical approximations discussed in this paper.

The main computational issues arise from the slow convergence of the sum over angular momenta l for the higher temperatures and the associated requirement for a greater number of points to be chosen for the integration over energy.

The radia1 equation describing the scattering wave function is integrated directly to determine the exact wave functions and their phase shifts for smaller values of l, $l \leq l_0$ say, and the Born approximation is then used to evaluate phase shifts for $l_0 < l \leq l_{max}$. The Born approximation for the scattering amplitude in its closed form is used to complete the summation up to $l = \infty$. Careful checks are made to determine the optimum values of l_0 and l_{max} at each energy.

Conclusions

In the present calculations we have demonstrated that the formalism and the computational techniques that have been developed can be successfully applied to obtain complete line profiles from the line centre to the line wings for all temperatures and for the lower perturber densities for which the one-perturber approximation is valid. Calculations are in progress to obtain the contribution from transitions where the emitter-perturber system occupies a bound state supported by the initial or final potentials for the molecular states Λ_i and Λ_f. These are known to contribute significantly in the far red wings of the lines considered in this paper.

Comparisons will be made with other theoretical approaches, see for example
N.F. Allard, F.Spiegelman and J.F. Kielkopf A&A, **589**, A21 (2016). Their theory differs in various ways from the theoretical approach described here.

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)

T(K)	one-perturber width	Baranger Theory width	shift
100.0	0.1741	0.1733	-0.0303
200.0	0.2310	0.2306	-0.0343
300.0	0.2713	0.2711	-0.0368
500.0	0.3319	0.3318	-0.0407
700.0	0.3792	0.3791	-0.0433
1000.0	0.4373	0.4372	-0.0457
1500.0	0.5146	0.5146	-0.0483
2000.0	0.5775	0.5775	-0.0502
2500.0	0.6314	0.6314	-0.0517
3000.0	0.6789	0.6789	-0.0529
5000.0	0.8307	0.8307	-0.0570
10000.0	1.0855	1.8055	-0.0622

Transition K $4p^2P$–$4s^2S$ at 767.83 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)

	one-perturber	Baranger Theory	
T(K)	width	width	shift
100.0	0.1979	0.1979	-0.0325
200.0	0.2713	0.2713	-0.0378
300.0	0.3233	0.3233	-0.0380
500.0	0.3986	0.3986	-0.0359
700.0	0.4551	0.4551	-0.0341
1000.0	0.5222	0.5222	-0.0329
1500.0	0.6101	0.6100	-0.0334
2000.0	0.6819	0.6813	-0.0353
2500.0	0.7446	0.7427	-0.0377
3000.0	0.8012	0.7971	-0.0402
5000.0	0.9861	0.9702	-0.0490
10000.0	1.2808	1.2504	-0.0620

Transition K $4p^2P$–$4s^2S$ at 767.83 nm broadened by helium.

Half half-widths $w(DW)/N$ (in units of 10^{-21}MHz m^3/atom $= (2\pi)^{-1} \times 10^{-9}$rad s^{-1} cm^3/atom)

Frequency separations from the line centre are +/-DW(cm^{-1}),T= $1000K$

DW	w(-DW)/N	w(+DW)/N
0.0	0.5222	0.5222
5.0	0.5271	0.5270
10.0	0.5368	0.5382
15.0	0.5508	0.5555
20.0	0.5687	0.5784
25.0	0.5900	0.6061
50.0	0.7347	0.7983
100.0	1.1150	1.2892
200.0	1.9677	2.2106
500.0	3.9393	4.3063
1000.0	3.4908	6.2594
1500.0	1.0390	5.6612
2000.0	0.1612	0.0192
2500.0	0.0171	0.0005
3000.0	0.0014	0.0000