Recent results for widths of lines important in the spectra of cool stars

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- Interatomic Potentials; their Modelling and Accuracy
- Spectral Line Broadening; Baranger Theory, Validity of Impact theory and Van der Waals Formula
- Results

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: two atomic cores and one active electron, i.e. $A^{m+} + B^{n+} + e^-$.

Examples: $Na^+ + H + e^-$; $Na^{2+} + H^+ + e^-$.

• 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 the cores A^{m+} and B^{n+}.

- 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 molecule is 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($1s^2$).

Calculation of potentials

• Extensive tests have been carried out on the Na*–H system. Quantum chemistry calculations exist for some electronic states which have been used to assess the accuracy of the present calculations at short range. The singlet states are strongly infuenced by curve crossings between the Na(nl)–H(1s) and the Na^+–H^- configurations. Results for the ground state and first excited states are shown in the following tables and the quantum chemistry calculations are taken from:

T. Leininger, F.X. Gadéa and A.S. Dickinson, *J. Phys. B: At. Mol. Opt. Phys.* **33**, 1805-17 (2000);
R.E. Olson and B. Liu, *J. Chem. Phys.* **73**, 2817-24 (1980);
W.T. Zemke, R.E. Olson, K.K. Verma, W.C. Stwalley and B. Liu
J. Chem. Phys. **80**, 356-64 (1984)

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

$V(R)^a$ Olson (1980), Zemke et al. (1984)

$V(R)^b$ 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

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

$V(R)^a$ Olson (1980), Zemke et al. (1984)

$V(R)^b$ 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

Interaction potential energies, $V(R)$, for $a^3\Sigma$ states of NaH in a.u.

$V(R)^a$ Olson (1980); $V(R)^b$ 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

Spectral line broadening

• Lindholm impact theory. The collision is treated semi-classically. The half-half width w and shift d are given by

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

where *'Av'* denotes an average over degenerate components of the line and $f(v)$ is the Maxwell distribution. The phase shift η is obtained from

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

For Van der Waals broadening $V(t)$ is replaced by $-C_6/R^6(t)$, a straight-line path for the relative motion is assumed and the integrals can be evaluated analytically.

G. Peach, *Adv. Phys.* **30**, 367-474 (1981).

• Quantum-mechanical impact theory. We make the transition

$$(Mv\rho)^2 \rightarrow \hbar^2\, l(l+1).$$

Then

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

the integral over ρ is replaced by a sum over l and

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

where $\eta_i(l,v)$ and $\eta_f(l,v)$ are elastic scattering phase shifts.

• Born impact theory. Born approximation is used for η_i and η_f, i.e. plane waves for the scattering wave functions plus first-order perturbation theory.

G. Peach and I.B. Whittingham,
New Astronomy Reviews, **53**, 227-30 (2009).

• Baranger's quantum-mechanical theory. The impact theory has been widely used, but is actually only an approximation to the general theory developed in his first important paper:

M. Baranger *Phys. Rev.* **111**, 481-93 (1958).

The line profile is given by

$$I(\omega) = \frac{1}{\pi}\mathrm{Re}\int_0^\infty \exp(-g(s))\,\mathrm{d}s \qquad (1)$$

where the exponent $g(s)$ can be separated into two parts, i.e.

$$g(s) = g_1(s) + g_2(s) \qquad (2)$$

and it is from the dominant term $g_1(s)$ that the impact approximation originates. However, $g_1(s)$ can be calculated directly and again gives a shifted Lorentz profile. The second term is much more difficult to calculate and leads to asymmetry.

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)

T(K)	Impact width	Theory shift	Baranger width	Theory 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

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

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

[a] V. Krsljanin and G. Peach, *Spectral Line Shapes* vol 7, New York: Nova Science, p. 527 (1993).

[b] G.Peach, present results.

[c] B. Kerkeni, P.S. Barklem, A. Spielfiedel and N. Feautrier, *J. Phys. B:* **37**, 677-88 (2004).

[d] T.S. Monteiro, A.S. Dickinson and E.L. Lewis, *J. Phys. B:* **18**, 3499-506 (1985); they obtain 10.6 from their approximation (iii).

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)

T(K)	Baranger Theory		vd Waals Theory	
	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

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)	Baranger Theory		vd Waals Theory	
	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

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)

T(K)	Baranger Theory		vd Waals Theory	
	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

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)

T(K)	Baranger Theory		vd Waals Theory	
	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