$\mathcal{R}$-matrix methods for the computation of Brown Dwarf spectral line shapes

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Abstract

Accurate profiles of alkali spectral lines pressure broadened by collisions with molecular hydrogen and atomic helium perturbers are of crucial importance for the modeling of atmospheres of brown dwarfs. Calculations of these Lorentzian profiles are computationally demanding as they involve the integration of coupled second order differential equations describing the colliding atoms out to large radial separations, for a wide range of energies and relative angular momenta of the perturbers. We report on the use of two $\mathcal{R}$-matrix packages, RPROP2 and FARM, to solve these equations for collisions of atomic helium with Na and K, the dominant alkalis in brown dwarf spectra. Overall we find that the FARM package to be far less transparent and, although

computationally faster, more cumbersome to use. For systems involving smaller sets of coupled differential equations, where there are no convergence problems with either method, RPROP2 appears to be the most appropriate method to use. However, for larger systems, where RPROP2 may become unreliable at higher temperatures, the FARM package appears to be our only feasible option.

Contents

1   Introduction

Accurate profiles of alkali spectral lines pressure broadened by collisions with molecular hydrogen and atomic helium are of crucial importance for the modelling of atmospheres of late M, L and T type brown dwarfs and for generating their synthetic spectra in the region 500–900 nm. A brown dwarf is an object heavier than a giant planet but with insufficient mass to initiate or sustain hydrogen fusion. The central cores of the profiles have a Lorentzian

form and highly accurate calculations of these Lorentzian cores are needed in order to estimate the effects of dust in brown dwarf atmospheres.

We are currently undertaking a study of the Lorentzian profiles of alkali spectral lines broadened by helium perturbers [3]. The calculations are an extension to higher temperatures ($\leq 3000\,\mathrm{K}$) of our previous study [4] of pressure broadening of Na lines by He at laboratory temperatures ($\leq 500\,\mathrm{K}$) and are based on a fully quantum mechanical description of the colliding atoms.

The calculations are computationally demanding in that they involve the integration of coupled second order differential equations describing the colliding atoms out to large radial separations where the solution is matched to a combination of the solutions for non-interacting atoms. This process has to be repeated for a wide range of energies and relative angular momenta of the colliding helium atoms. We chose to use $\mathcal{R}$-matrix propagation techniques as they have high numerical stability and are computationally efficient when large numbers of scattering energies are needed as the matrix diagonalisations, the dominant part of the propagation process, are energy independent.

We report here on two $\mathcal{R}$-matrix packages RPROP2 [1] and FARM [2] that we modified and implemented to calculate the temperature dependences of the widths and shifts of Lorentzian spectral profiles. The RPROP2 routine is extremely slow, but is simple to use and to modify where necessary. Conversely the FARM routine is extremely fast but considerably less transparent, incorporating a less computationally intensive potential-following propagator at intermediate radial separations where the potential is more slowly varying and an analytical, asymptotic solution fitting routine for large radial separations.

Section 2 outlines the background theory appropriate to the calculation of spectral line profiles. Numerical aspects of the calculations and details of the two R-matrix packages are presented in Section 3. Section 4 discusses results.

2   Background theory

The half half-width w and shift d at temperature T of the Lorentzian profile for a spectral line emitted by the alkali atom as it undergoes a transition between the initial and final states $|j_i\rangle$ and $|j_f\rangle$ (where $\mathbf{j}$ is total electronic angular momentum) is [4]

$$w + id = N \int_0^\infty f(E)S(E)\,dE\,, \tag{1}$$

where $f(E)$ is the normalized Maxwellian distribution

$$f(E) = 2\pi(\pi k_\mathrm{B}T)^{-3/2}\sqrt{E}\exp\left(-\frac{E}{k_\mathrm{B}T}\right)\,, \tag{2}$$

for the energies of the perturbing helium atoms, N is the perturber number density and

$$S(E) = \beta \sum_{l,l'} \sum_{J_i,J_f} c_{l,l'}^{J_i J_f}\left[\delta_{l,l'} - \langle j_i l' J_i|S|j_i l J_i\rangle\langle j_f l' J_f|S|j_f l J_f\rangle^*\right]. \tag{3}$$

describes the effects of collisions on the two states forming the spectral line. Here β is a constant, l and l' are the values of the relative emitter-perturber angular momentum $\mathbf{L}_R$ before and after the collision, $\mathbf{J} = \mathbf{L}_R + \mathbf{j}$ is the total angular momentum of the emitter-perturber system (which is conserved during collisions) and $c_{l,l'}^{J_i J_f}$ are known constants. The quantities $\langle j'l'J|S|jlJ\rangle$ are called scattering matrix elements and give the probability that the collision causes the system, initially in the state $|jlJ\rangle$, to undergo a transition into the final state $|j'l'J\rangle$.

The scattering matrix elements in (3) are determined from the asymptotic behaviour of the radial functions $G_{jl}^J(R)$ for each scattering channel (j,l,J) which satisfy the coupled radial Schrödinger equations [4]

$$\left[\frac{\partial^2}{\partial R^2} - \frac{l(l+1)}{R^2} + k_j^2\right] G_{jl,j''l''}^J(R) = \frac{2M}{\hbar^2}\sum_{j',l'} V_{jl,j'l'}^J(R)G_{j'l',j''l''}^J(R)\,. \tag{4}$$

Here (j'', l'') labels the linearly independent solutions of (4), M is the reduced mass of the emitter-perturber system and

$$k_j^2 = 2M \left[E - (E_j^{\text{atom}}) \right] / \hbar^2 \tag{5}$$

where E_j^{atom} is the energy level of the alkali atom before interaction. $V_{jl,j'l'}^J(R)$ are the matrix elements of the potential energy $V(R)$ describing the interaction between the colliding atoms. They are readily calculated for each atomic level. The equations (4) decouple into two sets of opposite parity $(-1)^{J \pm 1/2}$.

3   Numerical aspects

3.1 $\mathcal{R}$-matrix

The close coupled equations (4) were solved using the $\mathcal{R}$-matrix packages RPROP2 [1] and FARM [2], the latter as modified by Venturi et al. [5]. The $\mathcal{R}$-matrix is defined in terms of the inverse logarithmic derivative of the solution matrix $\mathbf{G}(R)$ via

$$\mathcal{R}(R) = \mathbf{G}(R) \left(R \frac{\partial \mathbf{G}}{\partial R} \right)^{-1}, \tag{6}$$

where $\mathbf{G}(R)$ satisfies

$$[\mathcal{H}(R) - \mathcal{E}] \, \mathbf{G}(R) = 0. \tag{7}$$

In equation (7), the scaled Hamiltonian matrix $\mathcal{H}(R)$ is

$$\mathcal{H}_{jl,j'l'}(R) = \left[-\frac{\partial^2}{\partial R^2} + \frac{l(l+1)}{R^2} \right] \delta_{j,j'} \delta_{l,l'} + \frac{2M}{\hbar^2} V_{jl,j'l'}^J(R), \tag{8}$$

and the diagonal scaled energy matrix $\mathcal{E}$ is

$$\mathcal{E} = k_j^2. \tag{9}$$

In the $\mathcal{R}$-matrix propagation method the total integration range for the coupled equations is divided into sectors $[R_L, R_R]$. The $\mathcal{R}$-matrix is then propagated across each sector such that the known $\mathcal{R}$-matrix at one boundary of the sector is used to calculate the $\mathcal{R}$-matrix at the other boundary.

The RPROP2 package uses the solution following propagator developed by Burke, Baluja and Morgan (BBM) whereas the FARM package incorporates a combination of the BBM solution following propagator at small distances where $V(R)$ is rapidly varying and the potential following Light–Walker (LW) propagator at larger distances where $V(R)$ is slowly varying. FARM also uses an accelerated Gailitis expansion to minimize the distance at which the matching procedure is undertaken.

3.2 The BBM $\mathcal{R}$-matrix propagator

The BBM $\mathcal{R}$-matrix propagator [1] for the pth sector $[R_L^p, R_R^p]$ is

$$
\begin{aligned}
R_R^p \mathcal{R}(R_R^p) \; = \; & \mathbf{G}^p(R_R^p, R_R^p) - \mathbf{G}^p(R_R^p, R_L^p) \left[\mathbf{G}^p(R_L^p, R_L^p) + R_L^p \mathcal{R}(R_R^p) \right]^{-1} \\
& \times \mathbf{G}^p(R_L^p, R_R^p) \,.
\end{aligned} \tag{10}
$$

The four matrices $\mathbf{G}^p(R_\alpha^p, R_\beta^p)$ are the Green's function matrices

$$
G_{ij}(R_\alpha^p, R_\beta^p) = \sum_k \frac{U_{ik}(R_\alpha^p)\tilde{U}_{kj}(R_\beta^p)}{\mathcal{E}_k - \mathcal{E}} \,, \quad \alpha, \beta = L, R \,. \tag{11}
$$

Here U_k and $\mathcal{E}_k$ are the eigenvectors and eigenvalues of $\mathcal{H} + \mathcal{L}_b$, where $\mathcal{L}_b$ is the Bloch operator

$$
\mathcal{L}_b = \left[\delta(R - R_R)\frac{\partial}{\partial R} - \delta(R - R_L)\frac{\partial}{\partial R} \right] \,, \tag{12}
$$

which has been introduced to ensure that $\bar{\mathcal{H}} \equiv \mathcal{H} + \mathcal{L}_b$ is Hermitian over the sectors $[R_L, R_R]$. The eigenvectors U_k and eigenvalues $\mathcal{E}_k$ of $\bar{\mathcal{H}}$ are found

by expanding U_k in terms of shifted Legendre polynomials and determining the expansion coefficients by QL matrix diagonalisation. The Hamiltonian $\bar{\mathcal{H}}$ over each sector is expressed in terms of integrations over shifted Legendre polynomials, and the integrations are performed using 32 point Gauss–Legendre quadrature.

3.3   The LW $\mathcal{R}$-matrix propagator

The Light–Walker $\mathcal{R}$-matrix propagator [6, 7] is a potential-following technique used for medium to large internuclear separations where the molecular potentials are more slowly varying. As the potential is slowly varying over short distances in this region, the interaction potential is assumed to be constant within each of the sectors and is therefore represented by the constant potential matrix at the centre of the sector.

The coupled differential equations for the pth sector $[R_L^p, R_R^p]$ have the form

$$\left[\frac{d^2}{dR^2} - \mathbf{V}(R^p) + \mathcal{E}\right]\mathbf{G}(R) = 0\,, \tag{13}$$

where $R^p = \frac{1}{2}[R_L^p + R_R^p]$ and the elements of $\mathbf{V}(R)$ are

$$V_{jl,j'l'}(R) = \frac{l(l+1)}{R^2}\delta_{j,j'}\delta_{l,l'} + \frac{2M}{\hbar^2}V_{jl,j'l'}^J(R)\,. \tag{14}$$

The Green's function matrix corresponding to the solution matrix $\mathbf{G}(R)$ is then

$$\left[\frac{d^2}{dR^2} - \mathbf{V}(R^p) + \mathcal{E}\right]\mathbf{G}(R, R') = \delta(R - R')\mathbf{I}\,. \tag{15}$$

The Light–Walker method requires the constant interaction potential matrix to be diagonalised for each sector in order to obtain the sector transformation matrix $\mathbf{T}^p$, that is

$$(\mathbf{T}^p)^{-1}\mathbf{V}(R^p)\mathbf{T}^p = \bar{\mathbf{V}}^p\,. \tag{16}$$

The matrix $\mathbf{T}^p$ converts (15) into a set of N_γ uncoupled equations for which analytical solutions are then found. $\mathbf{T}^p$ is also used to diagonalise the Green's function matrix

$$\bar{\mathbf{G}}^p(R, R') = (\mathbf{T}^p)^{-1}\mathbf{G}(R, R')\mathbf{T}^p \,, \tag{17}$$

and the $\mathcal{R}$-matrix,

$$\bar{\mathcal{R}}^p(R) = (\mathbf{T}^p)^{-1}\mathcal{R}(R)\mathbf{T}^p \,. \tag{18}$$

In terms of these matrices, the LW $\mathcal{R}$-matrix propagation equation is

$$
\begin{aligned}
R_R^p \bar{\mathcal{R}}^p(R_R^p) &= -\bar{\mathbf{G}}^p(R_R^p, R_R^p) + \bar{\mathbf{G}}^p(R_R^p, R_L^p)(\mathbf{Q}^p)^{-1} \left[\mathbf{Q}^p \bar{\mathbf{G}}^p(R_L^p, R_L^p)(\mathbf{Q}^p)^{-1} \right. \\
&\quad \left. - R_L^p \bar{\mathcal{R}}^{p-1}(R_R^{p-1}) \right]^{-1} \mathbf{Q}^p \bar{\mathbf{G}}^p(R_L^p, R_R^p) \,,
\end{aligned}
\tag{19}
$$

where the adiabatic overlap matrix is $\mathbf{Q}^p = (\mathbf{T}^{p-1})^{-1}\mathbf{T}^p$.

3.4   The Gailitis asymptotic solution method

The Gailitis method [8] allows fitting to the interaction-free solutions without propagating the $\mathcal{R}$-matrix all the way to the asymptotic $V(R) \approx 0$ region. It is computationally advantageous because it not only restricts the region over which the $\mathcal{R}$-matrix must be propagated but also addresses the problem that $\mathcal{R}$-matrix propagation methods actually decrease in efficiency with larger radial separation.

The matching is performed by expressing the interaction potential in the form of a multipole expansion so that the coupled equations take the form

$$\left[\frac{d^2}{dR^2} - \frac{l_i(l_i+1)}{R^2} + k_i^2 \right] M_i(R) = \sum_{j=1}^{N_\gamma} \sum_{\lambda=1}^{\Lambda} \frac{\alpha_{ij}^\lambda}{R^{\lambda+1}} M_j(R) \,, \quad i = 1, \dots, N_\gamma \,. \tag{20}$$

The asymptotic solution is then assumed to have the form

$$M_i(R) = S(R) \sum_{\mu=0} a_i^\mu R^{-\mu} + \dot{S}(R) \sum_{\mu=0} b_i^\mu R^{-\mu} \,, \tag{21}$$

where $S(R)$ and $\dot{S}(R)$ satisfy

$$\left[\frac{d^2}{dR^2} - \frac{L(L+1)}{R^2} + k^2\right] S(R) = 0\,, \tag{22}$$

and

$$\dot{S}(R) = \frac{1}{k}\frac{d}{dR}S(R)\,. \tag{23}$$

Recursion relations are then obtained for the expansion coefficients, a_i^μ and b_i^μ, for both open and closed channels, and these are in turn used to evaluate the wavefunctions (21) and their derivatives.

4   Results and discussion

RPROP2 was originally implemented for calculations of pressure broadening in neon. These calculations involved repeated solution of up to 20 coupled differential equations and were very time consuming, taking up to three months per spectral line. Also, as expected, RPROP2 became unstable at higher temperatures. Consequently, when the FARM package was released, we adapted it to line broadening applications and compared its performance to that of RPROP2 for the case of the Na line $3d\,^2D_{3/2} \rightarrow 3p\,^2P_{1/2}$ perturbed by He. This system is described by five coupled differential equations and FARM was found to be up to five times faster than RPROP2.

Both packages require extensive convergence testing before actual production runs are undertaken to produce the necessary S-matrix elements. This requires variation of up to ten parameters including step sizes for the inner and asymptotic regions, total integration distance and number of Legendre polynomials used in the BBM propagator. All combinations of these ten parameters need to be checked for each atomic level. However FARM utilises a number of automatic checks for varying step size, particularly for the Gailitis

method, which limits the range over which the convergence testing must be conducted and hence reduces the computational time.

The nature of the solutions to (4) varies with l and E so that different inner and asymptotic stepsizes are required for convergence. When l is small the required asymptotic stepsize is large but the effective origin and infinity of the integration range are small, whereas the converse is true for larger l.

Additional issues faced involve the convergence of the sum over partial waves l in (3) and of the integration (1) over perturber energies E. At low temperatures (small E) the maximum value of l needed for convergence is small but this increases with temperature. The present calculations required over 130 energy nodes up to $5000\,\mathrm{K}$, more than half of which were under $1000\,\mathrm{K}$, in order to obtain satisfactory convergence. In order to maximise the efficiency of the final production runs, the total energy range was broken up into seven sectors in which only the minimum number of partial waves required for convergence were used. This ranged from 350 for $T < 100\,\mathrm{K}$ to 800 for $T > 4600\,\mathrm{K}$.

The convergence of the real part of the collision function $S(E)$, which determines the broadened width of the spectral line for the given transition, with number of partial waves is illustrated in Figure 1 for several values of energy.

In summary, although the RPROP2 package is easy to use and modify, FARM is the only feasible option for calculations at higher temperatures where the coupled differential equations have to be integrated out to larger distances, especially for atomic systems requiring the solution of larger sets of equations.
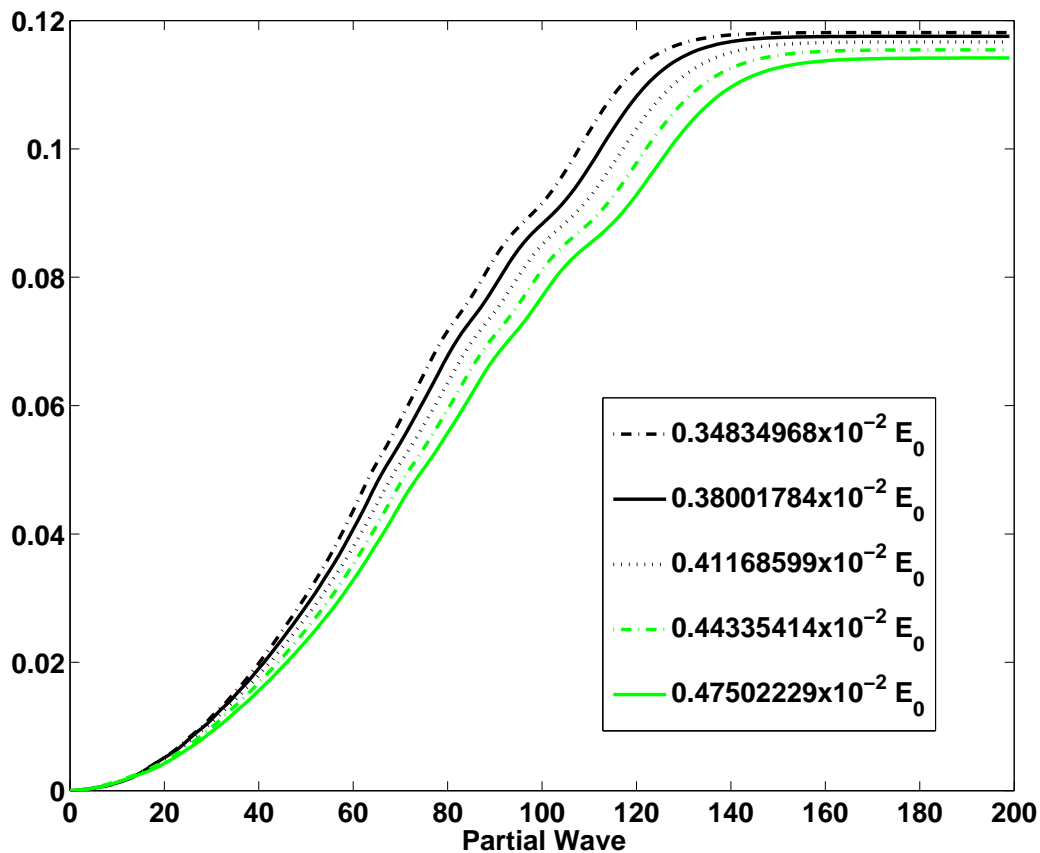
FIGURE 1: Convergence of $Re[S(E)]$ with l for the Na $3d$ $^2D_{3/2} \rightarrow 3p$ $^2P_{1/2}$ transition. The atomic unit of energy E_0 is equivalent to 3.1577×10^5 K.

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