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Self-broadening and shifting of the Li(2*s*–2*p*) and K(4*s*–4*p*) line cores

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ABSTRACT

The aim of this work is to determine quantum mechanically the width Γ and the shift Δ of the lithium Li($2p \rightarrow 2s$) and potassium K($4p \rightarrow 4s$) resonance lines when these atoms are evolving in their parent gases. The interaction potentials along which the atoms Li($2p$) + Li($2s$) and K($4p$) + K($4s$) approach each other are constructed from reliable data. The radial wave equation is then solved numerically by using these potentials to compute the elastic phase shifts. By adopting the simplified Baranger model for the pressure broadening, which assumes the impact approximation, the cross sections effective in linewidth and lineshift are analyzed. The analysis leads in particular to the determination of the width and shift rates and the computations show that these rates have constant values and, mainly, do not depend on temperature. An approximate method is further applied to the calculations of the cross sections. The results reveal the influence of the long-range $-C_3/R^3$ interactions and confirm the universality of the obtained formulas of Γ and Δ.

1. Introduction

The last decades have witnessed extensive theoretical and experimental investigations on the line cores and the far wings of atomic and molecular spectral profiles [1–3]. The corresponding spectroscopic parameters have demonstrated that they could be efficient tools for the diagnostics of astronomical objects and hot or cold plasmas. To fulfil this task, the theory of pressure broadening and shifting of resonance lines applied to ground and excited alkali-metal atoms perturbed by rare gases [4–9] or by their respective parent gases [10–13] has been especially developed.

The purpose of this work is to compute quantum mechanically the collisional width and shift of the lithium and potassium D lines, ^{7}Li($2p \rightarrow 2s$) and ^{39}K($4p \rightarrow 4s$), while the emitting atoms are perturbed by their ground parent atoms Li($2s$) and K($4s$), and to examine the temperature effect on the deduced broadening and shifting parameters. The work is also intended to find out the direct influence the interatomic potentials have on the broadening process. In the next section, the paper presents the most important results provided by the *simplified* quantal theory of pressure broadening developed by Baranger [14]. The simplified model may be sufficiently utilized, since the gas conditions allow one to suppose that the inelastic collisions, the degeneracy of the atomic states as well as the spin–orbit effects are negligible. Then, in Section 3, the required atom–atom potentials are constructed and, in Section 4, they are used to solve the wave equation and to

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deduce the width and shift parameters and their dependence with temperature. The last section employs a semiclassical technique to determine the same parameters and analyze the relationships they have with the potentials.

2. Theory

When an atom evolving in a gaseous environment is emitting or absorbing a radiation, the line core of its characteristic spectrum is most of the time symmetrically or asymmetrically broadened and shifted. Assuming the impact approximation, in which the surrounding monatomic gas of number density N is supposed dilute, i.e., where only binary and elastic collisions occur, this collisional broadening has been studied quantum mechanically by Baranger [14] and reviewed by Allard and Kielkopf [2] and Szudy and Baylis [3].

In the case of spherically symmetric interatomic potentials $V(r)$, with r being the radiator–perturber internuclear separation, the simplified Baranger model yields the relationship [3]

$$\frac{\Gamma}{2}+\mathrm{i}\Delta = N\left\langle \frac{\pi\hbar}{\mu k}\sum_{l=0}^{\infty}(2l+1)[1-\exp(2\delta_l)]\right\rangle_{\mathrm{av}} \tag{1}$$

between the full width at half maximum Γ and the shift of the maximum Δ, where $\hbar$ is the reduced Planck's constant and μ is the reduced mass of the interacting atomic pair. For one wavenumber vector $\mathbf{k}$ of magnitude k and one angular momentum l, the phase difference

$$\delta_l(k)=\eta_l'(k)-\eta_l''(k) \tag{2}$$

is between the elastic phase shifts η_l' and η_l'' corresponding, respectively, to the upper and lower molecular states which the radiating atom forms with one perturber. In expression (1), the average $\langle\cdots\rangle_{\mathrm{av}}$ is computed over the thermal Maxwellian distribution of the relative velocities $\mathbf{v}=(\hbar/\mu)\mathbf{k}$. It can be easily deduced from Eq. (1) that both Γ and Δ depend on the number density N of the perturbers and have, in terms of k, the forms [14]

$$\Gamma = +N\frac{\hbar}{\mu}\langle k\cdot Q_{\mathrm{w}}(k)\rangle_{\mathrm{av}} \tag{3}$$

$$\Delta = -N\frac{\hbar}{\mu}\langle k\cdot Q_{\mathrm{s}}(k)\rangle_{\mathrm{av}} \tag{4}$$

where Q_{w} and Q_{s} are, respectively, the width and shift cross sections defined as the summations [14]

$$Q_{\mathrm{w}}(k)=\frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \tag{5}$$

$$Q_{\mathrm{s}}(k)=\frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin(2\delta_l) \tag{6}$$

The various phase shifts $\eta_l(k)$ are obtained by integrating numerically the radial wave equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2}+k^2-\frac{2\mu}{\hbar^2}V(r)-\frac{l(l+1)}{r^2}\right]\phi_l(r)=0 \tag{7}$$

and forcing the lth partial wavefunction $\phi_l(r)$ to vary asymptotically as $r\to\infty$ like

$$\phi_l(r)\sim\sin\left(kr-\frac{l}{2}\pi+\eta_l\right) \tag{8}$$

It is worth noting that the values of the angular momentum l involved in Eqs. (5) and (6) are generally very large. In such a case, the scattering movement may be treated semiclassically and, consequently, the phase shifts can be approximated by [15]

$$\eta_l(k)\approx-\frac{\mu}{\hbar^2}\int_{r_0}^{\infty}\frac{rV(r)}{\sqrt{(kr)^2-l^2}}\mathrm{d}r \tag{9}$$

with $r_0\approx l/k$. As pointed out by Dalgarno et al. [16] , this integral can be evaluated analytically for most forms of $V(r)$ encountered in practice.

3. Interatomic potentials

Interatomic potentials have been determined in a large range of internuclear distances r for both molecules Li_2 and K_2, using for each region of r the more appropriate way to describe accurately $V(r)$.