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Diamagnetic spectra of alkaline earth barium in a magnetic field

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Abstract. We present theoretical diamagnetic spectra of Barium using R-matrix method combined with quantum defect theory. The nonhydrogenic character of the spectra is analyzed for Ba. Comparisons are made with similar calculations for hydrogen and with data of experiments in the l-mixing region and n-mixing region. The result shows that the theoretical results are in good agreement with the experimental ones.

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1 Introduction

Hydrogen and nonhydrogenic atoms are real physical systems whose behavior in external fields belongs to the fundamental problems in atomic physics. Over the past decades a great number of investigations on the atomic systems in magnetic fields have been carried out theoretically and experimentally and remarkable progresses have been made [1–4]. For example in 1969, Garton and Tomkins [5] in 1969 performed the first experiment on atoms in highly excited Rydberg states in an externally applied magnetic field and discovered the quasi-Landau resonances. These early experiments on alkaline-earth elements were important because they led to the discovery of many fundamental features of the quadratic Zeeman problem, including in particular those related to the chaotic behaviour of the underlying classical dynamics. However, they suffered from a hidden blemish, which was not initially appreciated. In all the early papers (both experimental and theoretical) it was assumed that

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the motional Stark effect, whose existence was uncovered and explained by Fano and Crosswhite [6], would have no significant influenced over the spectra of such heavy atoms. This has turned out not to be true. In fact, experiments with beams have shown that, under the conditions of the experiment performed by Garton and Tomkins [5], the spectra were strongly contaminated by motional Stark effects, to the extent that they do not really represent quadratic Zeeman structures. In fact, the first observation of a purely diamagnetic spectrum for Ba was reported by Elliott *et al.* [7] and to verify its interpretation. So far, there has been only one set of calculations since the work of Elliott *et al.*, namely those of Rao and Taylor [8]. In the present paper, we report a new set of calculations, which are based on similar principles, and we compare them both with earlier theoretical work and with the experimental data. We also note that recent experiments by Connerade and co-workers have led to new data on diamagnetic Stark spectra [9, 10]. In absence of electric fields, however, the system possesses rotational symmetry. This allows us to reduce the problem to a two-dimensional one, but the remaining two-dimensional system is still nonseparable. Especially if the influence of the external field and the inner-atomic forces are comparable, which is the case for highly excited atoms under laboratory field strengths, the system becomes highly nonintegrable, and classically behaves chaotically [11]. Semiclassical techniques and full quantum theories have been developed to study the highly excited Rydberg atoms in magnetic fields. Du *et al.* [12] presented semiclassical closed orbit theory and studied the hydrogen atom in a magnetic field by semiclassical methods. A series of papers have been published [8, 13] using the full quantum theories.

2 Model and method

In this work we study the spectra of Ba in a magnetic field by the R-matrix method with quantum defect theory that was developed by Halley, Delande and Taylor [14] and compare theoretical result with experimental one. This method combines a variant of the R-matrix method with quantum defect theory. The configuration space is divided into an inner region $(r \le a)$ and an outer region $(r \ge a)$. The boundary must be chosen large enough to encompass the multi-electron core, but also small enough for magnetic field terms in Hamiltonian to be neglected. In the outer region, we consider this system as a one-electron system. The Hamiltonian for outer electron of Ba in magnetic fields directed along the z-axis is given by (in atomic units)

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r} + \frac{\gamma L_z}{2} + \frac{\gamma^2}{8}(x^2+y^2), \qquad a \le r \le \infty, \tag{1}$$

where $\gamma = B/B_0$ and $B_0 = 2.35\times10^5$ Tesla, $\gamma L_z/2$ and $\gamma^2(x^2+y^2)/8$ are the linear and quadratic Zeeman terms, respectively. The linear term $\gamma L_z/2$ provides a uniform shift for all the energy levels in a specified subspace of magnetic quantum number m, and so can be omitted. The physics in the inner region where $r \le a$, is very complicated, but according to quantum defect theory we only require the wavefunction solutions on the boundary $r = a$. This