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The Lanczos method applied to quasi-static stark broadening of spectral lines

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ABSTRACT

The quasi-static ion approximation of Stark broadened spectral lines involves an average of the field-dependent line shape over the microfield probability distribution. In the conventional approach, this can become computationally expensive since the calculation at each field point requires inverting a possibly large matrix. It is shown that these calculations are well suited to the "Padé Via Lanczos" approach, which allows for an efficient and accurate numerical integration over the quasi-static field. In turn, the integration forms the basis for determining convergence with Lanczos iterations. Simple examples are used to demonstrate improved performance over conventional methods.

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1. Introduction

In the standard theory of spectral line broadening the ion motion is assumed negligible during the average lifetime of the radiating states [1,2]. Thus, the line shape calculation involves averaging the field induced state mixing and energy shifts over the field distribution. In the absence of external fields the line shape can be written in the form, [1,2]

$$I(\omega) = \int_0^\infty \mathrm{d}\varepsilon P(\varepsilon) J(\omega;\varepsilon) \tag{1.1}$$

where hω is the photon energy, $P(\varepsilon)$ is the probability of finding a Stark field of magnitude ε at the ion or atom (hereafter the radiator), and J(ω;ε) represents the line shape due to electron–radiator interactions in the presence of this field.

The numerical evaluation of the line shape replaces the integral in Eq. (1.1) with the sum.

$$I(\omega) = \sum_{i=1}^{N_\varepsilon} w_i P(\varepsilon_i) J(\omega;\varepsilon_i) \tag{1.2}$$

where N_ε is the number of field points and w_i are weights appropriate to the integration scheme. The challenge is using enough field points in Eq. (1.2) to provide satisfactory accuracy, but in the conventional method, which uses explicit matrix inversion [1,2], the calculation at each field point is expensive requiring m^3 operations for a matrix of size m [3].

The matrix size in line shape calculation can increase rapidly with the number of radiator levels. For example, consider the 1s to 2p helium-like satellites to the Hydrogenic Lyman-α line with lower and upper electronic configurations 1s2l and 2l2l', respectively. There are 448 line space elements and block diagonalization yields matrices with size ~100 [4]. Adding the interaction between the $n = 2$ and $n = 3$ levels (but not including the 1s to 3p line) so that the initial configurations include 1s3l and the final include 2l3l' and 3l3l', increases the number of line space elements to more than 16,000 and block diagonalization yields matrices with size ~3000. This example is relatively simple, so it is expected that multi-electron radiator calculations could involve matrices with sizes of order 10^4 or larger.

Computer codes have been developed to address Stark broadened line shapes from multi-electron radiators extending the capabilities beyond one- or two-electron systems [4–7]. For large numbers of atomic levels these codes, which rely on explicit matrix inversion, can require considerable computer resources. For example, assuming a modest number of frequency and field points totaling 10^4 pairs and an optimistic machine performance, then a line shape calculation involving a matrix of size 10^4 would need several months on a single processor. As a result, approximations are usually made to reduce the size of the problem. In the example above, neglect of interference terms [1,2] reduces the matrices from size ~3000 to less than 800, a decrease in computation time by a factor of ~50. Some approximations have been introduced to

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mitigate the problem that are difficult to quantify and are only validated by more complete calculations [6]. Consequently, accurate results are necessary not only to validate approximate schemes, but also for cases not satisfying the approximation criteria.

Recently a method [8] based on a Hessenberg decomposition was presented that is formally exact, numerically stable, and computationally more efficient than the conventional approach for large matrices. Still, calculations of very large problems would benefit from further increases in computational speed. The purpose here is to take advantage of that formulation and apply the "Padé Via Lanczos" (PVL) method to evaluate $J(\omega;\varepsilon)$. The proposed approach follows that used in large-scale linear systems involving non-Hermitian matrices [9] providing high efficiency compared to traditional calculations. It is stressed that the PVL does not make any physical approximations; instead it is a reduced-order model that reproduces the essential features of the problem. The PVL method is a well-documented technique that has enjoyed great success in efficiently solving extremely large problems [9]. Comparison of the Hessenberg method [8] and the PVL approaches to quasi-static line broadening calculations is analogous to a comparison of direct and iterative solutions to a system of linear equations.

Not only is the functional form of $J(\omega;\varepsilon)$ ideally suited for the application of the PVL method, but also the quasi-static line shape has the advantage that the complicated problem of establishing convergence, and consequent numerical accuracy, of the Lanczos iterations can be resolved using a simplified procedure. Furthermore, the method provides an efficient way for calculating $J(\omega;\varepsilon)$ at any given field value so that an adaptive quadrature scheme for evaluating Eq. (1.1) should prove satisfactory. Alternatively, the PVL method can also reveal the structure of $J(\omega;\varepsilon)$ through a dispersion formula [8] allowing optimization of the field mesh to perform accurately the integration over Stark fields.

2. Padé Via Lanczos

The field-dependent line shape in Eq. (1.1) can be written in "line space" as [8]

$$J(\omega;\varepsilon) = -\pi^{-1}\mathrm{Im}\left\{\ell^t[A(\omega)-\varepsilon B]^{-1}u\right\} \tag{2.1}$$

where ℓ and u are vectors simply related to the radiator dipole operator, the t superscript denotes transpose, $A(\omega)$ represents line broadening in the absence of the Stark field, and B depends only on the internal coordinates of the radiator. The form of Eq. (2.1) is amenable to the PVL method, which is an efficient and, with certain precautions, a stable algorithm [9,10].

2.1. Method

To proceed, for each frequency and $m \times m$ diagonal block rewrite Eq. (2.1) in the form.

$$J(\omega;\varepsilon) = -\pi^{-1}\mathrm{Im}\left\{\ell^t[I-(\varepsilon-\varepsilon_o)C]^{-1}r\right\} \tag{2.1.1}$$

where I is the identity matrix,

$$[A-\varepsilon_o B]r = u, \tag{2.1.2}$$

$$[A-\varepsilon_o B]C = B, \tag{2.1.3}$$

ε_o is a reference expansion point, and the frequency dependence was suppressed for brevity.

The tridiagonal decomposition of the matrix C is accomplished by the Lanczos method [10], which after k Lanczos iterations leads to

$$J(\omega;\varepsilon) \approx J_k(\omega;\varepsilon) = -\pi^{-1}\mathrm{Im}\left\{\ell^t Q[I-(\varepsilon-\varepsilon_o)T_k]^{-1}P^h r\right\} \tag{2.1.4}$$

with

$$C = QT_kP^h \tag{2.1.5}$$

$$QP^h = P^hQ = I \tag{2.1.6}$$

where the h superscript denotes Hermitian conjugate, Q and P are $m \times k$ matrices, and T_k is a tridiagonal matrix of size k. All field independent quantities are evaluated once at each frequency.

Although Eq. (2.1.4) appears similar to the results using the Hessenberg decomposition [8], there are fundamental differences. By exploiting the remarkable properties of the Lanczos method, the PVL approach yields significant savings for large problems [9]. Firstly, for $J(\omega;\varepsilon)$ with a relatively small number of distinct features, the number of Lanczos iterations can be small; that is, $k \ll m$ (see Sect. 2.2). Furthermore, Eq. (2.1.4) can be written in the form [9,10]

$$J_k(\omega;\varepsilon) = -\pi^{-1}\mathrm{Im}\left\{(\ell^t r)\, e_1^t[I-(\varepsilon-\varepsilon_o)T_k]^{-1}e_1\right\} \tag{2.1.7}$$

where $e_1 = [1,0,\ldots,0]^t$ is a unit vector of length k. This is an important result since only the [1,1] element of $[I-(\varepsilon-\varepsilon_o)T_k]^{-1}$ is required. Since T_k is a tridiagonal matrix, it is possible to derive a Padé expansion for the [1,1] element in terms of ε (hence, Padé Via Lanczos) [9]. In practice, however, the evaluation of Eq. (2.1.7) is safer with a stable tridiagonal matrix solver involving order k complex number operations. Further details are provided in the Appendices.

2.2. Order-reduction and convergence

The Lanczos approach provides an approximation to $J(\omega;\varepsilon)$ that improves with the number of iterations until it reaches its best value when the number of iterations is equal to the size of the matrix C. A function with a relatively small number of distinct features, however, can be satisfactorily reproduced with a few iterations. Thus, it is not the size of the matrix C that determines the number of iterations. This order-reduction provides a significant computational advantage over traditional methods for large matrices [9].

Unfortunately, it is impossible to determine the optimal number of Lanczos iterations in advance. It is then necessary to use an incremental approach until a convergence criterion is satisfied. The usual procedure is not only complicated but concentrates on the convergence of the eigenvalues [9]. The quasi-static line shape has the advantage that only the part of $J(\omega;\varepsilon)$ contributing to the relevant range of integration in Eq. (1.1) is of interest. This feature allows for a simplified and physically motivated approach to determine convergence.

The focus is on a robust property of the Lanczos method that holds without regard to the convergence of the eigenvalues. Performing k iterations in the Lanczos process yields a rational function approximation to $J(\omega;\varepsilon)$ that reproduces the first k coefficients in a Taylor series expansion about the reference point $\varepsilon = \varepsilon_o$. It is known that such rational functions have a larger range of validity than the Taylor series [11]. In an average sense, additional iterations increase the rational function range of validity relegating errors to regions further away from the reference value. Due to the presence of the microfield distribution, choosing ε_o near the peak of in the integrand in Eq. (1.1) diminishes the impact of these errors.

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