

Calculation of Resonance S-Matrix Poles by Means of Analytic Continuation in the Coupling Constant

Jiří Horáček^{1,*} and Lukáš Pichl²

¹ Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic.

² International Christian University, 3-10-2 Osawa, Mitaka, Tokyo 181-8585, Japan.

Received 12 May 2016; Accepted (in revised version) 4 September 2016

Abstract. The method of analytic continuation in the coupling constant in combination with the use of statistical Padé approximation is applied to the determination of complex S-matrix poles, i.e. to the determination of resonance energy and widths. These parameters are of vital importance in many physical, chemical and biological processes. It is shown that an alternative to the method of analytic continuation in the coupling constant exists which in principle makes it possible to locate several resonances at once, in contrast to the original method which yields parameters of only one resonance. In addition the new approach appears to be less sensitive to the choice of the perturbation interaction used for the analytical continuation than the original method. In this paper both approaches are compared and tested for model analytic separable potential. It is shown that the new variant of the method of analytic continuation in the coupling constant is more robust and efficient than the original method and yields reasonable results even for data of limited accuracy.

PACS: 31.15.-p

Key words: Analytical continuation in the coupling constant, resonance parameters, complex energy, statistical Padé approximation.

1 Introduction

Resonances defined as complex poles of the S-matrix [1] play an essential role in many areas of physics, chemistry, astronomy, biology, etc. The reason is that the presence of a resonance may increase the rate of a dynamical process by many orders of magnitude and in fact make it the dominant process. Let us mention for example the atomic processes controlling formation of stars and galaxies [2], radiation damage in biological tissues [3], formation of metastable long-lived states in molecular hydrogen [4], etc.

*Corresponding author. *Email addresses:* jiri.horacek@mff.cuni.cz (J. Horáček), lukas@icu.ac.jp (L. Pichl)

There exist several methods for the determination of resonance parameters (i.e. the real and imaginary part of the complex energy of the S-matrix pole). Let us mention just a few of them: stabilisation methods [5–7], Stieltjes imaging techniques [6], complex rotation [8,9], complex absorbing potential [10,11], etc. All the methods are computationally demanding requiring usually the use of complex arithmetics. The method of analytic continuation in the coupling constant represents the less computationally demanding method which uses real arithmetics only. This is a very important fact because for the determination of resonances of extended many electron systems which are essential in various biological and chemical processes (for example radiation damage of DNA) one has to use commercial quantum chemistry codes which are limited to real arithmetics only. The method of analytic continuation in coupling constant (ACCC) has been introduced in nuclear physics by Krasnopolsky and Kukulin [12,13] and is described in detail in the monograph [1]. The ACCC approach has found several applications mainly in nuclear physics, see e.g. [14–18]. Recently Horáček et al. [19] and Papp et al. [20] have applied the ACCC method to real molecular resonances, discussing the $^2\Pi_g$ state of N_2^- resonance of molecular nitrogen and resonance of amino acid molecules (alanine, glycine and valine). In addition Horáček, Paidarová and Čurík applied a modification of the ACCC method to the determination of resonance energy and width of the $^2B_{2g}$ shape resonance of ethylene [21] and diacetylene [22] proving that the ACCC method can yield accurate resonance energies and widths for non-model situations based on data obtained by using standard quantum chemistry codes. It therefore seems worthwhile to study the properties and numerical efficiency of the method in order to get a deeper insight into its properties. One of the open questions is the right selection of the perturbation interaction; this problem seems to be of crucial importance. It is the purpose of this work to propose a new form of the ACCC method, to test the role and choice of the perturbation potential and to compare the numerical efficiency of both approaches. In what follows we shall use units $\hbar=1$ and $m=\frac{1}{2}$ unless explicitly stated.

2 Description of resonances

In its simplest form (i.e. one dimensional radial problem) the resonances are defined as solutions of the following integro-differential Schrödinger equation

$$-\frac{d^2\psi_l(r)}{dr^2} + V(r)\psi_l(r) + \frac{l(l+1)}{r^2}\psi_l(r) + \int_0^\infty W(r,r')\psi_l(r')dr' = k^2\psi_l(r) \quad (2.1)$$

satisfying the boundary conditions of Siegert [27]

$$\psi_l(0) = 0, \quad \frac{\psi_l'(R)}{\psi_l(R)} = ik', \quad (2.2)$$

where R is a distant point at which the interaction V and W is negligible and l is the angular momentum of the resonance. For realistic molecular resonance the equation is of