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Numerical Continuation of Resonances and Bound States in Coupled Channel Schrödinger Equations

Przemysław Kłosiewicz*, Jan Broeckhove and Wim Vanroose

Department of Mathematics and Computer Science, Universiteit Antwerpen, Middelheimlaan 1, B-2020 Antwerpen, Belgium.

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Abstract. In this contribution, we introduce numerical continuation methods and bifurcation theory, techniques which find their roots in the study of dynamical systems, to the problem of tracing the parameter dependence of bound and resonant states of the quantum mechanical Schrödinger equation. We extend previous work on the subject [1] to systems of coupled equations.
Bound and resonant states of the Schrödinger equation can be determined through the poles of the S-matrix, a quantity that can be derived from the asymptotic form of the wave function. We introduce a regularization procedure that essentially transforms the S-matrix into its inverse and improves its smoothness properties, thus making it amenable to numerical continuation. This allows us to automate the process of tracking bound and resonant states when parameters in the Schrödinger equation are varied. We have applied this approach to a number of model problems with satisfying results.

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Key words: Resonances, numerical continuation, coupled channels, Schrödinger equation.

1 Introduction

The appearance of resonances is of ever-growing interest in the study of wave phenomena as they are considered among the most important features of systems described by wave equations. They appear in systems that are penetrable by an impacting wave. Such systems allow the interior field to couple to the external domain which leaves a characteristic fingerprint on the far-field pattern of the scattered wave. Many examples appear naturally in acoustic scattering [2] and in fluid-mechanical structure interaction [3]. In all cases the appearance of resonant states has a profound and important influence on the system's dynamics.

*Corresponding author. *Email address:* przemyslaw.klosiewicz@ua.ac.be (P. Kłosiewicz)

In the context of quantum mechanical scattering, resonant behavior also strongly influences the interactions between microscopic particles, which in turn has its influence on the reactivity of molecules and atoms described by such quantum mechanical models. In molecular systems these resonances can easily turn into bound states if the molecular configuration changes.

In [1] we developed a framework for applying numerical continuation techniques in the context of bound states and resonances in spherically symmetric short-range potentials. We have shown that numerical continuation methods, originally developed in the study of dynamical systems, can be applied successfully to track bound and resonant states efficiently in terms of a varying system parameter. Moreover, this technique can be used to reveal subtle and interesting transitions and connections between states automatically.

The present work focuses on the extension of that procedure to coupled channel short-range systems. This extension is a logical step towards automated, efficient and robust methods for the study of interactions in scattering experiments. In all generality, these techniques can be applied to systems of coupled Helmholtz equations with variable wave numbers, as long as the short-range conditions are met.

The outline of the paper is as follows. Section 2 sets the coupled channel Schrödinger equations in the context of non spherically symmetric quantum mechanical problems. In Section 3 a regularization procedure is discussed that allows application of numerical continuation even though the underlying functions that characterize resonances and bound states are numerically and analytically not very well-suited. Section 4 provides a brief overview of basic numerical continuation methods and gives some pointers on the available implementations. Finally, in Section 5 we present several results obtained with our implementation of the discussed methods.

2 Quantum scattering in coupled channel problems

In this paper we discuss a coupled channel problem that derives from a one particle Schrödinger equation with a non-spherical potential

$$\left(-\frac{1}{2\mu}\Delta+V(\boldsymbol{r},\lambda)-E\right)\psi(\boldsymbol{r})=0, \tag{2.1}$$

where Δ is the three-dimensional Laplacian, $V(\boldsymbol{r},\lambda)$ is a potential with a system parameter λ and E is the complex-valued energy of the system. The problem is such that for all $\boldsymbol{r}$ outside a bounded domain $V(\boldsymbol{r},\lambda)\approx 0$, i.e. the potential becomes negligibly small. Formally, the limitation to potentials that are negligible outside a certain radius is termed as the restriction to so called short-range potentials: $V(\boldsymbol{r},\lambda)$ must decay faster than r^{-3} as $r=|\boldsymbol{r}|\to\infty$ and must be less singular than r^{-2} in the origin $r=|\boldsymbol{r}|\to 0$ [4]. The long-range Coulomb interaction requires a significantly different approach and is not discussed here. The boundary conditions that are appropriate in the short-range case require the solution