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Solving the Faddeev-Merkuriev Equations in Total Orbital Momentum Representation via Spline Collocation and Tensor Product Preconditioning

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Abstract. The computational approach for solving the Faddeev-Merkuriev equations in total orbital momentum representation is presented. These equations describe a system of three quantum charged particles and are widely used in bound state and scattering calculations. The approach is based on the spline collocation method and exploits intensively the tensor product form of discretized operators and preconditioner, which leads to a drastic economy in both computer resources and time.

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Key words: Faddeev-Merkuriev equations, total orbital momentum representation, spline collocation, tensor product preconditioner.

1 Introduction

Since the pioneering work of Hylleraas [1], quantum three-body systems remain the source of challenges and inspirations for theoretical and experimental physicists. New effects specific to three-body systems have been predicted, such as Thomas effect [2], Efimov effect [3], the Phillips line [4, 5]. Direct modeling of nuclear and molecular three-body systems paved a way to develop and to fine-tune realistic models of inter-atomic and inter-nucleon interactions [6–9]. Ab-initio calculations of some specific three-atomic systems may give essential contributions to metrology [10]. The Coulomb quantum three-body systems are also of great importance. For instance, delicate calculations of asymmetric heavy-hydrogen molecular ions gave an insight on *mu*-catalysis [11], studies of positron-atom interactions are valuable for positron-emission tomography.

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Even though the basic mathematical model for such a broad spectrum of physical systems is the Schrödinger equation, the diversity of model interactions and particular physical states leads to a variety of employed computational methods [12–25]. Thus, our ability to perform direct model-free calculations for such wide range of systems is of utmost importance for many branches of physics.

Our goal is to present a universal and efficient computational framework applicable to this broad variety of physical systems and states. In order to achieve this goal we start from the following presuppositions. The approach should be based on a physically correct and mathematically sound representation of the problem. The Faddeev equations formalism [26–28] fulfills all of these requirements. Clear separation of asymptotic channels corresponding to different clusterisations of the system is one of the main advantageous features of the formalism from the point of view of practical applications. Coulomb systems are incorporated into the original formalism by the Merkuriev's version of the Faddeev equations in [29, 30], where the splitting of the Coulomb potentials into long-rage and short-range parts was introduced. Being mathematically equivalent to the Schrödinger equation [29, 30], the Faddeev-Merkuriev (FM) equations have advantages of much simpler boundary conditions and much simpler behavior of their solutions. This leads to much weaker requirements for the basis employed in the calculations.

Direct solution of the FM equations is not, however, a simple task. In order to reduce the dimensionality of the configuration space the symmetries of the solutions must be taken into account. We base our computational approach on total orbital momentum representation which leads to systems of partial differential equations in three-dimensional space. Solving such systems numerically is still a challenging task which calls for developing an effective and robust preconditioning technique. Here we propose a preconditioning scheme based on the tensor-trick algorithm and compare our numerical scheme with solving the corresponding sparse linear system using PARDISO direct solver. Our approach clearly outperforms the direct method both in time and memory requirements, which paves a way to accurate calculations of rather challenging systems, including highly rotationally excited three-body states.

In the following sections we give a description of the FM equations formalism, describe our numerical scheme, and give a few computational examples for some well-studied systems of diverse physical nature.

Throughout the paper we assume $\hbar = 1$ and we use bold font for vectors as, for instance, $\boldsymbol{x}$ and normal font for their magnitude $x = |\boldsymbol{x}|$.

2 The Faddeev-Merkuriev equations

2.1 Notation and basic equations

The FM equations for three quantum particles are of the form