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A Preconditioned Iterative Solver for the Scattering Solutions of the Schrödinger Equation

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Abstract. The Schrödinger equation defines the dynamics of quantum particles which has been an area of unabated interest in physics. We demonstrate how simple transformations of the Schrödinger equation leads to a coupled linear system, whereby each diagonal block is a high frequency Helmholtz problem. Based on this model, we derive indefinite Helmholtz model problems with strongly varying wavenumbers. We employ the iterative approach for their solution. In particular, we develop a preconditioner that has its spectrum restricted to a quadrant (of the complex plane) thereby making it easily invertible by multigrid methods with standard components. This multigrid preconditioner is used in conjunction with suitable Krylov-subspace methods for solving the indefinite Helmholtz model problems. The aim of this study is to report the feasibility of this preconditioner for the model problems. We compare this idea with the other prevalent preconditioning ideas, and discuss its merits. Results of numerical experiments are presented, which complement the proposed ideas, and show that this preconditioner may be used in an automatic setting.

AMS subject classifications: 65F08, 65F10, 65F15, 65M55

Key words: Scattering, Schrödinger equation, exterior complex scaling, preconditioning, multigrid, complex-shifted Laplacian (*CSL*), complex-scaled grid (*CSG*), quadrant-definite (*QD*).

1 Introduction

Acoustic, electromagnetic or seismic waves can all be modeled by a Helmholtz equation with a wave number that has properties specific to the problem area. In some acoustic scattering applications, for example, the wave number is space independent but the

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boundary of the domain can be very complicated depending on the shape of the object. In electromagnetic scattering there are jumps in the material parameters which lead to a piecewise constant wavenumber. In a similar way, the wavenumber in seismic waves will contain information about the geological layers in the earths crust. Each of these problems pose different challenges to the numerical methods.

In this article, we focus on the iterative solution of the Helmholtz equations with a wave number that is specific to models for breakup problems in chemical systems. These breakup dynamics are described by a Schrödinger equation that reduces, in the energy range of breakup problems, to Helmholtz equation with a wavenumber that is continuous in the space variables and can become very large near the boundary of the domain. One example is the disintegration into four charged particles of the H_2 molecule when it is hit with a single photon [1].

The prevalent practice for solving this type of problem requires massively parallel computers [2] and they use a significant portion of the resources of large computer facilities. The long term aim of this research is to replace this practice by efficient iterative methods.

The Helmholtz equation has often outgoing wave boundary conditions. Fixing homogeneous Dirichlet boundary conditions, on the boundaries of the truncated numerical domain, leads to artificial reflections in the domain of interest. These reflections are numerical errors and must be diminished by damping the outgoing waves at the domain boundaries. To bring this about in our numerical solution method, we employ *exterior complex scaled* [3] absorbing boundary layers (henceforth ECS-ABL). There is a long history of this type of absorbing boundary condition for chemical reactions [4]. This treatment is equivalent to the use of perfectly matched layers (PML) [5, 6] and leads to a non-Hermitian discrete problem [7]. For a review on transparent and absorbing boundary conditions for the Schrödinger equation we refer to [8].

For Krylov-subspace methods, the main challenge is to find a good preconditioner. Over the years there have been different approaches to preconditioning the indefinite Helmholtz equation. One line of research is based on a shifted Laplacian preconditioner that started with the work [9,10] (Bayliss, Goldstein and Turkel). They used the Laplacian and the positively shifted Laplacians as preconditioner.

This was later successfully generalized into a robust method, known as the *complex shifted Laplacian* (CSL) preconditioner, by Erlangga, Vuik and Oosterlee using complex valued shifts in [11, 12]. Introducing a complex shift pushes the spectrum of the Helmholtz operator into a region that is favorable for multigrid methods [13–15] to approximately invert the preconditioning problem. It is well-known that multigrid efficiency can readily be exploited only for problems having (positive or negative) definite spectra. In the indefinite case [15], both vital components of multigrid, i.e., smoothing, and coarse grid correction suffer severe degradation, and consequently this results in divergence of the method [16].

An alternative preconditioner that, in addition to shift, also scales the Laplacian was derived from frequency shift time integration by Meerbergen and Coyette [17]. By appro-