An Optimized Perfectly Matched Layer for the Schrödinger Equation

Anna Nissen* and Gunilla Kreiss

Department of Information Technology, Uppsala University, P.O. Box 337, SE-75105 Uppsala, Sweden.

Abstract. We derive a perfectly matched layer (PML) for the Schrödinger equation using a modal ansatz. We derive approximate error formulas for the modeling error from the outer boundary of the PML and the error from the discretization in the layer and show how to choose layer parameters so that these errors are matched and optimal performance of the PML is obtained. Numerical computations in 1D and 2D demonstrate that the optimized PML works efficiently at a prescribed accuracy for the zero potential case, with a layer of width less than a third of the de Broglie wavelength corresponding to the dominating frequency.

1 Introduction

Propagating waves are important in many fields of applications, such as electromagnetism, acoustics, aerodynamics and quantum mechanics. These types of problems are often formulated on very large or unbounded domains and an important aspect in performing efficient numerical simulations is to restrict the original domain to a much smaller computational domain. In order to mimic the behavior of outgoing waves on an unbounded domain, artificial boundary conditions need to be imposed on the boundary of the computational domain. An important feature of this boundary is that it should not reflect outgoing waves, which would contaminate the solution of the original problem. Such artificial boundary conditions can be divided into two classes: non-reflecting or absorbing boundary conditions (ABC) and absorbing layers. An ABC is posed precisely on the boundary, whereas an absorbing layer is an extension of the computational

---

*Corresponding author. *Email addresses:* `anna.nissen@it.uu.se` (A. Nissen), `gunilla.kreiss@it.uu.se` (G. Kreiss)

domain where outgoing waves are dampened (see, e.g., Hagstrom [1, 2] and Givoli [3] for extensive reviews on ABCs).

Here, we consider solving the time-dependent Schrödinger equation with a member from the second class, a perfectly matched layer (PML), in order to study the behavior of quantum mechanical systems without having spurious reflections from waves traveling out of the domain. This is an important issue when studying the dynamics of a chemical reaction, e.g., when the quantum mechanical system consists of a molecule that dissociates into two smaller molecules with a certain probability. The Schrödinger equation is formulated in terms of a wavefunction, where the squares of the absolute values of the wavefunction give the probability density of the states of the system. For the dissociating molecule, this means that as the distance between the two subsystems increases a "probability cloud" propagates towards the far-field. Another application of interest is quantum optimal control. Through the calculation of pulse shapes, e.g., finding the optimal shape of a laser pulse that drives a system from one state to another in a finite time, the control of chemical reactions is enabled. If the problem at hand can experience dissociation, absorbing boundary conditions should be imposed to take care of boundary effects [4].

The perfectly matched layer (PML) method was developed for Maxwell's equations by Berenger [5] in 1994 and has been successfully used in computational electromagnetics, where it has become the standard method. The idea of the PML method is to surround the computational domain by an artificial damping layer of finite width, where a modified set of equations have to be solved. Ideally, the incoming waves are damped to such an extent that the outer boundary conditions are of no importance. Also, the interface between the computational domain and the damping layer should not cause any reflections. The PML fulfils this criteria in theory, although some reflections occur in practice due to the discretization of the problem. We will refer to these as numerical reflections.

In comparison, much work has been done on developing exact ABCs and local approximations of ABCs for the Schrödinger equations. See for instance the review article of Antoine et al. [6]. A very recent result is Jiang and Greengard [7], where a fast algorithm for the exact, global condition is presented. However, specific geometries are required for global ABCs and extension to multi-dimensions is not trivial. Alternatively, local conditions can be derived for a more efficient implementation, at the expense of accuracy. The PML method is not as restricted as ABCs in terms of geometries and application in several dimensions, which makes it suitable for large-scale problems. Also, the PML approach is closely related to absorbing boundary methods used in chemical physics, and our results can be extended to such methods.

The aim of this work is to show how to systematically choose damping parameters and discretization parameters for optimal performance of a Schrodinger PML. A related study for Maxwell's equations in second order formulation was done in [8]. We focus on spatial discretization by finite difference methods and consider orders 2, 4, 6 and 8. In time we use a finite difference scheme of order 2, but the study is also relevant for more efficient time propagation methods. In particular we have the Magnus-Arnoldi