Examiner Report – Doctoral Thesis

Thesis title: Algorithms for time-independent Schrödinger equations

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Subject and Significance

The purpose of the described study is to find high-performance numerical techniques to manipulate and solve the Schrödinger equation. The significance of the Schrödinger equation is referred to its important contribution in solving quantum-mechanical problems. Finding the eigenvectors and eigenvalues of a given Hamiltonian, i.e., solving the steady state Schrödinger equation, is a fundamental element to understand a problem of quantum mechanics and is central in many applications. Analytical solutions of this equation can only be obtained for a small number of simple systems, and one soon needs to resort to computational methods to obtain approximate solutions. Numerically solving the Schrödinger equation is however a complex problem. Standard solution techniques or off-the-shelf packages become hopelessly demanding in terms of computational time and fail at providing accurate results. The development of approaches which are both fast and precise is an interesting and challenging task and forms the recurring theme throughout the thesis. The subject of this thesis is considered relevant and scientifically significant.

Scientific Content

In addition to providing a comprehensive and well-developed overview of the history, intuitions, and mathematical ideas behind constant perturbation and other algorithms for time-independent Schrödinger equations, the author's scientific contributions can be found in:

- An extension of the theory of constant perturbation methods for one-dimensional time-independent Schrödinger equations. The new theoretical results have main value in an extension of the approach to problems with periodic boundary conditions; and in enabling the evaluation of eigenfunctions in an unprecedented efficient and very flexible way.
- An extension of the theory of constant perturbation based shooting methods for the two-dimensional time-independent Schrödinger equation. The theoretical advancements allow to bring the autonomous "matslise"- approach to the 2D case by introducing new techniques for automatic partitioning and for an improved location of the eigenvalues.
- A new approach towards the solution of time-independent two-dimensional Schrödinger problems. The new procedure is no longer using a shooting process to locate the eigenvalues but translates the Schrödinger problem into a matrix eigenproblem. In contrast to other grid-based methods, the technique has not been restricted to rectangular domains and a procedure is delivered to evaluate the eigenfunctions in arbitrary points. Despite the particular attention which is given to the computational cost in the algorithmic choices, the author succeeds in demonstrating accurate results.

These new scientific findings are presented in a comprehensible manner. His contributions confirm the author's ability to master, apply and further develop very advanced solution techniques, and to interpret numerical results accurately. The author exercises honesty about work done by others and in his assessment of the numerical results.

The candidate has also contributed to the scientific community by publicly sharing the outcome of his work in easy-to-use software packages. This adds significant value to his research. Making reliable mathematical software packages is not easy and goes far beyond the limited numerical experimenting to confirm theoretical reasonings often seen in scientific publications. My (not so extensive) experimenting and inspection of the developed software was a positive experience. The python interface and the chosen design will allow users to easily integrate and use the methods in their own research and variety of applications.

Questions and Remarks

The developed approaches and software packages are shown to be considerably faster than earlier versions or other codes. Theoretical reasonings make clear why the proposed approaches can be considered computationally more efficient. But, as the comparison tables only show execution times, it is difficult to determine how much of the speedup can be attributed to the performant c++ implementation.

The contributions are undoubtedly scientifically relevant. It was however not always clear to me in how much a pursuit was given in by real applications or a user need, e.g., was there a specific reason to have experiments in quadruple floating point precision, or for some (non-rectangular) domain choices, … The discussion of the Schrödinger equation in chapter 1 felt rather short after reading about history of calculus and differential equations (nice but not all of it very essential for the rest of the thesis text).

Some aspects or results from the thesis work did not yet receive a fully satisfactory resolution or closure, but I acknowledge that this does not decrease the value of the already obtained results. At the end of chapter 3, I was left a bit puzzled, e.g. about Figure 3.23 which shows some results for N=18 being worse than N=12 results, and sudden jumps in the error between two consecutive eigenvalues almost forming vertical lines in the curves. It is unfortunate that the numerical problems identified in chapter 3 can not be clearly pinpointed as it makes it difficult to have more certainty about any (or no) possible further mitigation. was e.g. experimented with a very fine sector mesh to exclude any peculiarities in the automatic sector selection? Also, the numerical experiments in chapter 4 revealed some phenomena for which no definite explanation was given.

What might explain the observation that the relative errors for connected repeated eigenvalues seem to decrease with the eigenvalue index in for instance figures 4.1 and 4.8? In figure 4.7 the opposite behavior is seen.

Chapter 4 shows some nice eigenfunction plots. The author discusses the accuracy of the eigenvalue results in the numerical experiments section but does not describe how the accuracy of the proposed eigenfunction evaluation algorithm was verified. Did this receive some attention?

Structure, Presentation and Language

The PhD thesis is well structured, and the author quoted an appropriate number of bibliography sources. Furthermore, this thesis is well written in clear and concise manner. The language is comprehensive and coherent.

Overall Assessment

The thesis demonstrates a mastery of (and a love for) the mathematics involved. The thesis contains original contributions and advances knowledge in the field. The work is appropriately situated in a broader context. The results and conclusions are clear.

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Veerle Ledoux