UNIVERSITÀ DEGLI STUDI DI SALERNO
Dipartimento di Matematica

Report on the PhD thesis:

Algorithms for time-independent Schrödinger equations

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Overview:

The thesis is related to the numerical solution of time-independent Schrödinger equation by means of efficient and accurate numerical methods. It is organized into 4 Chapters: after an introductive chapter on differential equations, Chapter 2 is devoted to one dimensional time-independent Schrödinger equation, while Chapters 3 and 4 deals with the two dimensional case.
Theoretical and numerical results are presented, together with C++/Python packages implementing the derived numerical methods.

Main findings:

The author analyzes the numerical solution of time-independet Schrödinger equation both from a theoretical than from a practical point of view, by developing free access mathematical software in C++/Python languages. For one-dimensional Schrödinger equation, the developed software Matslise 3.0 is based on improved CP methods, with particular attention on an efficient implementation. The improvements are confirmed by several numerical experiments.
As regards 2D Schrödinger equation, an improvement of a numerical method introduced by Ixaru in

- L. G. Ixaru. "New numerical method for the eigenvalue problem of the 2D Schrödinger equation". In: Computer physics communications 181.10 (2010), pp. 1738–1742.

has been introduced. Also here the theoretical results are supported by interesting numerical experiments. In the last chapter a new method based collocation has been developed for 2D Schrödinger equation, obtaining the same accuracy of the method of Chapter 2, with a lower computational effort. Once again several numerical experiments illustrate the performances of the method.

Questions and comments:

The thesis is very well written and pleasant to read. I have just some small suggestions:

- when referring to a section, a chapter or a figure, I would use the capital letter (e.g. Section 2.4, Chapter 2.
- page 104, line one of Section 2.7: "In this chapter" instead of "in this section"

Conclusions:

In my opinion the thesis contains interesting and new high quality results. It is very well known for all mathematicians concerned with numerics how hard is performing codes related to numerical algorithms. The author of the thesis showed all necessary practical skills (related to the implementation of the numerical methods) as well as theoretical knowledge and high motivation for research work. Therefore I think the thesis fulfills all requirements for obtaining the PhD degree.

Salerno 23th May 2023

Prof. Dajana Conte

Dajana Conte