Report on PhD Thesis

Algorithms for time-independent Schrodinger equations
by Toon Baeyens

In my capacity as a jury member I formulate the report below.
The thesis has 233 pages and it is organized in four chapters.

Chapter 1 has an introductory character in the field of differential equations. Some pieces of history are presented, and also a number of physical problems where ordinary and partial diferential equations are involved is listed. Presentation is clear and pertinent. As a matter of fact, I must mention from the very beginning that I liked the style of presentation adopted in the whole thesis, open and aimed to disclose fine details, in a way to also sincerely unveil to the reader the attitude of the author on the investigated issues and the evolution of this along time.

Chapter 2 is concentrated on one-dimensional time-independent Schrodinger equation (1D). Here the author is considering mainly the problem of generating the eigenvalues and eigenfunctions for this equation. The two main ways of approaching this problem (final difference and CP methods) are presented and also an abundant set of illustrating numerical results obtained by Matslise2.0 (an existing code) and his Pyslise code is furnished.

As for an original contribution of the author on the theoretical side of the problem I mention Theorem 2.13 where the characteristics of a CP method version are established in terms of the desired accuracy.

Chapters 3 and 4 are devoted to the eigenvalue problem for the two-dimensional time-independent Schrodinger equation (2D).

In Chapter 3 the main attention is directed on the Ixaru’s method, based on the CP procedure, [43]. Many important original theoretical and computational contributions are brought, as, for example,

-an automatic procedure for finding the sector size in terms of the required precision,

-a formula to compute the inner products of two eigenfunctions, necessary for acccurate normalization of the these (Theorem 3.4),

-analytic expression for integral (3.15) which is needed in many contexts,
-a procedure tor computation of integrals involved in propagation of the solution along each sector,
-a robust way to locate the eigenvalues,
and, in my opinion the most important of them,:
-a procedure for correctly determining the eigenvalue index, section 3.3, with the main theorem presented in subsection 3.3.1.
Specifically, Theorem 3.10 answers a problem long addressed before: how to become sure that when building up the spectrum for the 2D no eigenvalue is missing ?
All these ingredients are included in the packages Matslise2d and psylise2d. The creation of these codes required a long and sustained effort, and this also deserves a high appreciation.
An intriguing issue in this chapter is that the numerical experiments do not exhibit the high accuracy expected from methods based on the CP procedure. In particular, the maximal accuracy seems to be blocked at approximately eight figures in spite that the codes are working in double precision arithmetic.
The author correctly assumed that the reason may lay somewhere in his source program, examined some parts of it but without a clear answer. I hope that meantime (I have received the text of the thesis on April 19, 2023) he was able to find the bug(s).

Chapter 4 investigates the treatment of 2D problems by means of finite difference (multistep) procedures. Here the author's attention is focussed on the procedure described in [96]. Some new properties are detected, such as, for example, the h and k dependence of the error (page 173). The author also developes associate codes, Strands (for the source) and strands (python), where a number of very interesting new ideas, presented in the thesis, are also added, and reports on a number of experiments to conclude that this 2D multistep method is fast, accurate and promissing.

As for a comparison between this and Ixaru's method, I think that there is still too early for making a final, pertinent conclusion because the bug(s) in the program for Ixaru's method is(are) not yet detected, on one hand, and the available set of experimental results is perhaps still limited (as I explain below), on the other hand.

A preliminary discussion, which tacitly assumes that the bug(s) do not affect the accuracy, is however possible. The central idea is that the comparison should follow the pattern of the 1D case. For this case it is well-known that the accuracies in the eigenvalues to be obtained on one and the same partition from multistep and CP methods of the same order are comparable for the low index eigenvalues, but when the index is increased the accuracy from the multistep method deteriorates, while that from the CP method improves, see e.g. [47].

The point is that not the index in itself is important but the fact that for the 1D case there is a special feature behind it: the index represents simply the number of internal zeros in the associate eigenfunction, or, in other words, it indicates how much is that eigenfunction oscillating inside the domain. This specification is important for the 2D case because now the index and the number of internal zeros of the eigenfunctions along each of the two directions are no more correlated. Graphs in all figures in the thesis where 2D eigenfunctions are presented show this. For example, on Figure 4.15 we see eigenfunctions with indexes 23, 24 and 25 but if, in each graph, we count the number of internal zeros (white colour) along any horizontal or vertical line we find that this number does not exceeds 7. On other figures this is even smaller; on Figure 4.9, for example, this number is 3. Seen in this way, the data available in the thesis are rather limited in the sense that, although they are assigned to rather high values for the index, they actually refer to sets of eigenfunctions with a small number of zeros on each axis. Consequently, these data cover situations when, by analogy with 1D, the two methods are expected to give comparable accuracies, and also that the multistep method is so accurate, as reflected in Chapter 4. The analogy with the 1D case also suggests that more and more significant differences, and in the favour of the CP-based method, will appear for higher and higher indexes. Having the bug(s) detected will become of much help for checking such predictions, of course.

Altogether, this thesis is of a very good quality. The author shows that he maturely masters his field and is able to bring important improvements and to advance new interesting directions for further research.

The thesis fulfills all standards for being admitted to the public defence. I suggest considering some of my remarks in his text, but only if the author also appreciates this as being helpful for increasing the quality of his work.

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