A substantive analysis of the different parts of the dissertation

The dissertation entitled "Algorithms for time-independent Schrödinger equations" consists of four chapters.

The first chapter gives a short introduction to differential equations. Surprisingly the author gives a quite nice overview of the development of the principal items in the history of mathematics and the position of differential equations in this science. Ordinary and partial differential equations are introduced, and some specific real-word applications taken from the world of physics are given.

Chapter two is completely devoted to the one-dimensional time-independent Schrödinger equation and its relation to the Sturm-Liouville equation. Attention is given to the code Matslise developed some ten years ago and the underlying mathematical techniques used in the numerical algorithms, such as finite difference schemes, piecewise constant approximation of the occurring potential and Prüfer's shooting techniques. As an illustration some numerical illustrations are added. Toon Baeyens concludes that the last version of the code dated from 2016 focuses on the fast and accurate computation of eigenvalues and the graphical representation of the corresponding eigenfunctions. There is one remark that the eigenfunctions are only computed in a limited set of points and that an eventual accurate computation of those entities over the whole integration interval however is very time-consuming. The used algorithms seem to be very useful for solving a particular Sturm-Liouville problem, but valuable computation time is lost if the detection whether a given problem is singular or the error estimation is not needed. These ideas have been motivated the author to look for a more efficient implementation of Matslise based on a more efficient implementation of the constant perturbation method. Besides considering only the Robin boundary conditions as in the existing Matslise code also generalized periodic boundary conditions are considered. For one-dimensional Schrödinger equations a more advanced Matslise 3.0 code is developed where C++-source files are used together with a python package. A quite large number of numerical experiments illustrates the efficiency of the new code. The author explained very openly the many occurring implementation challenges he has met by adapting the earlier version of Matslise with the new ideas. He also considered an efficient way of memory management and the automatic testing of the obtained results. By this he proves to be not only concerned with the mathematical correctness of his application, but also with the eventual occurring of software bugs. He ends the chapter with suggestions for future work.

Chapter three is devoted to the shooting method, introduced by Ixaru in 2010, for 2D time-independent Schrödinger equations. Toon Baeyens has studied very carefully this algorithm and concluded that this method is very promising, but that there exist possibilities to expand and improve the method. In four paragraphs the proposed adaptations are explained. The following adaptations are introduced: an automatically choice of the optimal sector size, a new formula for the inner product of eigenvalues, an occurring integral in the proposed algorithm is quite complicated to computed and is studied in the third paragraph, while at least a robust way to locate eigenvalues is presented. In a last part of this chapter the effectiveness of the provided theory is proved by some numerical results. Some important questions remain. Attaining extremely high accuracies proved to be difficult. A clear explanation for this phenomenon is not found.

In chapter four another method for approximating eigenvalues and eigenfunctions of time-independent two-dimensional Schrödinger equations with homogeneous Dirichlet boundary conditions on rectangular and non-rectangular domains is introduced. The author has found his inspiration by a simple method of Wang and Shao, which seems to be based on a finite difference scheme. It seems that such a simple method can reach very high accuracy. Inspired by this last method and with the knowledge of the algorithms studied and introduced in chapter three the author introduces a new method in which a continuous approximation of the eigenfunctions is introduced in both directions of the domain. After a lot of mathematical rearrangements, the method reduces into a generalized rectangular matrix eigenvalue problem. The author has studied three techniques to solve this problem. The last one, based on least squares approximations, is significant faster than the other ones and forms the basis for the new code Strands, a line-based collocation method. In a next paragraph the computation of eigenfunctions within Strands is tackled. The author shows the possibility to evaluate these eigenfunctions quite efficiently in any arbitrary point of the domain. Finally, the new method is tested thoroughly. The following time-independent two-dimensional Schrödinger problems with the following potentials are used as test: the harmonic oscillator problem, the Hénon-Heiles potential and the quartic oscillator potential, all tested on simple rectangular domains. The Schrödinger equation with zero potential is tested on a rectangular as well as a circular domain. The Schrödinger equation with Ixaru's potential is tested on a rectangle, a disc and 45° rotated rectangle. As a conclusion Toon Baeyens claims that Strands obtained extremely accurate results while using smaller matrix problems than the mentioned method of Wang and Shao, resulting in an overall significantly faster algorithm. We agree with the author that the new method shows a lot of promise. Further improvements are needed. This work can be the subject of further research work.

This thesis ends with a very large bibliography.

A motivated appraisal of the scientific value in comparison with the state-of-the-art in the field of research

Toon Baeyens has presented a very interesting and clearly written dissertation. He has studied all previously available research material in the considered field. The bibliography at the end of the work is very extensive and it shows really the state-of-the-art in the field of time-independent two-dimensional Schrödinger equations. He has studied all available software in the field and adapted it in a more up-to-date form using C++-source files instead of FORTRAN and Matlab codes. He introduces a python-package which provides a user-friendly interface to the efficiently implemented C++-code. He shows to be an excellent mathematician. This is reflected in a very good way in chapter 3 where he introduces and proofs the theorem 3.10. Although this dissertation is introduced in the field of mathematics Toon Baeyens also shows an extensive knowledge of software development. His skill of the different algebraical software packages is obvious. What he presents in his dissertation is an improvement of results in mathematical development and software which were already at a very high level of research. By reading his closing remarks it is obvious that he still has a lot of ideas to extend his results in different ways. Work perhaps for a new PhD-student or for post-doctoral work of Toon, himself.

Questions and/or remarks that will be points of attention during the meeting of the Examination Board

1. I have appreciated the historical introduction in chapter one. I was wondering on which reference work this short review is based. I have some problem with the sentence on page 15, "In this same century the complex numbers were discovered. And later in 1637 it was René Descartes who coined the terms real and imaginary numbers". The problem of complex numbers appears for the first time in the work "Ars Magna" published in 1545 of Girolamo

Cardano, where he solved cubic equations. At that time, he was not aware how to use these numbers. But later on Rafael Bombelli (1526-1572) studied for this same problem the square roots of negative numbers and published in his book “Algebra” in 1572 the word complex number, for which he introduces the calculation rules; In J.N. Crossley, The Emergence of number (Singapore 1980) one can read: “It seems to be quite fair to describe Bombelli as the inventor of complex numbers. Nobody before him had given rules for working with such numbers, nor had they suggested that working with such numbers might prove useful”. Also, the word “imaginary” was introduced in this context.

It should be nice to hear comments on that item.

2. I have some comment on the few lines in the Dutch language on pages 8-10. There are mentioned a lot of equations dedicated to famous mathematicians; “Schrödinger”, “Sturm-Liouville”, “Robin” and “Dirichlet”. In most of the cases these names are written with a capital and are followed by the words “vergelijking”, “problemen”, “randvoorwaarden”, except for the name “Schrödinger”, where the name is written without capital. It seems that there is no standard-rule in Dutch how one must handle this. I suggest using for all these kinds of expressions an identical form of notation with the family names written with a capital followed by the symbol hyphen.

3. On page 38 the author refers to a correction method whereby the error of eigenvalues obtained by Numerov’s method is improved. He only cites one reference. It is perhaps interesting to mention that in our numerical analyses group in Gent also research has been done concerning this error technique. I can cite the following papers: G. Vanden Berghe and H. De Meyer, A modified Numerov method for higher Sturm-Liouville eigenvalues, *Intern. J; Computer Math*. 37, pp.63-77 (1990). G. Vanden Bergh and H. De Meyer, Accurate computation of higher Sturm-Liouville eigenvalues, *Numer. Math.* 59, pp. 243-254 (1991).

4. On page 84 in table 2.4 I was surprised when I read the absolute error value on the first line, 4.5.10 (minus 1). Is this a typo or is there an explanation for this bad result?

5. On page 86 Toon mentioned that for beta= 15 and 25 there is a severe loose of accuracy. It is only a comment. Is there an acceptable reason for those phenomena?

6. On page 91 in table 2.9 some results of Siedlecki are given. I read in the title of the work of Siedlecki that he uses the “Control Volume method”. Can you describe in short, the algorithm behind this name.

7. On page 171 a table of central symmetric finite differences is given. Textbooks are cited on this topic. It perhaps worthwhile to mention that in our research group these finite difference schemes have been the topic of a lot of research in the context of one-dimensional Schrödinger problems. The first paper related to this research can be found in V. Fack and G. Vanden Berghe, *J. Phys. A, Math. Gen.*18 (1985) 335-3363. A FORTRAN 77 code was developed and described in V. Fack and G. Vanden Berghe, *A program for the calculation of energy eigenvalues and eigen states of a Schrödinger equation,* Computer Physics Communications 39 (1986) 187-196. The code was added to the CPC Fortran Library for public use.

8. On page 171 strange step lengths (19/40, 19/60 and 19/100) are used. Why using these numbers instead of for example (20/40, 20/60, 20/100)?

9. On page 180 in equation (4.10) twice the symbol “E” seems be missing after the equality signs.

10. On page 230 reference 62 gives no journal name. Is this an internal report or is some information missing?

11. On page 230 reference 63: I am honored to be a co-author of this paper, but as far as I know I am not.

Possible suggestions for modification of the doctoral thesis

I have in first instance no suggestions. If however some of the above questions or remarks should results in answers which changes drastically the spirit of the original text it should be desirable to modify where necessary.

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