Report on Ph.D. thesis

Metody aproksymacji numerycznej liniowego równania Kleina-Gordona z masą czasowo- i przestrzenno-zależną

by

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In this doctoral thesis the author is concerned with the construction, analysis, and validation of numerical methods for the linear Klein-Gordon equation of the form

$$\partial_t^2 \psi(\mathbf{x},t) = \Delta\psi(\mathbf{x},t) + f(\mathbf{x},t)\psi(\mathbf{x},t),$$

where $f(\mathbf{x},t)$ is time and space dependent mass function. It is assumed that this mass function can be approximated by the truncated Fourier series of the form

$$f(\mathbf{x},t) = \alpha(\mathbf{x},t) + \sum_{|n|\leq N} \alpha_n(\mathbf{x},t)e^{i\omega_n t},$$

where $n \in \mathbb{N}$, $N \leq \infty$, $\omega_n \in \mathbb{R}$, and the functions $\alpha(\mathbf{x},t)$ and $\alpha_n(\mathbf{x},t)$ are independent off ω_n.

In Chapter 2, which is based on the short note [1], the author proposed the method based on asymptotic expansion of the mass function $f(\mathbf{x},t)$ with $\alpha(\mathbf{x},t) = 0$, $N = \infty$, and $\omega_n = n\omega$, i.e.,

$$f(\mathbf{x},t) = \sum_{n=-\infty}^{\infty} \alpha_n(\mathbf{x},t)e^{in\omega t},$$

where the frequency of oscillations ω is assumed to be large, $\omega \gg 1$. The detailed derivation of this asymptotic method is presented in Section 2.1. There is no convergence or order analysis of this method, but the results of numerical experiments presented in Section 2.2 indicate that this methods is convergent with order depending on the splitting used to compute the terms of the form e^{hA}, where A are some anti diagonal matrices, which depend on the parameters of the problem. The author illustrate this for three splittings: first order splitting due to Lie and Trotter, second order splitting due to Strang, and third order splitting due to Ruuth. The author presents also costs versus accuracy graphs which illustrate that the method derived in this chapter are very efficient and competitive with other methods for this problem presented in the literature on this subject.

In Chapter 3, which is based on the report [2], the author constructed the numerical method for Klein-Gordon equation, which is based on Duhamel formula, and can effectively integrate equations with different mass functions with vastly different frequencies, such as, for example, $f(\mathbf{x},t) = \alpha_0(\mathbf{x},t)$, $f(\mathbf{x},t) = \alpha_2(\mathbf{x},t)e^{i10^6t}$, or $f(\mathbf{x},t) = \alpha_0(\mathbf{x},t) + \alpha_1(\mathbf{x},t)e^{it} + \alpha_2(\mathbf{x},t)e^{i10^6t}$. The detailed derivation of this method is described in Section 3.1, which starts with the short review of Duhamel's formula. The convergence and order of this method is then investigated in Section 3.2. It follows from error estimated derived in Section 3.2 that the numerical method based on Duhamel's formula is convergent with order 3. This is confirmed by the results of numerical experiments on two test problems on Klein-Gordon equation with mass functions depending on vastly different frequencies. These experiments are presented in Section 3.3. It is observed that the accuracy of the method is not degraded by high oscillation. This is achieved by embedding the oscillatory phases explicitly into the proposed numerical scheme.

In Chapter 4, which is based on the report [3] submitted for publication, the author design numerical schemes for Klein-Gordon equations, where the oscillations occur across a wide range of scales, from non-oscillatory to highly oscillatory. The main tool in the derivation of numerical method for Klein-Gordon equations with vastly different oscillations is truncation of Magnus expansion, described in Section 4.1.1, and the Strang splitting reviewed in Section 4.1.2. The detailed derivation of the resulting numerical scheme is described in Sections 4.1.3, 4.1.4, and 4.1.5. The theoretical analysis of the resulting numerical method is then provided in Section 4.2, where the estimates of leading error terms of Magnus truncated expansions (Section 4.2.1) and Strang splittings (Section 4.2.2) are derived. The results of numerical experiments presented in Section 4.4 on four test problems confirm the theoretical properties of the derived numerical schemes and illustrate high accuracy and efficiency of these methods.

The thesis concludes with Chapter 5, where short summary of the thesis is provided and plans for future research are briefly described.

Summary statement

The results of the first part of the thesis (Chapter 2) has been already published in the Elsevier journal Applied Mathematics Letters, the results obtained in the second part (Chapter 3) and third part (Chapter 4) appeared as arXiv preprints, and were also submitted for publication.

This thesis provides an important and essential contribution to the numerical solution of Klein-Gordon equation of quantum mechanics. The proposed new methods for this equation are accurate, efficient, and competitive with other methods proposed in the literature on this subject.

I believe this Ph.D. dissertation satisfies the criteria for granting Ph.D. degree in mathematics. Hence, I support granting Ph.D. degree to Karolina Agata Lademann.

References

[1] Marissa Condon, Karolina Kropielnicka, Karolina Lademann, and Rafał Perczyński, Asymptotic numerical solver for the linear Klein–Gordon equation with space- and time-dependent mass, Applied Mathematics Letters 115(2021), Paper No. 106935.

[2] Karolina Kropielnicka and Karolina Lademann, Third order, uniform in low to high oscillatory coefficients, exponential integrators for Klein-Gordon equations, arXiv:2212.13762, submitted to Mathematical Modeling and Numerical Analysis.

[3] Karolina Kropielnicka, Karolina Lademann, and Katharina Schratz, Effective highly accurate time integrators for linear Klein-Gordon equations across the scales, arXiv:2112.08908, submitted.

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