Description for the general public

In the last few years Karolina Kropielnicka has been a member of an international team that developed new and highly effective methods to solve the equations of quantum mechanics. The main purpose of this project is to build upon this success in new and important directions. We will focus on differential equations in semiclassical regime, where the small parameter, $\varepsilon = \frac{\hbar}{2m}$, ($\hbar$-Planck constant, m-mass of the underlying particle), causes extremely high oscillations and, therefore, problems in numerical analysis. We wish to develop numerical analysis for equations in quantum mechanics and to use it in the theory of quantum control. This project consists of two work packages:

1. Challenging equations in quantum mechanics. Nonlinear Schrödinger equation, Klein–Gordon, Wigner, Pauli and Dirac equations are in the centre of our attention, and we wish to propose adequate numerical methods. We will focus on gaining higher accuracy without prohibitively increasing computational cost. We intend to provide full *efficiency and cost analysis* of new methodologies and compare them with other existing approaches in computational chemistry and physics.

2. Quantum control. We will commence with quantum control of systems modelled by Schrödinger equations. Having methods from the previous work package established, we will move to other generic equations (Klein-Gordon, Wigner, Pauli...). We will also investigate various cost functions.

Equations in quantum mechanics are motivated by questions in theoretical physics and chemistry, and the ability of controlling quantum states by means of laser opens new technological possibilities. However those equations hardly ever can be computed exactly, so we need to resort to numerical approximation, which is very difficult due to the extremely high oscillations and modest computational power. Richard Feynman, motivated by seeking alternatives to classical computing, proposed quantum computers in 1982. Ironically, the design of quantum computers will itself require computational solutions of various complex equations of quantum mechanics on the only devices available to us – the classical computers.

Therefore, numerical problems in quantum mechanics are not only nontrivial but also necessary; this is the reason why the development of this part of science is so lively and attracts so many international leaders in physics, chemistry and mathematics.

In the light of effectiveness of our methodology, we wish to continue our investigations to other equations in quantum mechanics and to apply the results to quantum control theory.

The project will be implemented in collaboration with Arieh Iserles (University of Cambridge, UK), a great expert in numerical analysis, definitely one of the leading international authorities with extremely wide scope of mathematical knowledge. We hope that Arieh Iserles's activity in Polish environment will also be fruitful for Polish research, and will bring closer Polish and international researchers working in this field of mathematics and open some new collaboration perspectives.