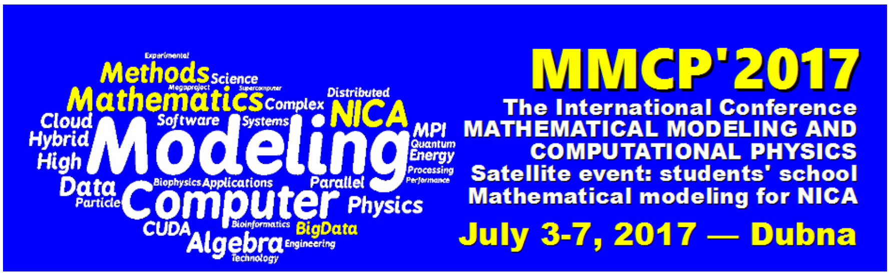

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Finite-difference splitting scheme for three-dimensional Schroedinger equation, describing tunneling from anharmonic atomic traps

Monday, 3 July 2017 15:30 (15 minutes)

We present an efficient computational scheme to integrate the time-dependent three-dimensional Schroedinger equation. The time-evolution operator is calculated with a second order split-operator technique and spatial derivatives are approximated with a sixth-order finite-difference method.

The efficiency of our implicit scheme is demonstrated in comparison with a high-order direct method [1] for an exactly solvable problem of a harmonic oscillator.

Our method was successfully applied to a tunneling problem of two interacting atoms confined in a one-dimensional optical trap by "walls" of an anharmonic potential [2]. By computing a time-evolution of a population of the trap states we extract tunneling rates of the atoms [2].

By using the above examples, we demonstrate a linear dependence of a computational time of the method on a number of spatial grid points and a fast convergence with respect to a step of integration over time and spatial variables. The computational method can be extended to more complicated problems in higher dimensions.

Short biography note

[1] I. Gonoskov and M. Marklund, Single-step propagators for calculation of time evolution in quantum systems with arbitrary interactions, Comp. Phys. Comm. 202, 211-215, (2016);
[2] I.S. Ishmukhamedov and V.S. Melezhik, Tunneling of two bosonic atoms from a one-dimensional anharmonic trap (accepted to Physical Review A).

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