PARALLEL ALGORITHM FOR CALCULATING THE WIGNER FUNCTION FOR A QUANTUM SYSTEM WITH A POLTNOMIAL POTENTIAL

E.E. Perepelkin, B.I. Sadovnikov, N.G. Inozemtseva, E.V. Burlakov, R.V. Polyakova, P.N. Sysoev, M.B. Sadovnikova

LIT, JINR, Dubna

When considering quantum systems in phase space, the Wigner function is used as a function of quasidensity of probabilities. Finding the Wigner function is related to the calculation of the Fourier transform from a certain composition of wave functions of the corresponding quantum system. As a rule, knowledge of the Wigner function is not the ultimate goal, and calculations of mean values of different quantum characteristics of the system are required. The explicit solution of the Schrödinger equation can be obtained only for a narrow class of potentials, so in most cases it is necessary to use numerical methods for finding wave functions. As a result, finding the Wigner function is connected with the numerical integration of grid wave functions. When considering a one-dimensional system, the calculation of N² Fourier intervals from the grid wave function is required. To provide the necessary accuracy for wave functions corresponding to the higher states of the quantum system, a larger number of grid nodes is needed. The article considers the construction of a parallel algorithm on the GPU computing architecture for finding the Wigner function of a quantum system with a polynomial potential. A numerical-analytical method for constructing the Wigner function, which is based on calculating the trace of the product of the density matrix and the matrix of the Weyl operator, is described. The operators are represented in the basis of a quantum harmonic oscillator, for which the Moyal equation transforms into the Liouville equation. This approach enables to visually analyze the degree of anharmonicity of the system in terms of the off-diagonal elements of the density matrix. The parallel implementation on the GPU massively parallel architecture has reduced the calculation time by two orders of magnitude compared to the single-threaded version on the x86 architecture.

The results described were obtained within a unified consideration of classical and quantum systems in the generalized phase space on the basis of the infinite self-interlocking chain of Vlasov equations. It is essential that using the apparatus of quantum mechanics in the phase space, one can estimate the required parameters of quantum systems, and the proposed numerical methods make it possible to perform such calculations efficiently. The availability of exact solutions to model nonlinear systems plays a cardinal role in designing complex physical facilities, for example, such as the SPD detector of the NICA project. Such solutions are used as tests when writing a program code and can also be encapsulated in finite difference schemes within the numerical solution of boundary value problems for nonlinear differential equations. The proposed efficient numerical algorithm can be applied to solve the Schrödinger equation and the magnetostatics problem in a region with a non-smooth boundary.

The work was supported by the RFBR grant No. 18-29-10014.