PATH INTEGRAL MONTE-CARLO METHOD FOR THERMOPHYSICAL PROPERTIES CALCULATIONS OF QUANTUM SYSTEMS OF PARTICLES

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Interest in modeling quantum particle systems at finite temperatures has been growing significantly, especially in the last 10–20 years. This is primarily due to the rapid development of supercomputing technology, which makes it possible to take into account an increasing number of particles in modeling and to reach the thermodynamic limit for a number of problems. Great success has been achieved in calculations using the density functional method (DFT). However, the Kohn-Sham approximation, on which all existing DFT implementations are based, has no theoretical basis, and it is often necessary to introduce fitting parameters into expressions for exchange-correlation energy in order to achieve agreement with the experiment. To date, one of the few theoretically sound methods for calculating the thermodynamic properties of quantum particle systems at a finite temperature is the path integral Monte-Carlo method (PIMC). This method is based on the Feynman formulation of quantum mechanics and uses the statistical sum of a quantum system of particles expressed in terms of a density matrix.

The report will examine the modern achievements of the PIMC method, including those related to the "mitigation" of the so-called fermion sign problem. A new expression for the high-temperature density matrix will be presented, taking into account the effects of long-range interaction [1]. Various variable substitutions will be discussed, as well as problems of numerical implementation. The results of calculations for various quantum particle systems will be demonstrated: an ideal Fermi gas, a homogeneous electron gas (jellium model), a system of quantum soft spheres, and He^3 [2]. Issues related to the calculations of the momentum distribution function, the density of states, and the dynamic structure factor [3] will be discussed. The work was supported by the Russian Science Foundation, grant No. 24-19-00746.

References

1. **Demyanov, G. S.**, Levashov P. R. // Comp. Phys. Comm. – 2024. – Vol. 305. – P. 109326.
2. **Filinov, V. S.**, Levashov P. R., Larkin A. S. // Phys. Rev. E. – 2024. – Vol. 109. – P. 024137.
3. **Filinov, V. S.**, Syrovatka R. A., Levashov P. R. // Phys. Rev. E. – 2023. – Vol. 108. – P. 024136.