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Degeneracy and interference quantum effects in phase space distribution functions: Path integral approach

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Quantum effects may strongly disturb the momentum maxwellian distribution function and are important in studies of kinetic properties of matter at low temperatures and under extreme conditions (for example, for combustion, detonation and even warm nuclear fusion). In this case, particles are strongly coupled and perturbative methods cannot be applied. Therefore, for theoretical studies of these systems the *ab initio* approaches in phase space are required. In this paper, we propose the path integral representation of Wigner function in phase space and two quantum Monte Carlo methods for calculations of Wigner functions and thermodynamic values of strongly coupled systems. The phase space distribution Wigner function is Fourier transform of density matrix where the Bose/Fermi statistics are counted for by the sum over permutations.

$$W(p,q;\beta,V) = \int d^{3N}\xi\, e^{i\langle\xi|p\rangle/\hbar} \sum_{P} (\pm 1)^{\kappa} \int_{q(0)=(q-\xi/2)}^{q(1)=P(q+\xi/2)} D^{3N}q(\tau)\; e^{-\int_0^1 d\tau \left[\frac{\dot{q}^2(\tau)}{2} + \beta U(q(\tau))\right]}$$

To avoid difficulties of calculations of 3N-dimensional Fourier transform we have developed two different approaches. The first one is the linear/ harmonic approximation, which use expansion of potential energy of interaction into Taylor series up to first/second order:

$$U(\lambda z(\tau) + q + \xi(\tau - 1/2)) \approx U + (\tau - 1/2)\xi_{\alpha,i}\frac{\partial U}{\partial q_{\alpha,i}} + \frac{1}{2}(\tau - 1/2)^2 \xi_{\alpha,i}\xi_{\beta,j}\frac{\partial^2 U}{\partial q_{\alpha,i}\partial q_{\beta,j}}$$

It allows to do Fourier transform analytically and to obtain explicit expression of Wigner function for further Monte Carlo calculations. This quasiclassical method allows calculating Wigner functions and to study thermodynamic properties for systems of particles without taking into account quantum many body bound states.

The second single momentum approach is based on the reduced Wigner function integrated over all momentums except one:

$$W_{sm}(\mathbf{p}, \mathbf{q}_1, \dots, \mathbf{q}_N; \beta, V) = \int d^3\mathbf{p}_2 \dots d^3\mathbf{p}_N W(\mathbf{p}_1, \dots, \mathbf{p}_N, \mathbf{q}_1, \dots, \mathbf{q}_N; \beta, V)$$

Here calculations of distribution functions and thermodynamic values can be carried out by the usual Monte Carlo method for density matrix in path integral representation and subsequent 3-dimensional Fourier transform. This method allows to a great extent to overcome the well-known sign problem for degenerate Fermi systems of particles. Both methods have been tested on some simple models: Single particle in one and three dimensional potential wells and degenerate ideal many particle Fermi systems. Results of both methods are in very good agreement with available analytical expressions and independent numerical data. Below, as example, we present some results of our calculations.

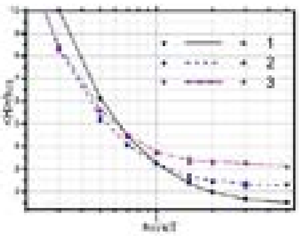

Figure 1 : dependence of average energy < E > on inverted temperature $\beta = 1/kT$ [illegible]

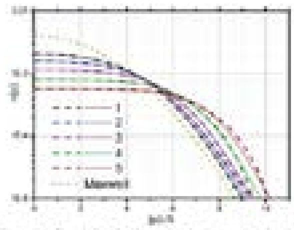

Figure 2 : Fermi distribution [illegible]

Biography

A S Larkin has completed his Master's degree from Moscow Institute of Physics and Technology (MIPT). He is a graduate student at MIPT and Junior Researcher at Joint Institute for High Temperatures, RAS. He published 4 papers in reputed journals.

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