

THEORETICAL AND CONDENSED MATTER PHYSICS

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Treatment of the 'sing problem' by pair phase space pseudopotentialV S Filinov¹, A S Larkin^{1,2} and V E Fortov¹¹Joint Institute for High Temperatures of the Russian Academy of Sciences, Russia²Moscow Institute for Physics and Technology, Russia

The main difficulty for path integral Monte Carlo studies of Fermi systems results from the requirement of antisymmetrization of the density matrix and is known in literature as the 'sign problem'. To overcome this issue the new numerical version of the Wigner approach to quantum mechanics for treatment thermodynamic properties of degenerate systems of fermions has been developed. The new path integral representation of quantum Wigner function in the phase space has been obtained for canonical ensemble. Explicit analytical expression of the Wigner function accounting for Fermi statistical effects by effective pair pseudopotential has been presented. Derived pseudopotential depends on coordinates, momenta and degeneracy parameter of fermions and takes into account coordinate - momentum principle uncertainty. The new quantum Monte-Carlo method for calculations of average values of arbitrary quantum operators has been proposed. To test the developed approach calculations of the momentum distribution function of the degenerate ideal system of Fermi particles has been carried out in a good agreement with analytical Fermi distributions. On other hand the first results on influence of interparticle interaction on momentum distribution functions show appearance of quantum "tails" in the Fermi distributions.

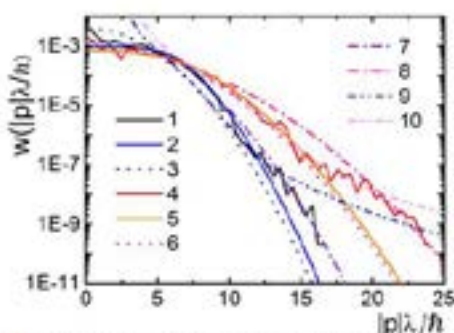


Figure 1. Momentum distributions for non-ideal plasma of electrons (1, 2, 3, 7, 9) and two times heavier holes (4, 5, 6, 8, 10); Lines: 1, 4 – MC results versus momentum scaled by ratio of Planck constant to thermal electron wavelength; 2, 5 – Fermi distributions; 3, 6 – Maxwell distributions; 7, 8 – Maxwell approximation of MC results with effective temperature [7, 8]; 9, 10 – consp^h correction [7, 8] to Maxwell distributions 3, 6. Degeneracy parameter of electrons is equal to 4, plasma classical coupling parameter is 2.1.

Biography

V S Filinov is Doctor Phys&Math. Sc., Prof.. Education: Moscow Power Engineering Institute, M. Sc.degree in Physical Optics, Moscow State University, M. Sc.degree in Mathematics. He is a principal researcher in Joint Institute for High Temperatures Russian Academy of Sciences. He has published more than 200 papers in reputed journals and has been serving as Organizing Committee Member of several International conferences.

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