WIGNER PATH INTEGRAL REPRESENTATION OF DENSITY OF STATES AND RESPONSE FUNCTIONS. MONTE CARLO SIMULATION OF THE ONE- AND TWO-COMPONENT PLASMA MEDIA

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The Wigner formulation of quantum mechanics and the Wiener–Khinchin theorem are used to derive a new path integral representation of the quantum density of states (DOS), dynamic structure factor (DSF) and response function (RF) of the strongly coupled electron-proton plasma (two-component plasma, TCP) and electron gas in the uniformly distributed in space of uncorrelated positive discrete charges ("protons") forming a neutralizing background (one-component plasma, OCP). The DSFs and RFs characterize the excitation spectrum of the system and the amount of energy absorbed by the system when perturbed by an external field. These functions contain information about inter-particle correlations and their time evolution.

The derived Wigner function resembles the modified Maxwell–Boltzmann distribution, which allows to take into account quantum effects. A path integral Monte Carlo approach for the simulation of DOS and other thermodynamic functions is suggested for plasma media in the canonical ensemble. The calculated properties include the DOS, RFs, momentum distribution functions and the spin–resolved radial distribution functions (RDFs).

The RDFs for electrons with the same spin projection revealed the exchange–correlation cavities with the characteristic "size" of the order of the thermal wavelength. In the TCP the Coulomb attraction results in the appearance of high peaks on the electron–proton RDFs at small inter-particle distances, while for the OCP the analogous RDFs demonstrate the unexpected significant depression arising due to a three-particles effect caused by electron repulsion preventing any two electrons to be in the vicinity of any third non-correlated "neutralizing charge".

The TCP DOS in general are larger than the OCP and ideal ones. For negative energy the TCP DOS is a fast decaying (five order of magnitude) function and demonstrates oscillations describing discrete energy bound states. Quantum effects make momentum distribution functions a non-maxwellian with a power-law high-momentum asymptotics ("quantum tail").