ON THE PLASMA PHASE TRANSITION IN WARM DENSE CESIUM

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The existance of plasma phase transition in warm dense cesium is discussed in [1] and associated with an abrupt increase in the ionization degree. In an attempt to verify this prediction, quantum molecular modelling of cesium within the framework of the finite temperature density functional theory was carried out, for that VASP software package is used. An approximation of generalized gradients is applied to the exchange-correlation functional with PBE parameterization (Perdew, Burke, Ernzerhof). The electron-ion interaction is described by means of the projector augmented wave method with 9 valence electrons.

Calculations were performed for a system of 64 cesium atoms under periodic boundary conditions. Equation of state was obtained in the density range from 2 $\frac{g}{cm^3}$ to 18 $\frac{g}{cm^3}$ and at temperatures 200–10000 K. The dynamic electrical conductivity, averaged over various independent configurations of atoms in the system, is computed. Electron density, ionization degree and average ion charge were estimated by Drude model approximation of frequency-dependent conductivity in metals.

Static electrical conductivity was found to reach the minimum at a density of 3–4 $\frac{g}{cm^3}$ on all studied isotherms. A monotonous increase in the average charge of ions, while increasing density up to 9 $\frac{g}{cm^3}$, is followed by a steep decline from 5–6 e at 9 $\frac{g}{cm^3}$ to 1–1.5 e at 14 $\frac{g}{cm^3}$. A further increase in density again leads to an increase in the value of the average charge.

In the density range of 10–14 $\frac{g}{cm^3}$ two branches of the isotherms can be seen with different mean ion charges, yet same density.

Additional calculations were performed for a different numbers of cesium atoms in a supercell (27, 64, 125) and demonstrate a more dramatic increase in the ionization degree when number of particles is redused, which is the result of finite size effects on the properties of the system.

The presence of extremums in dynamic electrical conductivity and mean ion charge functions of density, as well as the occurrence of various branches (ambiguities) in the vicinity of these extremes, imply emergence of metastable states and predict possible plasma phase transition.

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1. Vorob'ev V.S., Grushin A.S., Novikov V.G. Investigation of the phase transitions in cesium by the average atom model // Keldysh Institute Preprints. 2016. No. 100. 16 p.