Plasma Phase Transition in Dense Hydrogen and Electron-Hole Plasmas

V.S. Filinov¹, M. Bonitz², P. Levashov¹, V.E. Fortov¹, W. Ebeling³ and M. Schlanges⁴
1 Institute for High Energy Density, Russian Academy of Sciences, Izhorskay 13/19, Moscow 127412, Russia
2 Fachbereich Physik, Universität Rostock, D-18051 Rostock, Germany
3 Institut für Physik, Humboldt-Universität Berlin, Invalidenstrasse 110, D-10115 Berlin, Germany
4 Fachbereich Physik, Universität Greifswald, D-17489 Greifswald, Germany

Plasma phase transitions (PPT) in dense hydrogen and electron-hole plasmas are investigated by direct path integral Monte Carlo methods (DPIMC). The phase boundary of the electron-hole liquid in Germanium is calculated and is found to agree reasonably well with the known experimental results. Analogous results are found for high-density hydrogen. For a temperature of $T = 10,000$K it is shown that the internal energy is lowered due to droplet formation for densities between $10^{23}$ cm$^{-3}$ and $10^{24}$ cm$^{-3}$.

1. Path integral Monte Carlo simulations

All thermodynamic properties of a two-component plasma are defined by the partition function $Z$ which, for the case of $N_e$ electrons and $N_p$ protons, is given by $Z(N_e, N_p, V, \beta) = \frac{Q(N_e, N_p, \beta)}{N_e! N_p!}$, with $Q(N_e, N_p, \beta) = \sum_\sigma \int dq dr \rho(q, r, \sigma; \beta)$, where $\beta = 1/k_B T$. The exact density matrix is, for a quantum system, in general, not known but can be constructed using a path integral representation [1, 2] $\int dR(0) \sum_\sigma \rho(R(0), \sigma; \beta) = \int dR(0) \ldots dR(n) \rho^{(1)} \cdot \rho^{(2)} \ldots \rho^{(n)} \times \sum_\sigma \sum_\rho \rho(\pm 1)^{k_p} \mathcal{S}(\sigma, \rho; a) \mathcal{P}(n+1)$, where $\mathcal{P}(i) \equiv \rho \left( R(i-1), R(i); \Delta \beta \right) \equiv \left( R(i) \right) e^{-\Delta \beta H(R(i))}$, whereas $\Delta \beta \equiv \beta/(n + 1)$ and $\Delta \lambda^2 = 2 \pi h^2 \Delta \beta / m_a$. $a = e, p$. $H$ is the Hamilton operator, $\hat{H} = \hat{K} + \hat{U}_e$, containing kinetic and potential energy contributions, $\hat{K}$ and $\hat{U}_e$, respectively, with $\hat{U}_e = \hat{U}_e^p + \hat{U}_e^e + \hat{U}_e^p$ being the sum of the Coulomb potentials between protons ($p$), electrons ($e$) and electrons and protons ($ep$). Further, $\sigma$ comprises all particle spins, and the particle coordinates are denoted by $R(i) = \left( q(i), r(i) \right) = \left( q_e(i), q_p(i), \ldots, q_e(n), q_p(n) \right)$, for $i = 1, \ldots, n + 1$, $R(0) \equiv \left( q, r \right) \equiv \left( q_e(0), q_p(0), \ldots, q_e(n), q_p(n) \right)$, and $R(n+1) \equiv R(0)$ and $\sigma = \sigma$. This means, the particles are represented by fermionic loops with the coordinates (beads) $[R] \equiv [R(0); R(1); \ldots; R(n); R(n+1)]$, where $q$ and $r$ denote the electron and proton coordinates, respectively. The spin gives rise to the spin part of the density matrix $\mathcal{S}$, whereas exchange effects are accounted for by the permutation operator $\mathcal{P}$, which acts on the electron coordinates and spin projections, and the sum over the permutations with parity $\kappa_p$.

To compute thermodynamic functions, the logarithm of the partition function has to be differentiated with respect to thermodynamic variables, so for internal energy $E$ we have $\beta E = -\beta \partial \ln Q / \partial \beta$

2. Numerical Results

Since the PPT in dense hydrogen is still hypothetical and has not been observed experimentally, it is reasonable to look for other systems where similar conditions exist. A suitable example is electron-hole plasma in low-temperature semiconductors, for which droplet formation is well established and observed ex-
We, therefore, performed DPIMC simulations for electron hole plasmas. Below the critical temperature the simulations exhibit anomalously large fluctuations and an unstable behavior of the pressure. The e-h-plasma is found to phase separate and form large droplets. The phase boundary of the electron-hole liquid (e-h-droplets) in Germanium obtained by our DPIMC method is presented in Fig. 1 together with the experimental data. We observe good agreement. Deviations may be connected with complex band structure of Germanium approximated in our simulations by a two-band parabolic mass model.

Figure 1: Phase boundary of the electron-hole liquid in bulk Germanium. Experiment - [3]. Temperature is presented in units of the exciton binding energy.

Figure 2: Pressure and energy of hydrogen for \( T = 10,000K \), DFT - [5], RPIMC - [4].

between plasma particles is of the order of the size of a hydrogen molecule the homogeneous plasma state becomes unstable, and many-particle clusters appear. Results of one independent well tested method based on density functional theory (DFT) are presented on Fig. 2, where PPT was obtained at smaller density [5].

References


