# Der Alte würfelt nicht - wir schon

## Extending DFT-MD simulations of Warm Dense Matter using *ab initio* Quantum Monte Carlo Input

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### In Short

- QMD investigation of high temperature Warm dense matter made possible by our recently proposed ext-FPMD method
- Our recent QMC calculation of finite-temperature uniform electron gas provides a better description of electron behaviors in warm dense regime
- Using QMC derived finite-temperature exchange-correlation functionals as an input in ext-FPMD method to investigate warm dense matter will yield promising results for plasmas physics, astrophysics and geophysics etc.

Warm dense matter (WDM) refers to a state between solid and ideal plasma, whose typical density is comparable to or a few times higher than solids, and temperature varies from a few electron volts to a few hundred electron volts. Until recently, the properties of WDM remain poorly understood. WDM exists widely in our universe, such as brown dwarfs, giant planets, and the core of the Earth. More importantly, the fuel of the inertial confinement fusion undergoes WDM region for quite a long period of time during the implosion. Therefore, it is of great scientific and practical significance to study the properties of WDM [1].

FPMD combines quantum treatment for the fast moving electron part with classical treatment for the slow varying ionic part [2]. For electrons, the finite temperature density functional theory(FT-DFT) are used. With Born-Oppenheimer approximation, under a certain configuration of ions, Kohn-Sham-Mermin equations are solved self-consistently to find the electron charge density corresponding to the minimum free energy, and then the forces act upon each ion can be obtained by Hellmann-Feynman theorem. The ions can be treated as classical particles conforming to Newton's second law. After the new positions of the ions are updated using Verlet algorithm, the electrons are recalculated under this new ionic potential field. Such process continues for a sufficiently long period of time when statistical mechanics begin to involve in to determine the bulk properties of WDM. FPMD is a natural and successful extension of density functional theory (DFT) from solid state physics to WDM regime. However, since the electrons are under Fermi-Dirac distribution, with the increase of the temperature, the number of orbitals needed to be included in the calculation grows rapidly, making this method inefficient or even prohibitive for high temperature.

Using plane wave approximation to account for the contribution of high energy electrons analytically in Kohn-Sham-Mermin equation, Dr. S. Zhang, et al. recently developed an extended-FPMD (ext-FPMD) method that can coherently deal with WDM with a wide range of temperature[3]. This new method is shown to be accurate, efficient and consistent for the study of equation of states (EOS) of WDM. Meanwhile, the ext-FPMD method also provides information of electronic structure, giving it an edge to the further study of X-ray spectra and other diagnostic technology [4].

Within DFT scheme, the many-body effect of the electrons is accounted for by the exchange-correlation energy. If the exchange-correlation functional is constructed correctly, one can reproduce the exact solution of the original many-body problem. This term, however, cannot be obtained within DFT itself. Practically, with the help of Monte Carlo method, people can solve the special case of uniform electron gas, and use these data to construct the exchange-correlation functional for all the rest systems. As a result, how the exchange-correlation is constructed is crucial to the application of DFT method. Unfortunately, previous exchange-correlation functionals are constructed using MC results without considering temperature effects, which is adequate for condensed matter systems but is doomed to fail when it comes to WDM.

In order to numerically investigate degenerated electrons in the range of warm dense matter with high accuracy, the group of Prof. Dr. M. Bonitz developed two novel PIMC methods [5]. The Configuration-PIMC (CPIMC) method achieves the highest available accuracy in the simulation of strongly degenerate electrons at finite temperatures [6]. However, the Fermi-sign problem with increasing coupling strength limits the accuracy of the results. To solve this problem, one of us developed another PIMC method. The so-called permutation-blocking PIMC (PB-PIMC) method [7] circumvent the sign problem and thus considerably expands the parameter range to increasing degeneracy. The combination of these two complementary quantum Monte Carlo methods therefore allows the simulation of electron gas in the entire range of warm dense matter with unprecedented accuracy.

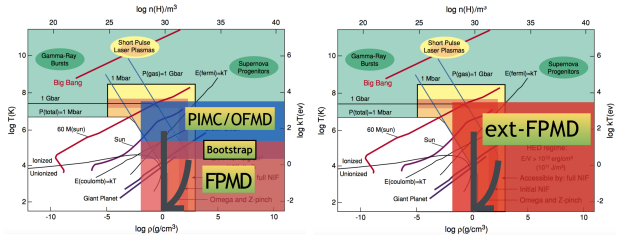


***Abbildung 1:*** *Schematic valid boundary for PIMC, OFMD, FPMD, and ext-FPMD. The thick grey lines represent three typical experimental technique to create warm dense matter in the lab. The vertical line represents isochoric heating, the horizontal line represents static compression, and the curve represents shock compression. Background picture from [8]*

We plan to combine our previous efforts from both ends to better benefit the community. It is very appealing to apply the temperature-dependent exchange-correlation functional in our ext-FPMD because it provides a more advanced theoretical description to the electrons in WDM [9]. The temperature-dependent exchange-correlation will affect not only the EOS, but also transport properties such as reflectivity, thermal and electrical conductivity, etc. Meanwhile, the quantification of the effect of the newly-proposed temperature-dependent exchange-correlation functional with respect to the old ones without temperature effects will help us evaluate all the previous first-principles calculations in this field.

Specifically, materials like hydrogen, water, carbon, methane, silicon, and complex compounds such as silicates, can be good candidates to test out ideas. Hydrogen is the lightest element in nature, since it has only one electron around its nucleus. Also, the study of hydrogen can be of great interest to inertial confinement fusion because the deuterium-tritium (DT) fuel cell goes through WDM region for a relatively long period during the implosion. Water and methane arouses much interests recently because they are very important components of exoplanet, whose properties under warm dense regime is key parameter to determine the formation and structure of such celestial bodies. Warm dense silicates consist a large part of the inner core of our planet earth. In fact, its wide range of EOS and other properties are crucial to understand the structure of the earth and the model to predict geophysical events such as earthquakes.

## WWW

http://www.theo-physik.uni-kiel.de/bonitz/

## More Information


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