Equation of state of warm dense matter: Reproducing quantum molecular dynamics results at high temperature

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In the thermodynamic domain of warm dense matter (WDM), there is no clear definition of the chemical species present and various effects like bonding, exchange-correlation or electron degeneracy must generally be taken into account. Quantum molecular dynamics (QMD), a first-principles approach in which the system is regarded as a mixture of electrons and nuclei and in which the quantum nature of electrons is taken into account [1], is appropriate for addressing the equation of state (EOS) of WDM. However, QMD is limited at high temperature by computational cost. In the present work, our aim is to construct an approach allowing to reproduce the QMD EOS at high temperature.

If an orbital-free approximation of the kinetic electronic free energy is used, QMD is made into orbital-free molecular dynamics, an approach which can be implemented at high temperature [2,3]. In the present work, we consider orbital-free-Weizsacker molecular dynamics (OFWMD) [4] and we define the ionic excess pressure for QMD and OFWMD as the difference between the excess pressure and an average atom pressure. We present the case of deuterium in the domain above 1 eV and 0.2 g/cc, and we show that we have been able to perform QMD calculations at sufficiently high temperature to demonstrate that the OFWMD ionic excess pressure is the limit of the QMD ionic excess pressure as temperature increases at given mass density. As a result, the QMD ionic excess pressure can be reproduced at high temperature. And, since the quantum average atom model can be implemented at high temperature, the QMD pressure can be reproduced at high temperature. The same is true for internal energy. The EOS which allows to reproduce the QMD results at high temperature is denoted OFWHMD.

With the approach described above, we have constructed an EOS table for deuterium in the domain above 1 eV and 0.2 g/cc [5]. Although the QMD and OFWHMD results are obtained independently, the convergence of QMD to OFWHMD is observed within statistical error or within a few tenths of a percent of total pressure [5]. The sensitivity of the EOS constructed to the exchange-correlation functional is shown.

In conclusion, we note that, while the QMD EOS cannot be reproduced at high temperature by the OFWMD EOS because of a non-monotonic convergence due to shell effects, it is reproduced by the OFWHMD EOS we have constructed [5]. We also evoke the applicability of our approach to atoms of higher atomic numbers and we consider what future work could consist in.

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