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Ab initio path integral Monte Carlo simulations of hydrogen snapshots at warm dense matter conditions

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We combine ab initio path integral Monte Carlo (PIMC) simulations with fixed ionic configurations, obtained by DFT-MD simulations, in order to solve the electronic problem for hydrogen under warm dense matter conditions. To solve the divergence problem in the Ewald-sum for attractive potentials we employ the pair-approximation. This approach is compared against the much simpler Kelbg pair-potential. We find very favorable convergence behavior towards the former. Since PIMC does not require any further assumptions regarding exchange and correlations of the many-body system, we then compare electronic densities obtained from our snapshot PIMC calculations with DFT calculations in the metallic regime. Furthermore, we investigate the manifestation of the resulting fermionic sign problem in our snapshot PIMC simulations. This gives us the unique capability to study the properties of warm dense hydrogen from ab initio simulations without any further assumptions, like the functional form of the exchange- correlation effects or fixed fermionic nodes. Thus, snapshot PIMC enables us to obtain the exact density response of warm dense hydrogen. This is extremely valuable to both experiments, like X-Ray Thomson scattering, as well as the development of new XC-functionals.

References

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