Influence of finite temperature Exchange-Correlation effects in Hydrogen

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We use density functional molecular dynamics (DFT-MD) to study the effect of finite temperature exchange-correlation (xc) in Hydrogen. Using the Kohn-Sham approach, the xc energy of the system, $E_{xc}(r_s)$ is replaced by the xc free energy $f_{xc}(r_s, \Theta)$ within the local density approximation (LDA) based on parametrized path integral Monte Carlo (PIMC) data for the uniform electron gas (UEG) at warm dense matter (WDM) conditions. We observe insignificant changes in the equation of state (EOS) at the region of metal-insulator transition compared to the regular LDA form, whereas significant changes are observed for $T>10000$ K, i.e., in the important WDM regime. Thus, our results further corroborate the need for temperature-dependent xc functionals for DFT simulations of WDM systems. Moreover, we present the first finite-temperature DFT results for the EOS of Hydrogen in the electron liquid regime up to $r_s = 14$ and find a drastic impact (the EOS changes by more than 20%) of thermal xc effects, which manifest at lower temperatures compared to WDM. We expect our results to be important for many applications beyond DFT, like quantum hydrodynamics and astrophysical models.

I. INTRODUCTION

Over the last decade or so, the interest on the properties of matter under extreme conditions has drastically increased due to new experimental and theoretical methods$^1$. Of particular importance is the so-called warm dense matter (WDM) regime$^{2,3}$, which is defined by two characteristic parameters being of the order of one: 1) the density parameter $r_s = \pi/\alpha_B$ (with $\pi$ and $\alpha_B$ being the average inter-particle distance and first Bohr radius, respectively) and 2) the reduced temperature $\Theta = k_B T/E_F$ (with $E_F$ being the usual Fermi energy$^4$). We note that the latter can be viewed as a degeneracy parameter$^5$, and $\Theta \ll 1$ ($\Theta \gg 1$) indicates when a quantum description or a non-degenerate treatment, respectively, of the (electronic subsystem) is appropriate.

In nature, WDM occurs in astrophysical objects such as brown and white dwarfs$^6$–$^8$, interiors of giant planets$^9$–$^{11}$, and meteor impacts$^{12,13}$. Moreover, these conditions can be realized experimentally using different methods such as laser or ion beam compression$^{14}$–$^{16}$, see Ref. 17 for a topical review article. Finally, we mention that WDM is predicted to occur on the pathway towards inertial confinement fusion$^{18,19}$, which makes a thorough understanding of this regime highly desirable.

From a theoretical perspective, the condition $r_s \sim \Theta \sim 1$ implies an intricate interplay of quantum scattering, electronic degeneracy effects and thermal excitations, which renders the accurate description of WDM a formidable challenge. More specifically, there are no small parameters and, hence, perturbative methods break down$^{20}$. This leaves computationally expensive $ab\initio$ simulations as the only option. In this work, we focus on density functional theory (DFT), which has emerged as the de-facto work horse in modern many-body theory$^{21,22}$. In particular, the possibly unrivaled success of DFT regarding the description of real materials was facilitated by the availability of accurate exchange-correlation (xc) functionals, which, however, cannot be obtained within DFT itself and have to be supplied as input. While the exact functional is, in general, not known, this quantity can often be reasonably approximated on the basis of the properties of a uniform electron gas$^{2,23}$ (UEG). In this context, the key quantity is given by the xc-energy of the UEG, which, at zero temperature, was accurately computed by Ceperley and Alder$^{24}$. These data were subsequently used as input for different parametrizations$^{25}$–$^{27}$ of $E_{xc}(r_s)$, which allow for DFT calculations on the level of the local density approximation (LDA). Moreover, these results constitute the basis for more advanced functionals like the celebrated work by Perdew, Burke, and Ernzerhof$^{28}$ (PBE).

While the generalization of DFT from the ground-state to finite temperature was introduced over 50 years ago by Mermin$^{29}$, most results for WDM up to this date have been obtained on the basis of the zero-temperature approximation (e.g., Refs. 30–35), i.e., using xc-functionals that were designed for the ground-state. However, this assumption is highly questionable, as the thermal DFT formalism requires as input a parametrization of the xc-free energy $f_{xc}(r_s, \Theta)$ that explicitly depends both on density and temperature$^{36,37}$. Therefore, carrying over the success of DFT from the ground state to finite temperature requires an accurate description of the UEG in the WDM regime.

This need has sparked a surge of new developments regarding quantum Monte Carlo simulations of electrons in this regime$^{38}$–$^{50}$, which culminated in the first accurate parametrizations of $f_{xc}(r_s, \Theta)$ of the UEG covering the entire WDM regime$^{49,51}$, see Ref. 2 for a topical review article. Here, we focus on the xc-functional by Groth and co-workers$^{49}$ (hereafter denoted as GDSMFB), which is not biased due to the fixed node approximation$^{38,52}$ (see also Ref. 53 for the first extensive quantification of nodal
errors) and exhibits an overall accuracy of 0.3%. Shortly thereafter, Karasiev et al.\textsuperscript{54} presented a small set of data which indeed highlight the impact of these new functionals on DFT simulations of WDM systems followed by an improvement in the Hugoniot of deuterium based on a finite-temperature GGA functional\textsuperscript{55,56}. Yet, a comprehensive study of the impact of finite-temperature exchange–correlation effects on thermal DFT simulations at extreme conditions is still lacking.

In this work, we aim to fill this gap by carrying out extensive thermal DFT calculations of hydrogen and comparing different zero-temperature approximations to the GDSMFB functional\textsuperscript{49}. In this context, we mention that hydrogen constitutes the most abundant element in our universe and offers a plethora of interesting physical effects\textsuperscript{57} such as the infamous liquid-liquid insulator-to-metal phase transition, the holy grail of extreme-conditions research\textsuperscript{58–65}. Further actively investigated questions regarding hydrogen at extreme conditions include ionization potential depression\textsuperscript{66,67} and proton crystallization\textsuperscript{68,69}, which makes it the system of choice for our current investigation.

Our new results allow us to unambiguously study the impact of the finite-temperature contributions to the xc functional on various quantities such as the EOS and the electronic density of states over a broad range of temperatures and densities going from $r_s = 0$ up to $r_s = 14$, where the electrons are strongly coupled and start to exhibit a liquid-like behavior\textsuperscript{70}.

The paper is organized as follows: In Sec II., we discuss the computational methods including the choice of the basis set, system size and the employed $k$-point sampling. The subsequent Sec III. is devoted to our simulation results, starting with the metal-insulator transition (Sec. III.A) and the warm dense matter regime (Sec. III.B). In Sec. III.C, we extend these configurations to the previously unexplored electron liquid regime at finite temperature. In addition, we present simulation results for the electronic density of states (DOS) and the density in coordinate space in Secs. III.D and III.E, respectively. The paper is concluded by a brief summary and outlook in Sec. IV.

II. COMPUTATIONAL DETAILS

The simulations are performed using the CP2K code\textsuperscript{49,71}. The Kohn-Sham equations are solved using the Gaussian plane waves method with the basis set using the Gaussians along with the additional plane waves as the auxiliary basis. The electron-proton potential is approximated using the Goedecker-Teter-Hutter pseudopotentials of LDA form\textsuperscript{72}. The standard $T=0$ LDA xc functional is hereafter referred to as PZ\textsuperscript{26} (Perdew-Zunger) and the parametrized temperature dependent LDA form of the xc functional is referred to as GDSMFB. The temperature dependent GDSMFB functional is accessed in the CP2K code using the library of exchange-correlation functionals (LIBXC)\textsuperscript{73,74}.

The choice of the basis set is important for obtaining accurate energies. We performed convergence tests in order to find the right basis set that also satisfies the computational demands. The best accuracy with sufficient speed
is met by the double zeta valence polarized (DZVP) basis set for the computations based on the energy minimization to obtain the pressure summarized in Fig. 1a for the PZ functional. The choice of the computationally more expensive basis sets can be ignored as the results are converged to within 0.3%. The DZV/DZVP basis set have been previously utilized in the simulations of warm dense hydrogen and hydrogen-helium mixtures\cite{75, 76}. Based on the DZVP basis set, the choice of the system size influences the energy convergence. The smallest system size feasible for our DFT-MD simulations (N= 32) shows differences at a range of densities and temperatures and the minimum size required for sufficient accuracy is given by N= 256 as shown in Figure 1b. Yet, we are forced to resort to N= 32 for extreme cases of small/large densities due to high computational demands required, which is explicitly mentioned in those cases. Note that a similar effect of the system size on the EOS is also observed by Lorenzen et al. for dense hydrogen\cite{77}. The effect is seen in Fig. 1b for \( r_s = 3.0 \) with a pressure variation of 4.7\% with the change in system size from N= 32 to 256. At \( r_s = 4.0 \), the pressure variation with system size is 2.5\% and at lower densities a system size of N= 32 or \( N = 108 \) is feasible for simulations also considering the requirement of more plane waves for big simulation boxes.

The choice of \( k \)-point sampling can influence the computed energy and pressure of the system. At \( r_s = 3 \), \( T = 15625 \) K, we see no dependence on \( k \)-point sampling based on the system size for obtaining the convergence as shown in Fig. 1c. For a system size of \( N= 108 \), the pressure difference between \( \Gamma \)-point sampling and \( 3 \times 3 \times 3 \) is \( < 0.1\% \). Higher \( k \)-point sampling has a smaller effect for bigger supercells as the case of \( N= 256 \) particles demonstrates where the change in pressure is still \( < 0.1\% \) going from \( \Gamma \)-point sampling to a \( 3 \times 3 \times 3 \) grid of \( k \)-points. For these reasons, we consider a system size of \( N= 256 \) sampled at the \( \Gamma \)-point.

The plane wave energy cutoff of the system is set between 450-800 Ry and the Gaussian basis set cutoff is set to 90-180 Ry depending on the density and the temperature of the system. The simulation time step was chosen so as to account for the large kinetic energies of the protons at higher temperatures. It ranges in between 0.02 fs for the highest temperatures and 0.1 fs for the lowest temperatures considered. Simulations ran for 10000 steps and more until the system equilibrated and the equilibrated time steps of sizes 4000-5000 are considered for obtaining the statistics. We use a Fermi occupation of the bands/eigenvalues to set the electronic temperature\cite{79, 86} and employ a Nosé-Hoover thermostat to control the ionic temperature in the canonical ensemble\cite{78, 79}. The simulation box consisted of an hexagonal cell (\( a=b, c=1.63a \)) under periodic conditions and the cell size varied depending on the \( r_s \) (density). The simulations cover the density range from \( r_s = 0.7 \ldots 14 \) for a wide range of temperatures \( T = 250 \ldots 400000 \) K. For completeness, we mention that simulations of temperature ranges beyond 400000 K are at present computationally too expensive using KS-DFT. Alternatives include orbital-free DFT\cite{80–83} and an extended KS-formalism\cite{82}, which, however, are beyond the scope of this work.

### III. RESULTS

#### A. Metal-Insulator transition and metallic hydrogen

![FIG. 2: EOS at \( T = 1000K \) using various xc functionals and \textit{ab initio} methods. Lorenzen Ref. 77; Morales Ref. 84; Lu Ref. 85; Alavi Ref. 86. PZ, GDSMFB and PBE results of this work.](image)

We have performed simulations for a system size \( N = 256 \) and the \( k \)-point sampling is performed only at the \( \Gamma \)-point. The first order phase transition (LLPT) has a characteristic signature\cite{84} in the PVT diagram, \( \left( \frac{dP}{d\rho} \right)_{T=0} \). While nuclear quantum effects (NQE) have been shown to influence the transition pressure\cite{84, 91}, they are not considered in this work as we focus on thermal xc effects on the electrons. Figure 2 shows the EOS at 1000 K computed with various xc functionals and \textit{ab initio} methods. CEIMC gives a very clear signature of the LLPT. The DFT-MD results, which can be calculated for a finer grid of points and have to utilize a dense \( k \)-point grid near the transition region, show a slightly lower transition pressure\cite{77}. First and foremost, we find no significant change in the EOS due to the incorporation of finite-temperature exchange and correlation effects as the reduced temperatures are low at these densities, \( 0.003 < \Theta < 0.004 \). At \( T = 1000 K \), the LDA results (PZ/GDSMFB) are in the range obtained by Alavi et al.\cite{86}. The differences between PBE results from Lorenzen et al.\cite{77} and ours could stem from the employed \( \Gamma \)-point sampling, which is known to lead to a lower pressure at high densities\cite{77}. This is evident in the lower pressures reported at higher densities in Figure 2. There are obviously differences to the pressure isotherms ob-
higher rungs of xc functionals especially with non-local density functionals. Thus, Lu et al. recently reported a higher transition pressure comparable to CEIMC and BOMD (Born-Oppenheimer molecular dynamics) using PIMD with rVV10 and vDW-DF1 functionals.85

In Figs. 3a-3c, we compare the computed EOS with QMC and BOMD at temperatures 6000 K, 8000 K and 10000 K, respectively. The relative difference in pressure shown in the inset plot is given by

\[
\left( \frac{P_{\text{GDSMFB}} - P_{\text{PZ}}} {P_{\text{GDSMFB}}} \right) \times 100\%.
\]

(1)

Our LDA results and the BOMD results obtained by Morales et al. consistently exhibit deviations from each other with smallest deviations for the highest densities (lowest \(r_s\)).87 The pressure difference between our LDA results and CEIMC do not feature any consistency but exhibit lower relative difference than the BOMD results with decreasing density.87 In Fig. 3a, we also show the close agreement for lower densities (\(r_s > 1.4\)) between our results with DFT/QMC and BOMD obtained by Mazzola et al.89 and Vorberger et al.11. The GDSMFB results in a higher pressure compared to PZ by 0.2 – 0.5% at these conditions, which is reasonable as \(\Theta \approx 0.01 – 0.03\). A similar trend can also be observed in the Figs. 5b-5d discussed in section III B where the pressure difference is positive for similar densities at low temperatures.

For completeness, we show the phase diagram with LLPT boundaries in Fig. 4. Our PBE data is only shown at 1000 K as a reference to other simulation results and experiments. Moreover, the LDA (PZ/GDSMFB) results of this work are not included into the diagram as they fail to capture the LLPT and the EOS is inconsistent compared to other xc functionals and experimental results.
FIG. 5: EOS at a) $r_s = 0.7$, b) $r_s = 0.8137$, c) $r_s = 1.1$, d) $r_s = 1.4$ comparing our results with the previous results obtained using PIMC and DFT. The inset plot shows the relative difference (Eq. 2) in total pressure for the finite temperature case with respect to the LDA case. Hu Ref. 18; Wang Ref. 95; Danel Ref. 96; Karasiev Ref. 54.

B. Warm dense matter

Let us next explore the warm dense matter regime, where thermal xc effects are expected to be important. In Figs. 5a-5d, we compare the equation of state for $r_s = 0.7 - 1.4$ corresponding to densities in the range of 0.98 - 7.855 g/cm$^3$. Due to the drastically increased computational cost at high densities and temperatures, we choose $N = 32$ for all of the simulations shown in this section. Moreover, the $k$-point sampling is performed only at the Γ-point. The resulting finite-size effects have been demonstrated for lower temperatures at $r_s = 3$, where we have obtained higher pressures for smaller system sizes. Consequently, our results for the pressure deviate from the data by Wang$^{95}$ et al at WDM conditions ($r_s = 0.7$ and 0.8137) as can be seen in Figs. 5a-5b. Wang et al.$^{95}$ use a system size ranging from 8-512 atoms sampled at the Γ-point with the Kohn-Sham DFT simulations restricted to $T < T_F$ for $\rho > 0.5$ g/cm$^3$. Yet, this does not necessarily constitute a problem, since we are only interested in the pressure differences due to the use of the GDSMFB functional instead of PZ, and the finite-size effects are expected to mostly cancel. For example, a similar cancellation of finite-size effects has been reported for $ab$ initio PIMC calculations of the static local field correction, see, e.g., Refs. 50 and 97.

Thus, the relative difference in the total pressure calculated using

$$\frac{(P_{PZ} - P_{GDSMFB})}{P_{PZ}} \times 100\%.$$  \hspace{1cm} (2)

shown in the inset plot in Fig. 5 is in good agreement with the Kohn-Sham DFT and orbital-free DFT results obtained by Karasiev et al.$^{54}$. The variation of the electronic pressure with respect to temperature and density is shown in Fig. 6. In accordance with Ref. 54, we obtain the electronic pressure by subtracting the ideal ion pressure from the total pressure. The ionic excess pressure as can be obtained for instance by integrating over the pair correlation function, has not been subtracted$^{98}$. With a decrease in density,
First and foremost, we note that $\Delta P$ exhibits a sign change for intermediate $T$, which is shifted to larger temperatures for increasing density. This is again a consequence of the $r_s$-dependence of the reduced temperature $\Theta$, which decreases with $r_s$. For completeness, we mention that a similar sign change has been found for the xc-detection of the associated negative dispersion relation of the dynamic structure factor constitutes an exciting opportunity for future research\textsuperscript{102}.

Figure 7a shows the EOS for $r_s = 2.0 - 10$ corresponding to densities in the range $2.7 \times 10^{-3} - 0.34 \text{ g/cm}^3$. The system size is $N = 256$ except at $r_s = 10$ where the system size is reduced to $N = 32$ due to the large simulation box required at extremely low densities. The $k$-point sampling is performed only at the $\Gamma$-point. The EOS fits well with the PIMC and DFT-MD data of Hu et al. and Wang et al., respectively across a gamut of temperatures for the densities considered\textsuperscript{18,34}. The relative difference in total pressure between PZ and GDSMFB is shown in Fig. 7b.

With decreasing density (i.e., increasing $r_s$), electronic correlations become more important and the system will eventually form an electron liquid\textsuperscript{3,100-103} for $r_s \gtrsim 10$. 3D electron liquids can be found in metals such that the Fermi surface of the conducting electrons be spherical to facilitate the movement of electrons as free particles. This is also possible with semiconductors by controlling the amount of dopants\textsuperscript{4,104}. While these exotic conditions are rather difficult to realize experimentally at present, they offer the valuable opportunity to study the nontrivial interplay of temperature and Coulomb coupling ($\Gamma = 1/(a k_B T)$) with quantum diffraction and exchange effects. For example, Takada\textsuperscript{104} predicted the emergence of a collective excitonic mode for large $r_s$ based on ground-state many-body theory, which was recently substantiated by more accurate \textit{ab initio} path-integral Monte-Carlo calculations at finite temperature\textsuperscript{102,103}. Moreover, the possibility of an experimental

**FIG. 6**: The electronic pressure as a function of temperature at various densities. The inset plot shows the relative difference (Eq. 2) in electronic pressure for the finite temperature case with respect to the LDA case.
part of the kinetic energy of the UEG, see, e.g., Ref.\textsuperscript{105}. Between $r_s = 5 - 10$, the relative difference in pressure is more pronounced with positive differences at low temperatures and negative differences at higher temperatures being of a similar magnitude. The maximum changes for $r_s = 10$ are observed in a broad range of reduced temperatures of $\Theta = 0.6 - 6.0$. For comparison, we mention that the positive maximum deviation for $r_s = 5$ is found for $\Theta = 0.3 - 0.7$, whereas the negative maximum deviation extends to temperatures beyond the depicted range. At $r_s = 2.0 - 3.0$, the onset of the significant changes begin near the maximum of the temperature considered in Fig. 7b. This can be observed in Fig. 8a, where the temperature is held constant and the relative difference in total pressure is evaluated with the change in density and the electron degeneracy. The positive pressure difference is maximal for the density range $r_s = 2.0 - 3.0$ in the vicinity of $\Theta \sim 1$ and $\Gamma \sim 2$. At $r_s = 14.0$, we compute the relative difference in total pressure across a wide range of temperature where the maximum differences ($\pm$) can be seen at the reduced temperatures $\Theta = 1.18(5.90)$ as shown in Fig. 8b. Remarkably, these deviations exceed 20\% and, thus, are even more pronounced than for the previously considered WDM regime. Finally, we note that the system size is set to $N = 32$ due to the large simulation box and sampled only at the $\Gamma$-point, with the finite size errors being unimportant as we are only interested in the relative differences in total pressure.

D. Density of states

The density of states (DOS) is computed for $r_s = 2.0$ simulating $N = 256$ atoms sampled at the $\Gamma$-point. We choose a set of 5 independent equilibrated configurations from different simulation runs which are averaged to obtain the corresponding density of states. In Figs. 9a-9d, the density of states is shown for a range of temperatures and compared to the ground-state GGA calculations by Collins et al.\textsuperscript{99} At 2000 K, the system is still insulating with a band gap shown in 9a while the results from Collins et al. show a slight increase in the DOS near the Fermi level. At a slightly higher temperature 5000 K, the system is metallic and our results match the trend obtained by Collins et al. Between 2000 and 5000 K, the DOS is hardly influenced by finite temperature xc-effects as the reduced temperature is still low. At 15625 K ($\Theta = 0.107$), the results follow the trend seen by Collins et al., with the $\sqrt{E}$ feature being clearly visible at 62500 K ($\Theta = 0.43$). Noticeable differences between the DOS computed with the PZ $T=0$ functional and the GDSMFB finite-$T$ functional start to appear at these two temperatures, which are still below the regime where the maximum change in finite temperature xc effects can be observed.

E. Electronic density

Figure 10a-10b shows snapshots of a electronic density iso-surface computed using PZ and GDSMFB for $r_s = 2.0$, $T = 62500$ K (i.e., $\Theta = 0.43$, which is located in the WDM regime) and for the same ionic configuration. More specifically, we have simulated $N = 256$ atoms sampled at the $\Gamma$-point in a hexagonal cell. The snapshot has been obtained by performing DFT-MD simulations with the PZ functional until the system equilibrated and a random ionic configuration is chosen, which is subsequently used to compute the density with the different xc functionals. The visualization of the results are generated using VESTA\textsuperscript{106}. Overall, the two snapshots in panels a) and b) exhibit a similar structure, with the electronic iso-surfaces being mostly located around the ions. Yet, there appear
FIG. 9: The density of states at $r_s = 2.0$ and a) $T = 2000$ K b) $T = 5000$ K c) $T = 15625$ K and d) $T = 62500$ K using LDA and the finite-temperature case. The Fermi energy is set to zero. The blue and the yellow areas represent DOS calculated using PZ and GDSMFB respectively. The overlap between them is indicated by the red area. Collins Ref. 99.

distinct systematic differences, which can be seen particularly well in Figs. 11a-11b showing a magnified segment around the bottom left corner of the simulation cell: using the PZ-functional, there appears a pronounced overlap between the electronic orbitals around individual atoms; the GDSMFB-functional, on the other hand, leads to substantially reduced overlap, as we shall explain heuristically in the following. With increasing temperature, the thermal wavelength $\lambda \sim 1/\sqrt{T}$ decreases and, consequently, the electronic orbitals are less extended. Ultimately, this leads to the convergence to classical point-like particles in the high temperature limit. The PZ-functional, which has been constructed solely based on ground-state data for the UEG, cannot consistently capture this behaviour, and the extension of the electronic iso-surfaces is drastically overestimated.

We thus conclude that including finite-$T$ xc effects in a thermal DFT simulation of a WDM system is crucial to capture the relevant physics, even though the impact on averaged quantities like the total pressure (3%, cf. Fig. 8) might be comparably small. The local electronic density and it’s fluctuation are for instance important for the calculation of scattering quantities.

IV. CONCLUSIONS

In summary, we have studied in detail the impact of finite-temperature xc effects on DFT simulations of hydrogen over a vast range of different conditions. More specifically, we have carried out extensive DFT calculations using the ground-state functional by Perdew and Zunger (PZ) and the recent finite-$T$ analogue by Groth et al.49 (GDSMFB). This has allowed us to unambiguously quantify the impact of finite-$T$ xc for different quantities and in different physical regimes. Firstly, we have found that electronic temperature effects do not play a significant role for the description of the LLPT, as the reduced temperature is small, $\theta \lesssim 0.01$. Thus, closing the gap between simulation and experiments will most likely require to further ascend Jacob’s ladder of xc functionals107, but in the ground state. Moving on to the warm dense matter regime, temperature-effects in the xc functional become more
FIG. 10: Snapshot of an electronic density isosurface for $r_s = 2.0$, $T = 62500$ K ($\Theta = 0.43$) using a) PZ and b) GDSMFB for the same ionic configuration with $N = 256$.

FIG. 11: Magnified segment around the bottom left corner of the density plots in Fig. 10. The left and right panels correspond to the PZ and GDSMFB functionals, respectively.

important, and we find deviations in the electronic pressure clearly exceeding 5%. Moreover, these deviations are non monotonous with respect to $T$, and we find a sign change in the pressure difference, which is shifted to larger temperatures with increasing density. We thus conclude that the further development of xc functionals to consistently take into account thermal excitations is of central importance to achieve predictive capability for DFT calculations in the WDM regime.

In addition, we have presented the first finite-$T$ DFT results for hydrogen in the strongly coupled electron liquid regime, $r_s \geq 10$. At these conditions, electronic xc effects are even more important for an accurate description, and, consequently, the temperature-dependence of the xc functional is crucial. More specifically, we find pressure differences between the PZ and GDSMFB functionals exceeding 20% at $r_s = 14$ in the vicinity of the Fermi temperature. We expect this point to be of high importance for the future investigation of interesting phenomena such as the possible emergence of an incipient excitonic mode, which might occur at even lower density$^{104}$.

Finally, we have extended our consideration to other physical properties of hydrogen like the density of states, and the electronic density in coordinate space. Regarding the DOS, we have found that finite-$T$ xc effects do indeed significantly influence the DFT results in the WDM regime, as it is expected. Our simulation results for the
electronic iso-surfaces in coordinate space are even more remarkable, as the PZ functional is not capable to describe the reduction of electronic overlap at finite temperature. Possible topics for future research include the consideration of other materials such as helium or carbon (see Ref. for first results) and the investigation of transport properties like the electrical conductivity. As a concluding remark, we note that thermal xc effects are highly important for many applications other than DFT, such as quantum hydrodynamics and astrophysical models.

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