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Self-energy shift and energy band theory for warm dense matter

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Energy band structures caused by self-energy shifting that results in bound energy levels broadening and merging are found in the warn dense matter (WDM), which is a partially-ionized quantum plasma under high density and temperature and is numerically intractable to deal with by the traditional thermal density functional theory (DFT) due to existing thousands of high-excited atomic states. We proposed an energy band theory for WDM and developed a new code based on the energy band theory to improve the traditional DFT. Massive data of equation of state and transport coefficients for WDM in medium and low Z have been simulated and investigated. The transition from the fully degenerate to partially degenerate (related to WDM) and finally to non-degenerate state is studied using the Lorenz number varying with the degeneracy parameter, and lower and upper parameter boundaries for WDM are achieved. It is shown that the pressure ionization results in the Wiedemann-Franz law no longer available for WDM.

References

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