A unified modelization from condensed matter to plasmas

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During the last twenty years, Density functionnal theory has emerged mostly to describe cold condensed matter. When one wants to describe warm dense matter at high electronic temperature ($\approx$ 10 eV), plane waves DFT codes pain to get the ground state. Indeed, at these temperature ranges, one has to consider many electronic orbitals which lead to a drastic increase of the number of plane waves needed to describe the ground state wave functions. The diagonalization procedure of the Hamiltonian will be impacted by the number of plane waves, and the calculation will became numerically impossible.

To overcome this limitation, orbital free methods have been developped. Unfortunately, these methods are not able to describe matter at ambiant temperature because of the absence of orbitals. Fortunately some simplifications to this problem [1] can be applied to plane waves DFT codes, which will allow a unification of these methods, and will lead to a better understanding of warm dense matter at a quantum level.

References

[1] Shen Zhang, Hongwei Wang, Wei Kang, Ping Zhang, and X. T. He. Extended application of Kohn-Sham first-principles molecular dynamics method with plane wave approximation at high energy—From cold materials to hot dense plasmas. *Physics of Plasmas*, 23(4):042707, April 2016.