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NEW ADVANCEMENTS IN THE STUDY OF THE UNIFORM ELECTRON GAS WITH FULL CONFIGURATION INTERACTION QUANTUM MONTE CARLO MICHELE RUGGERI, HONGJUN LUO, Max Planck Institute for Solid State Research, Stuttgart, ALI ALAVI, Max Planck Institute for Solid State Research, Stuttgart and University Chemical Laboratory, Cambridge — Full Configuration Interaction Quantum Monte Carlo (FCIQMC) [1] is able to give remarkably accurate results in the study of atoms and molecules. The study of the uniform electron gas (UEG) on the other hand has proven to be much harder, particularly in the low density regime. The source of this difficulty comes from the strong interparticle correlations that arise at low density, and essentially forbid the study of the electron gas in proximity of Wigner crystallization. We extend a previous study on the three dimensional electron gas [2] computing the energy of a fully polarized gas for N=27 electrons at high and medium density ($r_S = 0.5$ to 5.0). We show that even when dealing with a polarized UEG the computational cost of the study of systems with $r_S > 5.0$ is prohibitive; in order to deal with correlations and to extend the density range that to be studied we introduce a basis of localized states and an effective transcorrelated Hamiltonian.

[1] G. H. Booth, A. J. W. Thom and A. Alavi, J. Chem. Phys. **131** 054106 (2009)
[2] J. J. Shepherd, George H. Booth and A. Alavi, J. Chem. Phys. **136** 244101 (2012)

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