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Developing Quantum Fluid Theory of Electrons from First Principles

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The simulation of correlated fermions is important for various phenomena in warm dense matter, plasmonics, and ultracold atoms. In order to enable simulations at larger length and longer time scales, there is a need to develop quantum hydrodynamics (QHD) as a complementary method to commonly used first-principles methods. The key difference of the QHD from classical fluid equations is the inclusion of the quantum non-locality. This is usually done by using the Bohm potential. We performed the very first investigation of the Bohm potential for a correlated many-fermion system based on the data from KS-DFT. Despite its long history in quantum mechanics since its derivation by Bohm in 1952 and its importance for QHD, this has not been done before. Our key result shows the very limited applicability of the standard Bohm potential which is used in virtually all previous works of QHD. We showed that it is only valid for a very weakly perturbed electron gas. We illustrate that the many-fermion quantum Bohm potential is needed to model nonlinear phenomena in quantum plasmas and WDM [1, 2].

[1] Z. A. Moldabekov, T. Dornheim, G. Gregori, F. Graziani, M. Bonitz, A. Cangi, Towards a Quantum Fluid Theory of Correlated Many-Fermion Systems from First Principles, SciPost Physics [accepted for publication], scipost_202106_00020v3

[2] F. Graziani, Z. Moldabekov, B. Olson, M. Bonitz, Shock Physics in Warm Dense Matter–a quantum hydrodynamics perspective, arXiv:2109.09081

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