Theoretical Quantum Physics

Group Seminar

11:30 AM
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Online (Zoom)

Repulsively diverging gradient of the density functional in the Reduced Density Matrix Functional Theory

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Abstract

The general topic of the talk concerns the Reduced Density Matrix Functional Theory (RDMFT) where the object of interest is the RDMFT functional. The exact RDMFT functional depends only on the interaction term of the Hamiltonian and is universal for all the single-particle terms such as the kinetic energy or the external potential. The RDMFT functional is found via the **Levy-Lieb constrained search [1]** in multiparticle systems with a fixed particle number. The domain of this functional is the set of all **one-particle reduced density matrices**. The functional is real-valued and while looking for the ground-state energy of the system at hand, one has to minimise the total value of the functional plus the energy of the single particle terms which can be summarised in the formula Tr(\gamma h)+F_W(\gamma), where h are the single-particle terms of the Hamiltonian, F_W is the RDMFT functional and \gamma is a one-particle reduced density matrix.

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Because of this minimisation procedure, the knowledge of the gradient of the RDMFT functional is crucial. In particular, Christian together with his collaborators (Carlos Benavides-Riveros, Julia Lieber, Rolf Schilling and others) has discovered that in many quantum systems the gradient of the RDMFT functional is repulsive and divergent at the boundary of its domain (the set one-particle reduced density matrices which is a complicated geometric object!) – a phenomenon dubbed the "Bose-Einstein condensation force" (for bosons) or the "exchange force" (for fermions). This means that the minimiser can never lie on the boundary of the domain – a really remarkable fundamental fact for quantum physics. It has been conjectured that this is in fact a generic phenomenon occurring in multipartite quantum systems. However, due to the complicated nature of the Levy-Lieb constrained search, it is often impossible to find the formula for the exact RDMFT functional, so some other methods have to be found in order to prove the universal nature of this repulsively diverging gradient. My approach to this problem relies on finding appropriate upper bounds on the exact functional which bear some information about its gradient on the boundary of the functional's domain. In my talk, I will introduce the relevant constructions in the case of the Bose-Hubbard dimer and compare them with the known results for the exact RDMFT functional in this system [2]. Then, I will show how this is generalised to considerably more complicated higher-dimensional quantum systems using some tools from group theory [3].

[1] Lieb E H 1983 Density functionals for coulomb systems Int. J. Quantum Chem. 24 243

[2] Benavides-Riveros C L, Wolff J, Marques M A L and Schilling C 2020 Reduced density matrix functional theory for bosons Phys. Rev. Lett. 124 180603

[3] Maciazek T 2021 Repulsively diverging gradient of the density functional in the reduced density matrix functional theory New J. Phys. 23 113006

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