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

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The Reduced Density Matrix Functional Theory (RDMFT) is a remarkable tool for studying properties of ground states of strongly interacting quantum many body systems. As it gives access to the one-particle reduced density matrix of the ground state, it provides a perfectly tailored approach to studying interacting multi-particle quantum systems. In particular, for homogeneous Bose-Einstein condensates as well as for the Bose-Hubbard dimer it has been recently shown that the relevant density functional exhibits a repulsive gradient (called the Bose-Einstein condensation force) which diverges when the fraction of the non-condensed bosons tends to zero [2,3]. In my talk I will explain that the existence of the Bose-Einstein condensation force is completely universal for any type of the pair-interaction and also in the non-homogeneous gases [1]. To this end, I will outline a construction of a universal family of variational trial states which allows one to suitably approximate the relevant density functional in a finite region around the set of the completely condensed states. I will generalise these arguments to show the existence of an analogous repulsive gradient in the fermionic RDMFT for the N-fermion singlet sector in the vicinity of the set of the Hartree-Fock states. Such an approximate functional may perform well in density-functional calculations involving low numbers of electrons. This is demonstrated numerically in the electron transfer calculations for the Fermi-Hubbard model in the strongly correlated limit where some other approximate functionals are known to fail.

References

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