Reduced Density Matrix Functional Theory for Bosons

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Based on a generalization of Hohenberg-Kohn's theorem, we propose a ground state theory for bosonic quantum systems. Since it involves the one-particle reduced density matrix γ as a variable but still recovers quantum correlations in an exact way it is particularly well-suited for the accurate description of Bose-Einstein condensates. As a proof of principle we study the building block of optical lattices. The solution of the underlying v-representability problem is found and its peculiar form identifies the constrained search formalism as the ideal starting point for constructing accurate functional approximations: The exact functionals $\mathcal{F}[\gamma]$ for this N-boson Hubbard dimer and general Bogoliubov-approximated systems are determined. For Bose-Einstein condensates with $N_{\mathrm{BEC}} \approx N$ condensed bosons, the respective gradient forces are found to diverge, $\nabla_\gamma \mathcal{F} \propto 1/\sqrt{1 - N_{\mathrm{BEC}}/N}$, providing a comprehensive explanation for the absence of complete condensation in nature.