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【105】 Reduced Density Matrix Functional Theory for Superconductors

Tuesday 27 August 2019 15:00 (15 minutes)

In this talk I present a new ab-initio theory for superconducting systems with non-local external potentials based on the one-particle reduced density matrix $\rho(\mathbf{r},\mathbf{r}')$ and the anomalous density $\chi(\mathbf{r},\mathbf{r}')$. All the equilibrium properties of the system are determined uniquely by these two quantities. By replacing the local electronic density with the non-local one-particle reduced density matrix, our theory is able to solve difficulties which arise in DFT for superconductors. I sketch the proof of the existence of a non-interacting Kohn-Sham system that is able to reproduce ρ and χ of the interacting system at finite temperature. On the basis of the Kohn-Sham system, one obtains a set of Bogoliubov-de Gennes-like single particle equations.

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