Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Wednesday, Sept. 6th, 2016 – 11:00 a.m.
CFEL Seminar room III (Bldg. 99)

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Reduced formula for the macroscopic polarization including quantum Fluctuations

The macroscopic polarization of a solid is an fundamental quantity from which permittivity and piezoelectric tensors can be derived. The Berry phase formula of King-Smith and Vanderbilt expresses the macroscopic polarization in terms of the Bloch states of a mean-field band structure, almost invariably taken from density functional theory. Although this procedure has been successful for many materials, quantum fluctuations cause it to break down in strongly correlated systems.

In this talk, I introduce a novel many-body Berry phase formula for the macroscopic polarization that maintains the simplicity of the King-Smith--Vanderbilt formula while accounting for genuine quantum fluctuations. The polarization is approximated by a sum of natural orbital geometric phases with fractional occupation numbers accounting for the dominant quantum fluctuations.

Numerical exact diagonalization calculations for the Rice-Mele-Hubbard model demonstrate that the formula accurately reproduces the exact polarization throughout the phase diagram, including the vicinity of the band insulator-Mott insulator quantum phase transition. As a final example, I show that the theory can be used to calculate topological invariants in interacting systems.

Host: Angel Rubio

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