



Recent Developments in Full Configuration Interaction Quantum Monte Carlo

- 講師** : **Professor Ali Alavi**
Max Planck Institute for Solid State Physics, Germany and
University of Cambridge, United Kingdom
- 日程** : 11月16日(木) 16:00-
- 場所** : 本館2階 H284A 物理学系輪講室

概要

Full Configuration Interaction Quantum Monte Carlo (FCIQMC) is a stochastic technique for solving the electronic Schrödinger equation in the configuration interaction (CI) representation. Here we will present some recent developments in this methodology, including the extension to real-time propagation, which allows for the calculation of spectral functions along the real frequency axis, and photo-emission and inverse-photo-emission spectra.

If time allows, we will also present developments in using more sophisticated wavefunction ansatz than a linear CI expansion, including the transcorrelated method of Boys and Handy, which allows for a much more rapid convergence to the basis set limit.

連絡教員 物理学系 Bhanu Das (内線 3045)