A wave-function approach to solids

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Hartree-Fock (HF) method is a useful first-step tool for investigating electronic structure and total energy of atoms and molecules: it gives very good electron density, reasonably accurate total energy, and molecular orbitals and orbital energies that are helpful for understanding the electronic structure. The HF method is, however, not commonly applied to solids nowadays, since electronic screening effect is neglected, thereby resulting in vanishing density of states at the Fermi level of metals and serious overestimation of band gap of semiconductors. Although systematic improvement is considered to be an advantage of wave function theory (WFT) against the density functional theory (DFT), so-called post-HF methods are computationally too demanding for solids. For long, therefore, variational Monte Carlo (VMC) method and diffusion Monte Carlo (DMC) method have been only practical ways to calculate accurate total energy of solids within WFT.

We are developing another wave function approach to solids based on the transcorrelated (TC) method by Boys and Handy [1, 2]. In the TC method, an explicitly correlated wave function of Slater-Jastrow-type is adopted. After similarity transformation of the Hamiltonian with the Jastrow function, one obtains a HF-like self-consistent-field equation to determine one-electron orbitals in the Slater determinant, which also provides TC orbital energies. Koopmans' theorem holds for the TC orbital energies and so we can easily draw electronic band structure of solids with taking account of the electron correlation effect through the Jastrow function. This is an advantage of the TC method against VMC or DMC. Total energy of solids can be calculated without Monte Carlo sampling.

In this talk I review recent applications of the TC method to solids and demonstrate how the HF results are improved by taking account of the electron correlation effect [3-5].

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