Multi-reference density functional theory for Mott's insulators and electron-electron interaction mediated superconductivity

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We have found that an effective Hamiltonian of an interacting Fermion system representing the many electron system in the non-relativistic description is determined by referencing Coulomb interaction driven fluctuation in the multi-reference density functional theory (MR-DFT).[1-5] In our MR-DFT, an effective Hubbard-type Hamiltonian is defined as an extended Kohn-Sham Hamiltonian,[1,2] which gives a self-consistent calculation scheme applicable for the materials design. The effective interaction may be determined by adjusting local fluctuation determined by a reference calculation. A kinetic energy functional may be used as an indicator to detect occurrence of the strong suppression of fluctuation, which provides us a self-contained calculational scheme within MR-DFT.

In this presentation, we focus on the *N* representability satisfied in our MR-DFT. Two geometries to detect occurrence of the Mott insulating transition and the electron-electron interaction mediated superconductivity are proposed for the rigorous MR-DFT. The momentum boost technique may be used by adopting a twisted boundary condition in one direction of the Born-von-Karman boundary condition. The Harriman construction is easily generalized for the twisted boundary condition.[5] The Meissner effect may happen for a sample with a cylinder geometry. The internal vector potential should appear, if the superconducting current flows on the surface of the ring. This broken symmetry state can be detected as a stable solution within a symmetry restricted phase space, where the *N* representability is again ensured. Test calculations using simplified model systems are shown.

References

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