# LCAO method for finite-temperature systems and self-consistent perturbation scheme beyond the GW approximation

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The linear combination of atomic orbitals (LCAO) method, which was originally developed for calculating the electronic structure of systems at zero temperature, is extended to treat finite-temperature systems. The new method yields an approximate free energy that is an upper bound to the true free energy of a real system. The approximate free energy is given in the space spanned by an LCAO basis and in a parameterized form. When a mean field approximation is adopted and the approximate free energy is minimized with respect to the parameters, this method includes the conventional LCAO method at zero temperature as a limiting case.

As further development of the above method, we propose a scheme based on a kind of self-consistent perturbation theory, where both the non-interacting Hamiltonian and charge fluctuation are determined self-consistently. The non-interacting Hamiltonian is given within the Hartree-Fock approximation in which the interacting electron density is used instead of the non-interacting one. To describe the charge fluctuation dynamics, we use a functional-integral representation of the free energy [1]. Our main approximation is to replace the exact free energy functional by a variationally chosen quadratic form in the fluctuating field. This procedure leads to the inclusion of electron correlation beyond the GW approximation.

We also mention the application of our scheme to electron transport in carbon nanotubes and superconductivity in carbon-based materials.

[1] J. Hubbard, Phys. Rev. Lett. 3 (1959) 77-78