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An Extension of the Kohn-Sham Equations for the Correlated Electron Systems

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Knowledge on the Mott metal-insulator transition and the Kondo effects has revealed that description of several kinds of electron-correlation effects inevitably requires multi-Slater determinants. In this talk, we reconsider possibility of the so-called first-principles approach for the electronic state calculation based on the density functional theory (DFT) as a standard theory for the interacting electron systems showing these interesting correlation effects.

Tractable calculational methods have been developed by utilizing an additional strategy of DFT, i.e. the Kohn-Sham scheme. In this formulation, one considers an imaginative non-interacting model system which is assumed to reproduce the single-particle density \( n(r) \) of the true ground state. Then, an effective potential problem is obtained, which is described by the Kohn-Sham equation.

In the present theory, we start from an assumption similar to the Kohn-Sham scheme. Namely, we assume existence of an imaginative interacting system which reproduces \( n(r) \), then we can derive a many-body problem describing the model system as follows.

\[
\begin{align*}
\{ -\frac{\hbar^2}{2m}\Delta + v_{\text{eff}}(r) \} \phi_{ij}(r) &= \epsilon_i \phi_{ij}(r) \\
\sum_{\sigma} \epsilon_i c_{ij\sigma}^\dagger c_{ij\sigma} + \sum_{ij} V^{(1)}_{\text{eff}}(ij\sigma)c_{ij\sigma}^\dagger c_{ij\sigma} + \sum_{ijkl;\sigma\sigma'} V^{(1)}_{\text{eff}}(ijkl;\sigma\sigma')c_{ik\sigma}^\dagger c_{kj\sigma'} c_{ij\sigma'} c_{kl\sigma} + \hat{H}_{\text{exe}} \}
\end{align*}
\]

Here, the effective potential, \( v_{\text{eff}} \), in eq. (1) is essentially similar to the Kohn-Sham effective potential, but we note that the ground state of this model is determined by solving eq. (2) including a two-particle interaction, \( V^{(2)}_{\text{eff}} \), and a Hartree-type mean-field, \( V^{(1)}_{\text{eff}} \). This set of self-consistent equations are determined by a variational method.

To obtain formula for \( v_{\text{eff}}, V^{(1)}_{\text{eff}} \) and \( V^{(2)}_{\text{eff}} \), a key point is how to re-describe Levy's density functional, \( F[n] \), by a model functions. The solution is given below.

\[
\begin{align*}
F[n] &= T_0[n] + V_{\text{exe}}[n] + E_{\text{exe}}[n] \\
T_0[n] &= \langle \Psi | \sum_{ij} \int d^3r \phi_{ij}(r) \left( -\frac{\hbar^2}{2m}\Delta + \phi_{ij}(r)c_{ij\sigma}^\dagger c_{ij\sigma} \right) |\Psi \rangle \\
V_{\text{exe}}[n] &= \frac{1}{2} \int \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} n(r)n(r')d^3rd^3r' + \sum_{ijkl;\sigma\sigma'} \int \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \phi_{ij\sigma}(r)\phi_{ij\sigma'}(r')\phi_{kl\sigma'}(r')\phi_{kl\sigma}(r)d^3rd^3r' \rho^{(2)}(ijkl;\sigma\sigma')
\end{align*}
\]

Here the two-particle density matrix, \( \rho^{(2)}(ijkl;\sigma\sigma') \), is defined using the single-particle density matrix, \( \rho(ij;\sigma) = \langle \Psi | c_{ij\sigma}^\dagger c_{ij\sigma} |\Psi \rangle \), as follows.

\[
\rho^{(2)}(ijkl;\sigma\sigma') = \langle \Psi | c_{ik\sigma}^\dagger c_{kl\sigma'} c_{ij\sigma'} c_{kj\sigma} |\Psi \rangle - \rho(i;\sigma)\rho(j;\sigma')
\]

A residual many-particle interaction, \( \hat{H}_{\text{exe}} \), is a kind of the exchange-correlation correction coming from definitions of both \( E_{\text{exe}}[n] \) and \( v_{\text{eff}}(r) \) and is defined as

\[
\langle \Psi | \hat{H}_{\text{exe}} |\Psi \rangle = E_{\text{exe}}[n] - \int \frac{\delta E_{\text{exe}}}{\delta n(r)} n(r)d^3r
\]

In our new scheme, a summation, \( \sum' \), appearing in two-particle interactions is arbitrary. Thus, our formulation is applicable for description of any type of local interactions including the Hubbard interaction. Although an additional approximation on the new exchange-correlation term, \( E_{\text{exe}} \), is required, our scheme provides the Hubbard model, the Anderson-lattice model etc. starting from DFT without artificial inclusion of the \( U \)-term as performed in the LDA+U approach. If \( \sum' \) is taken for all possible terms, \( E_{\text{exe}}[n] \equiv 0 \). This property may be useful to discuss the v-representability problem remaining in the original Kohn-Sham theory.