

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 $n(\mathbf{r})$ 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 $n(\mathbf{r})$. Then, we can derive a many-body problem describing the model system as follows.

$$\left\{ -\frac{\hbar^2}{2m}\Delta + v_{\text{eff}}(\mathbf{r}) \right\} \phi_{i\sigma}(\mathbf{r}) = \varepsilon_i \phi_{i\sigma}(\mathbf{r}) \quad (1)$$

$$\left\{ \sum_{i\sigma} \varepsilon_i c_{i\sigma}^\dagger c_{i\sigma} + \sum_{ij\sigma} V_{\text{eff}}^{(1)}(ij\sigma) c_{i\sigma}^\dagger c_{j\sigma} + \sum'_{ijkl\sigma\sigma'} V_{\text{eff}}^{(2)}(ijkl; \sigma\sigma') c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{k\sigma'} c_{l\sigma} + \hat{H}_{\text{rxc}} \right\} |\Psi\rangle = E|\Psi\rangle \quad (2)$$

Here, the effective potential, v_{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, $V_{\text{eff}}^{(2)}$, and a Hartree-type mean-field, $V_{\text{eff}}^{(1)}$. This set of self-consistent equations are determined by a variational method.

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

$$F[n] = T_0[n] + V_{\text{ee}}[n] + E_{\text{rxc}}[n] \quad (3)$$

$$T_0[n] = \langle \Psi | \left[\sum_{ij\sigma} \int d^3r \phi_{i\sigma}(\mathbf{r}) \left(-\frac{\hbar^2}{2m} \Delta \right) \phi_{j\sigma}(\mathbf{r}) c_{i\sigma}^\dagger c_{j\sigma} \right] | \Psi \rangle \quad (4)$$

$$V_{\text{ee}}[n] = \frac{1}{2} \int \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} n(\mathbf{r}) n(\mathbf{r}') d^3r d^3r' + \sum'_{ijkl\sigma\sigma'} \frac{1}{2} \int \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \phi_{i\sigma}^*(\mathbf{r}) \phi_{j\sigma'}^*(\mathbf{r}') \phi_{k\sigma'}(\mathbf{r}') \phi_{l\sigma}(\mathbf{r}) d^3r d^3r' \bar{\rho}^{(2)}(ijkl; \sigma\sigma') \quad (5)$$

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

$$\bar{\rho}^{(2)}(ijkl; \sigma\sigma') = \langle \Psi | c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{k\sigma'} c_{l\sigma} | \Psi \rangle - \rho(il; \sigma) \rho(jk; \sigma')$$

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

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

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_{rxc} , 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, $E_{\text{rxc}}[n] \equiv 0$. This property may be useful to discuss the v -representability problem remaining in the original Kohn-Sham theory.

[1] W. Kohn and L.J. Sham, Phys. Rev. **140**, A1133 (1965).[2] M. Levy, Phys. Rev. A **26**, 1200 (1982).