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Kohn–Sham models

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Abstract
To construct an optimization scheme for an extension of the Kohn–Sham approach, I introduce
an operator form of the Coulomb interaction. This form is the sum of quadratic form pairs,
which can be redefined in a self-consistent calculation of a multi-reference density functional
theory. A detailed derivation of the form is given. A fluctuation term introduced in the extended
Kohn–Sham scheme is expressed in this form for regularization. The present procedure also
provides an exact derivation of effective negative interactions in charge fluctuation channels.
Relevance to high-temperature superconductors is discussed.

1. Introduction

A new scheme for the Kohn–Sham approach [1] in
density functional theory [2–5] was proposed by the present
author [6–11]. This formulation uses the energy density
functional by the Levy–Lieb definition [3–5], ensuring
that the N-representation of the density appears in the
simulation. The extension is made by introducing a
correlation term added to the kinetic energy density functional.
Thus the method naturally gives an interacting fermion
system, resulting in a multi-reference density functional
theory. But the present approach differs from other known
methods [13–16] in the sense that the correlation term can be
chosen arbitrarily keeping the N-representable energy density
functional untouched. To solve the problem of how to optimize
the correlation term depending on the system considered, I
need to introduce a controllable form of the correlation term.

Recently, topology of the model space given by extension
of the Kohn–Sham scheme was discovered by the present
author [12]. Definition of the functional derivative of each
energy functional is thus given. The new scheme enables
one to handle multi-reference density functional theory in a
self-consistent manner without any reference calculation. For
this purpose, a new operator form of the Coulomb correlation
term is required. In this paper, I give a detailed derivation
of the quadratic form of the Coulomb operator. The positive
semi-definite form gives a fundamental tool for constructing

a numerical minimization scheme of the energy density
functional. The new form is found to possess a positive part
and a negative part. I will also give a discussion on the effective
negative interactions in charge fluctuation channels, which has
great relevance to high-temperature superconductors.

2. A quadratic form of the Coulomb operator

I now derive a new form of the Coulomb operator. Let $\mathbf{r}_1$
and $\mathbf{r}_2$ be position vectors of two electrons in the spherical
coordinate, which are $\mathbf{r}_1 = (r_1, \theta_1, \phi_1)$ and $\mathbf{r}_2 = (r_2, \theta_2, \phi_2)$.
I introduce notations for distance as $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$, and $\gamma = \cos^{-1}(\mathbf{r}_1 \cdot \mathbf{r}_2/(r_1 r_2))$. Using spherical harmonics $Y_l^m(\theta, \phi)$, an
expansion of $1/r_{12}$ is given as

$$
\begin{aligned}
\frac{1}{r_{12}} &= \frac{1}{\sqrt{r_1^2 + r_2^2 - 2 r_1 r_2 \cos\gamma}} \\
&= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_l^m(\theta_1, \phi_1)^* Y_l^m(\theta_2, \phi_2).
\end{aligned}
\tag{1}
$$

Here, $r_>$ and $r_<$ represent a longer distance and a shorter
distance in r_1 and r_2.

I introduce the electron-field operator $\psi_\sigma^\dagger(\mathbf{r})$, $\psi_\sigma(\mathbf{r})$
with spin σ and the electron density operator $\hat{n}(\mathbf{r}) = \sum_\sigma \psi_\sigma^\dagger(\mathbf{r}) \psi_\sigma(\mathbf{r})$. The Coulomb interaction is given in an

operator form as

$$\hat{V}_{ee} = \frac{1}{2} \int d^3r_1 \, d^3r_2 \, \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \sum_{\sigma,\sigma'} \psi_\sigma^\dagger(\mathbf{r}) \psi_{\sigma'}^\dagger(\mathbf{r}') \psi_{\sigma'}(\mathbf{r}') \psi_\sigma(\mathbf{r})$$

$$= \hat{V}_d + \hat{V}_{SIC}. \tag{2}$$

Here, $\hat{V}_d$ and $\hat{V}_{SIC}$ are a position diagonal term and the self-interaction correction term,

$$\hat{V}_d = \frac{e^2}{2} \int d^3r_1 \, d^3r_2 \, \frac{1}{r_{12}} \hat{n}(\mathbf{r}_1) \hat{n}(\mathbf{r}_2), \tag{3}$$

$$\hat{V}_{SIC} = -\frac{e^2}{2} \int d^3r_1 \, d^3r_2 \, \frac{1}{r_{12}} \sum_\sigma \psi_\sigma^\dagger(\mathbf{r}_1) \psi_\sigma(\mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}_2). \tag{4}$$

Using a complete set of single particle wavefunctions, $\varphi_k(\mathbf{r})$, these operators are re-expressed. These orbitals may be the Kohn–Sham orbitals. Due to the orthogonality of $\varphi_k(\mathbf{r})$, I can introduce creation and annihilation operators, $c_{k,\sigma}^\dagger$ and $c_{k,\sigma}$. First, I note a unitary transformation:

$$\psi_\sigma^\dagger(\mathbf{r}) = \sum_k \varphi_k^*(\mathbf{r}) c_{k,\sigma}^\dagger, \qquad \psi_\sigma(\mathbf{r}) = \sum_k \varphi_k(\mathbf{r}) c_{k,\sigma}. \tag{5}$$

Using the expansion in equation (1), I have the next expression for $\hat{V}_d$:

$$\hat{V}_d = \int d^3r_1 \, d^3r_2 \, \frac{1}{r_{12}} \hat{n}(\mathbf{r}_1) \hat{n}(\mathbf{r}_2)$$

$$= \sum_{l=0}^\infty \sum_{m=-l}^l \sum_{k_1,k_2,k_3,k_4} \sum_{\sigma,\sigma'} \frac{2\pi e^2}{2l+1} \int r_1^2 \, dr_1 \, r_2^2 \, dr_2 \, \frac{r_<^l}{r_>^{l+1}}$$

$$\times \int d\theta_1 \, d\phi_1 \, Y_l^m(\theta_1, \phi_1)^* \varphi_{k_1}^*(\mathbf{r}_1) \varphi_{k_2}(\mathbf{r}_1) \sin\theta_1 c_{k_1,\sigma}^\dagger c_{k_2,\sigma}$$

$$\times \int d\theta_2 \, d\phi_2 \, Y_l^m(\theta_2, \phi_2) \varphi_{k_3}^*(\mathbf{r}_2) \varphi_{k_4}(\mathbf{r}_2) \sin\theta_2 c_{k_3,\sigma'}^\dagger c_{k_4,\sigma'} \tag{6}$$

$$= \int_0^\infty dp \sum_{l=0}^\infty \sum_{m=-l}^l X_{plm} \left\{ \hat{Y}_{plm}^\dagger \hat{Y}_{plm} - \hat{Z}_{plm}^\dagger \hat{Z}_{plm} \right\}. \tag{7}$$

This is the required form. Here X_{plm} is a constant and $\hat{Y}_{plm}$ and $\hat{Z}_{plm}$ are single particle operators. Since the Coulomb operator is positive semi-definite, our new form obtained as an identity is a positive semi-definite form.

To derive the above expression, I introduce a complete set $g_{p,l}(r)$ of radial functions:

$$\int_0^\infty dr_1 g_{p,l}(r_1) g_{q,l}(r_1) = 2\pi \delta(p - q). \tag{8}$$

The next equation holds for arbitrary $\Phi_1(r)$ and $\Phi_2(r)$:

$$\int_0^\infty r_1^2 \, dr_1 \int_0^\infty r_2^2 \, dr_2 \, \frac{r_<^l}{r_>^{l+1}} \Phi_1(r_1) \Phi_2(r_2)$$

$$= \int_0^\infty dr_1 \, r_1^2 \Phi_1(r_1) \int_{r_1}^\infty dr_2 \, r_2^2 \frac{r_1^l}{r_2^{l+1}} \Phi_2(r_2)$$

$$+ \int_0^\infty dr_2 \, r_2^2 \Phi_2(r_2) \int_{r_2}^\infty dr_1 \, r_1^2 \frac{r_2^l}{r_1^{l+1}} \Phi_1(r_1). \tag{9}$$

I insert the next expansions in two terms of the above expression:

$$r_1^2 \Phi_1(r_1) = \int_0^\infty dp \, f_{1,l}(p) g_{p,l}(r_1) \tag{10}$$

$$\int_{r_1}^\infty dr_2 \, r_2^2 \frac{r_1^l}{r_2^{l+1}} \Phi_2(r_2) = \int_0^\infty dq \, f_{2,l}^I(q) g_{q,l}(r_1). \tag{11}$$

Here, coefficients are given by

$$f_{1,l}(p) = \int_0^\infty dr_1 \, g_{p,l}(r_1) r_1^2 \Phi_1(r_1) \tag{12}$$

$$f_{2,l}^I(q) = \int_0^\infty dr_1 \, g_{q,l}(r_1) \int_{r_1}^\infty dr_2 \, r_2^2 \frac{r_1^l}{r_2^{l+1}} \Phi_2(r_2)$$

$$= \int_0^\infty dr_2 \, r_2^2 \frac{1}{r_2^{l+1}} \int_0^{r_2} dr_1 \, r_1^l g_{q,l}(r_1) \Phi_2(r_2)$$

$$= \int_0^\infty dr_2 \, \bar{g}_{q,l}(r_2) r_2^2 \Phi_2(r_2). \tag{13}$$

Then, I have

$$\int_0^\infty dr_1 \, r_1^2 \Phi_1(r_1) \int_{r_1}^\infty dr_2 \, r_2^2 \frac{r_1^l}{r_2^{l+1}} \Phi_2(r_2)$$

$$= \int_0^\infty dr_1 \int_0^\infty dp \, f_{1,l}(p) g_{p,l}(r_1) \int_0^\infty dq \, f_{2,l}^I(q) g_{q,l}(r_1)$$

$$= 2\pi \int_0^\infty dp \, f_{1,l}(p) f_{2,l}^I(p) \tag{14}$$

$$\int_0^\infty dr_2 \, r_2^2 \Phi_2(r_2) \int_{r_2}^\infty dr_1 \, r_1^2 \frac{r_2^l}{r_1^{l+1}} \Phi_1(r_1)$$

$$= \int_0^\infty dr_2 \int_0^\infty dp \, f_{2,l}(p) g_{p,l}(r_2) \int_0^\infty dq \, f_{1,l}^I(q) g_{q,l}(r_2)$$

$$= 2\pi \int_0^\infty dp \, f_{2,l}(p) f_{1,l}^I(p). \tag{15}$$

I may write equation (6) in the next form.

$$\hat{V}_d = \sum_{l=0}^\infty \sum_{m=-l}^l \int_0^\infty dp \, \frac{(2\pi e)^2}{2l+1} \sum_{k_1,k_2,k_3,k_4} \sum_{\sigma,\sigma'}$$

$$\times \{ c_{k_1,\sigma}^\dagger a_{k_2,k_1}(p,l,m)^* c_{k_2,\sigma} \cdot c_{k_3,\sigma'}^\dagger b_{k_3,k_4}(p,l,m) c_{k_4,\sigma'}$$

$$+ c_{k_1,\sigma}^\dagger b_{k_2,k_1}(p,l,m)^* c_{k_2,\sigma} \cdot c_{k_3,\sigma'}^\dagger a_{k_3,k_4}(p,l,m) c_{k_4,\sigma'}^\dagger \}$$

$$= \sum_{l=0}^\infty \sum_{m=-l}^l \int_0^\infty dp \, \frac{(2\pi e)^2}{2l+1} \sum_{k_1,k_2,k_3,k_4} \sum_{\sigma,\sigma'}$$

$$\times \{ (c_{k_2,\sigma}^\dagger a_{k_2,k_1}(p,l,m) c_{k_1,\sigma})^\dagger \cdot c_{k_3,\sigma'}^\dagger b_{k_3,k_4}(p,l,m) c_{k_4,\sigma'}$$

$$+ (c_{k_2,\sigma}^\dagger b_{k_2,k_1}(p,l,m) c_{k_1,\sigma})^\dagger \cdot c_{k_3,\sigma'}^\dagger a_{k_3,k_4}(p,l,m) c_{k_4,\sigma'}^\dagger \}. \tag{16}$$

This expression is easily rewritten in a summation of quadratic forms, which is the final form of equation (7). Definitions of the operators are given as follows:

$$\hat{Y}_{plm} = \sum_{k_1,k_2,\sigma} c_{k_1,\sigma}^\dagger f_{+,k_1,k_2}(p,l,m) c_{k_2,\sigma}, \tag{17}$$

$$\hat{Z}_{plm} = \sum_{k_1,k_2,\sigma} c_{k_1,\sigma}^\dagger f_{-,k_1,k_2}(p,l,m) c_{k_2,\sigma}, \tag{18}$$

$$f_{+,k_1,k_2}(p,l,m) = \frac{1}{\sqrt{2}} (a_{k_1,k_2}(p,l,m) + b_{k_1,k_2}(p,l,m)), \tag{19}$$

$$f_{-,k_1,k_2}(p,l,m) = \frac{1}{\sqrt{2}} (a_{k_1,k_2}(p,l,m) - b_{k_1,k_2}(p,l,m)), \tag{20}$$

$$a_{k_1,k_2}(p,l,m) = \int d^3r \, g_{p,l}(r) Y_l^m(\theta,\phi) \phi_{k_1}^*(\mathbf{r}) \phi_{k_2}(\mathbf{r}), \quad (21)$$

$$b_{k_1,k_2}(p,l,m) = \int d^3r \, \bar{g}_{p,l}(r) Y_l^m(\theta,\phi) \phi_{k_1}^*(\mathbf{r}) \phi_{k_2}(\mathbf{r}), \quad (22)$$

$$\bar{g}_{p,l}(r) = \frac{1}{r^{l+1}} \int_0^r dr' \, (r')^l g_{p,l}(r'). \quad (23)$$

The set of functions $g_{p,l}(r)$ gives the complete basis of the radial function. One possible set may be given by the spherical Bessel functions as

$$g_{p,l}(r) = 2pr j_l(pr) = (-1)^l \cdot 2 \cdot \frac{r^{l+1}}{p^l} \left(\frac{d}{r\,dr} \right)^l \frac{\sin pr}{r}. \quad (24)$$

In this case, the factor X_{plm} becomes

$$X_{plm} = \frac{(2\pi e)^2}{2l+1}. \quad (25)$$

but we can use the same $g_{p,l}(r)$ for any l.

The form in equation (7) is centered at a point in space. If we have a crystal, we can make use of the Dirac character [17] to obtain the operator having the crystal symmetry.

3. A fluctuation term giving effective interactions

The new form can be utilized in the extended Kohn–Sham scheme [6, 10]. Actually, I can introduce a fluctuation term $\langle \Psi | \hat{V}_{X_i} | \Psi \rangle$ with the self-interaction correction $\hat{V}_{SIC}$ in the next form:

$$\langle \Psi | \hat{V}_{X_i} | \Psi \rangle = \sum_n X_i^{(n)} \langle \Psi | \{ (\hat{Y}_i^{(n)} - \langle \hat{Y}_i^{(n)} \rangle)^\dagger (\hat{Y}_i^{(n)} - \langle \hat{Y}_i^{(n)} \rangle)$$
$$- (\hat{Z}_i^{(n)} - \langle \hat{Z}_i^{(n)} \rangle)^\dagger (\hat{Z}_i^{(n)} - \langle \hat{Z}_i^{(n)} \rangle) \} | \Psi \rangle$$
$$+ \langle \Psi | \hat{V}_{SIC} | \Psi \rangle. \quad (26)$$

Here, I use an index n to represent a set $\{p, l, m\}$ symbolically and thus the summation on n denotes the integration with respect to p and the summation on l and m. The reason why I number the fluctuation term as X_i is because a sequence of models given by the X_i terms is prepared in order to have a derivative of the energy functional. Thus the energy functional of the new extended Kohn–Sham scheme is

$$G_{X_i}[\Psi] = \langle \Psi | \hat{T} + \hat{V}_{X_i} | \Psi \rangle - \min_{\Psi' \to n_\Psi(\mathbf{r})} \langle \Psi' | \hat{T} + \hat{V}_{X_i} | \Psi' \rangle$$
$$+ F[n_\Psi] + \int d^3r \, v_{ext}(\mathbf{r}) n_\Psi(\mathbf{r})$$
$$= \langle \Psi | \hat{T} + \hat{V}_{X_i} | \Psi \rangle + \frac{1}{2} \int \frac{n_\Psi(\mathbf{r}) n_\Psi(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r \, d^3r'$$
$$+ E_{rxc}[n_\Psi] + \int d^3r \, v_{ext}(\mathbf{r}) n_\Psi(\mathbf{r}). \quad (27)$$

In the above definition, the kinetic energy operator $\hat{T}$ is

$$\hat{T} = -\frac{\hbar^2}{2m} \int d^3r \sum_\sigma \lim_{\mathbf{r}' \to \mathbf{r}} \psi_\sigma^\dagger(\mathbf{r}') \Delta_\mathbf{r} \psi_\sigma(\mathbf{r}), \quad (28)$$

with the electron mass m, and the universal energy functional $F[n]$ is given by

$$F[n] = \min_{\Psi' \to n} \langle \Psi' | \hat{T} + \hat{V}_{ee} | \Psi' \rangle. \quad (29)$$

To represent the Ψ dependence of the density, I use a notation $n_\Psi(\mathbf{r}) = \langle \Psi | \hat{n}(\mathbf{r}) | \Psi \rangle$. The definition of $E_{rxc}[n]$ is given by equation (27) itself.

In the process of searching for the model, strength of $X_i^{(n)}$ is a relevant variable. In equation (26), $X_i^{(n)}$ acts as a set of weights for the fluctuation of physical operators $\hat{Y}_i^{(n)}$, $\hat{Z}_i^{(n)}$, which are non-Hermitian in general. Note that the whole operation of $\hat{V}_{X_i}$ is Hermitian as well as $\hat{V}_d$. It is also important to find that the fluctuation term is always counted from a density $n_\Psi(\mathbf{r})$ in the simulation. Thus, instability against part of the fluctuation term implies that a tested $|\Psi\rangle$ is improper as a variational state appearing in the process of searching for the true ground state. Now, if each term in equation (26) is identical to the corresponding term given in the previous section and the interaction strength is the same as X_{plm}, and if the self-interaction correction terms are properly taken into account in the determination of the basis $\varphi_k(\mathbf{r})$, the universal energy density functional is reproduced when we count E_{rxc}. In other words, when we perfectly introduce all of the relevant fluctuations in the simulation process, the residual exchange–correlation energy vanishes:

$$E_{rxc}[n_\Psi] = F[n_\Psi] - \min_{\Psi' \to n_\Psi(\mathbf{r})} \langle \Psi' | \hat{T} + \hat{V}_{X_i} | \Psi' \rangle$$
$$- \frac{1}{2} \int \frac{n_\Psi(\mathbf{r}) n_\Psi(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r \, d^3r'$$
$$= F[n_\Psi] - \min_{\Psi' \to n_\Psi(\mathbf{r})} \langle \Psi' | \hat{T} + \hat{V}_d + \hat{V}_{SIC} | \Psi' \rangle = 0. \quad (30)$$

Before ending this section, I should comment on the arbitrariness and uniqueness of the fluctuation term given by the new form. The expansion given in equation (16) is uniquely determined once we fix a set $g_{p,l}(r)$. Seemingly, the equation has dependence on a basis given by the Kohn–Sham orbitals $\phi_k(\mathbf{r})$. However, the definition of $a_{k_1,k_2}(p,l,m)$ and $b_{k_1,k_2}(p,l,m)$ implies that these coefficients are matrix elements or projections of two waves given by $g_{p,l}(r) Y_l^m(\theta,\phi)$ and $\bar{g}_{p,l}(r) Y_l^m(\theta,\phi)$ with respect to $\{\phi_k(\mathbf{r})\}$. Indexes in the summation appearing in $\hat{Y}_{plm}$ and $\hat{Z}_{plm}$ operators run over the whole set of Kohn–Sham orbitals. In this sense, the final expression of the extended Kohn–Sham scheme requires a full configuration interaction calculation and gives no reduction in calculation steps. However, we hope that there is a big advantage in this expansion. We need to introduce a cut-off for each summation in an actual simulation. Efficiency of the series expansion can be evaluated when it is given as a converging series. There are two factors determining the speed of convergence. One is the expansion coefficients, X_{plm}, $a_{k_1,k_2}(p,l,m)$ and $b_{k_1,k_2}(p,l,m)$. Another is the expectation value of each fluctuation or each correlation function given by $\hat{Y}_{plm}$ and $\hat{Z}_{plm}$. To utilize a well converged set of Kohn–Sham orbitals will enhance the speed of convergence in each series expansion in $\hat{V}_{X_i}$. Thus, we may cut the doubled infinite sum off and approximate it by a finite series in a practical

calculation. For this purpose, we can and should optimize $g_{p,l}(r)$. The arbitrariness of $g_{p,l}(r)$ is another important point for the new quadratic form. Depending on the basis set $\{\phi_k(\mathbf{r})\}$, we can adjust $g_{p,l}(r)$ to have a rapidly converging series.

4. Relevance of the negative term for high-temperature superconductivity

To consider the relevance of the negative $\hat{Z}_{plm}$ term, let us treat some simplified test cases. First, if $l = m = 0$ and if $g_{p,0}(r)$ is a constant, we have $\bar{g}_{p,0}(r) = g_{p,0}(r)$. Then, $\hat{Z}_{p,0,0}$ is identically a zero operator. In this case we inevitably have k-diagonal terms in the double k summation appearing in $\hat{Y}_{p,0,0}$ operators. When we introduce the localized electron orbital, e.g. the Wannier representation, the index k is naturally interpreted as an index for the position of the Wannier center and the quantum level at the site. Thus, the diagonal terms correspond to the so-called on-site terms. The vanishing $\hat{Z}_{p,0,0}$ term means that only on-site repulsion appears and no diagonal attractive on-site (on a single orbital) interaction arises from the Coulomb positive definite form.

Assume that a quasi-two-dimensional electron system on a tetragonal crystal structure has a multi-band structure with two Fermi pockets around $(\frac{\pi}{a}, 0, \kappa)$ and $(0, \frac{\pi}{a}, \kappa)$. The constant a is the lattice constant. Quasi-two-dimensionality allows us to consider wavefunctions on a square lattice of relevant atoms. We select two of them, which are close in real space, and call them $\varphi_{(\mathbf{k},\kappa)}(\mathbf{r})$ with a two-dimensional wavevector $\mathbf{k} = (\frac{\pi}{a}, 0)$ or $(0, \frac{\pi}{a})$. Let me introduce the notation $k_1 = ((\frac{\pi}{a}, 0), \kappa)$, $k_2 = ((0, \frac{\pi}{a}), \kappa)$. The Bloch phases of $\varphi_{k_1}(\mathbf{r})$ and $\varphi_{k_2}(\mathbf{r})$ create a staggered profile of a phase factor from $\varphi_{k_1}^* \varphi_{k_2}$ on the square lattice. Thus, a channel with $l = 2$ is relevant, if we consider a center surrounded by four atomic sites.

If we introduce $g_{p,l}(r) = a \cos(pr)$ with a properly chosen p, we have

$$\bar{g}_{p,l}(r) = a' \left\{ \frac{\sin(kr)}{kr} + \frac{2}{(kr)^2} \left(\cos(kr) - \frac{\sin(kr)}{kr} \right) \right\}.$$

Here, a and a' are constants. The difference in $g_{p,l}(r)$ and $\bar{g}_{p,l}(r)$ immediately implies finite differences between $a_{k_1,k_2}(p, l, m)$ and $b_{k_1,k_2}(p, l, m)$. Thus it can be shown that $\hat{Z}_{p2m}$, which is constructed from the wavefunctions $\varphi_{k_1}(\mathbf{r})$ and $\varphi_{k_2}(\mathbf{r})$, creates an electron pair hopping term. The term is written as $-f_{12} f_{21}^* c_{k_1,\uparrow}^\dagger c_{k_1,\downarrow}^\dagger c_{k_2,\downarrow} c_{k_2,\uparrow}$ with

$$f_{12} = \frac{1}{\sqrt{2}} (a_{k_1,k_2}(p, l, m) - b_{k_1,k_2}(p, l, m)) \neq 0, \quad (31)$$

$$f_{21} = \frac{1}{\sqrt{2}} (a_{k_2,k_1}(p, l, m) - b_{k_2,k_1}(p, l, m)) \neq 0. \quad (32)$$

This attractive channel may be relevant for a superconductor with two-dimensional atomic structures, e.g. the copper oxide plane in cuprates and the iron-pnictide plane in oxypnictides, to stabilize the superconductivity.

It must be noted that the above term is a fluctuation term, so that only a negative channel can be developed without any fluctuation in the other positive channel. This is another relevant point for the present discussion. In the extended Kohn–Sham scheme, these pair hopping terms actually originate from the exchange–correlation term. The Hartree term, which is the mean-field term, is self-consistently determined, taking the diagonal repulsion between electrons into account.

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