Scheme for the energy-band calculation under the external magnetic field

Katsuhiko Higuchi [a,1], Masahiko Higuchi [b],

[a] *Department of Electrical Engineering, Hiroshima University, Higashi-Hiroshima 739-8527, Japan*
[b] *Department of Physics, Shinshu University, Matsumoto 390-8621, Japan*

Abstract

In the framework of the current-density functional theory (CDFT), we propose three kinds of approximation schemes for the exchange-correlation energy functional on the basis of the coupling-constant expression. These should be called the CDFT version of the local-density approximation, average-density approximation and weighted-density approximation. The validity of these approximations is estimated by using the sum rules which have recently been derived. We also discuss the symmetry of the noninteracting fictitious system of the CDFT.

Key words: current-density functional theory; exchange-correlation energy functional; coupling-constant expression;

The current-density functional theory (CDFT)[1] and its relativistic version, the relativistic current- and spin-density functional theory (RCSDFT)[2,3], provide a promising method for calculating the electronic structure of the system to which an external magnetic field is applied. For the practical use, the approximate forms of the exchange-correlation energy functional $E_{xc}[\rho, \boldsymbol{j}_p]$ must be developed in the applicable form. Here $\rho(\boldsymbol{r})$ and $\boldsymbol{j}_p(\boldsymbol{r})$ respectively denote the electron density and the paramagnetic current density, which are the basic variables in the CDFT. Two strategies are conceived for developing the approximate forms of $E_{xc}[\rho, \boldsymbol{j}_p]$. One is to utilize the exact conditions fulfilled by $E_{xc}[\rho, \boldsymbol{j}_p]$ as sum rules which should be satisfied by the approximate forms[4]. This strategy is similar to that used in the generalized gradient approximation (GGA). The exchange energy functional has already been constructed in accordance with this strategy[5]. Another strategy is based on the coupling-constant expression of $E_{xc}[\rho, \boldsymbol{j}_p]$. In the conventional DFT, the local density approximation (LDA), the average-density approximation (ADA) and the weighted-density approximation (WDA) have been developed on the basis of the coupling-constant expression for $E_{xc}[\rho]$. In this paper, we employ the latter strategy and develop three kinds of approximation schemes for $E_{xc}[\rho, \boldsymbol{j}_p]$, which should be called the CDFT-version of the LDA, ADA and WDA.

In the conventional DFT, the exact expression for $E_{xc}[\rho]$ was derived successfully by using the coupling-constant integration technique. Also in the CDFT, the exact expression can be derived by means of the same technique. We have

$$E_{xc}[\rho, \boldsymbol{j}_p] = \frac{e^2}{2} \iint \frac{\rho(\boldsymbol{r})\rho(\boldsymbol{r}')\{\bar{g}(\boldsymbol{r}, \boldsymbol{r}'; [\rho, \boldsymbol{j}_p]) - 1\}}{|\boldsymbol{r} - \boldsymbol{r}'|} \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{r}', \quad (1)$$

where $\bar{g}(\boldsymbol{r}, \boldsymbol{r}'; [\rho, \boldsymbol{j}_p])$ is the coupling-constant-averaged pair correlation function. The exact expression (1) is similar to that of the DFT, but the coupling-constant-averaged pair correlation function is the functional of both $\rho(\boldsymbol{r})$ and $\boldsymbol{j}_p(\boldsymbol{r})$ in the CDFT. Due to the gauge invariance, $E_{xc}[\rho, \boldsymbol{j}_p]$ depends on $\boldsymbol{j}_p(\boldsymbol{r})$ only through the vorticity $\boldsymbol{\nu}(\boldsymbol{r})$ defined by $\boldsymbol{\nu}(\boldsymbol{r}) \equiv \nabla \times \left\{ \boldsymbol{j}_p(\boldsymbol{r}) / \rho(\boldsymbol{r}) \right\}$ [1,6]. Therefore, Eq. (1) can also be referred to as the functional of $\rho(\boldsymbol{r})$ and $\boldsymbol{\nu}(\boldsymbol{r})$.

The LDA scheme is obtained if the exchange-correlation hole is replaced by the corresponding ho-

[1] E-mail:khiguchi@hiroshima-u.ac.jp

mogeneous electron liquid expression and evaluated at the local densities $\rho(\boldsymbol{r})$ and $\boldsymbol{\nu}(\boldsymbol{r})$. We have

$$E_{xc}^{LDA}[\rho,\boldsymbol{j}_p] = E_{xc}^{'LDA}[\rho,\boldsymbol{\nu}] \tag{2}$$
$$= \frac{e^2}{2}\iint \frac{\rho(\boldsymbol{r})^2}{|\boldsymbol{r}-\boldsymbol{r}'|}\left\{\bar{g}^{hom}(|\boldsymbol{r}-\boldsymbol{r}'|,\rho(\boldsymbol{r}),\boldsymbol{\nu}(\boldsymbol{r}))-1\right\}\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{r}',$$

where $\bar{g}^{hom}(|\boldsymbol{r}-\boldsymbol{r}'|,\rho(\boldsymbol{r}),\boldsymbol{\nu}(\boldsymbol{r}))$ is the coupling-constant-averaged pair correlation function of the homogeneous electron liquid. Equation (2) is just the LDA expression for the exchange-correlation energy functional of the CDFT. In Eq. (2) $\bar{g}^{hom}(|\boldsymbol{r}-\boldsymbol{r}'|,\rho(\boldsymbol{r}),\boldsymbol{\nu}(\boldsymbol{r}))$ can be obtained from the Fourier transform of the coupling-constant-averaged static structure factor $\bar{S}^{hom}(\boldsymbol{q})$ of the homogeneous electron liquid. Vignale and co-workers have evaluated $\bar{S}^{hom}(\boldsymbol{q})$ with respect to the ground-state of the homogeneous electron liquid in the uniform magnetic field[7,8]. Thus, it is possible to perform energy-band calculations within the LDA by utilizing the knowledge of the homogeneous electron liquid in the uniform magnetic field.

In the ADA, $\bar{g}(\boldsymbol{r},\boldsymbol{r}';[\rho,\boldsymbol{j}_p])$ is borrowed from the homogeneous electron liquid and evaluated at the averaged densities $\bar{\rho}(\boldsymbol{r})$ and $\bar{\boldsymbol{\nu}}(\boldsymbol{r})$. Furthermore the prefactor $\rho(\boldsymbol{r}')$ is replaced by the averaged density $\bar{\rho}(\boldsymbol{r})$. We are led to the ADA expression as

$$E_{xc}^{ADA}[\rho,\boldsymbol{j}_p] = E_{xc}^{'ADA}[\rho,\boldsymbol{\nu}] \tag{3}$$
$$= \frac{e^2}{2}\iint \frac{\rho(\boldsymbol{r})\bar{\rho}(\boldsymbol{r})}{|\boldsymbol{r}-\boldsymbol{r}'|}\left\{\bar{g}^{hom}(|\boldsymbol{r}-\boldsymbol{r}'|,\bar{\rho}(\boldsymbol{r}),\bar{\boldsymbol{\nu}}(\boldsymbol{r}))-1\right\}\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{r}',$$

where

$$\bar{\rho}(\boldsymbol{r}) = \int \mathrm{d}\boldsymbol{r}' w(|\boldsymbol{r}-\boldsymbol{r}'|,\bar{\rho}(\boldsymbol{r}'),\bar{\boldsymbol{\nu}}(\boldsymbol{r}'))\rho(\boldsymbol{r}'), \tag{4}$$

$$\bar{\boldsymbol{\nu}}(\boldsymbol{r}) = \int \mathrm{d}\boldsymbol{r}' w(|\boldsymbol{r}-\boldsymbol{r}'|,\bar{\rho}(\boldsymbol{r}'),\bar{\boldsymbol{\nu}}(\boldsymbol{r}'))\boldsymbol{\nu}(\boldsymbol{r}'). \tag{5}$$

$w(|\boldsymbol{r}-\boldsymbol{r}'|,\bar{\rho}(\boldsymbol{r}'),\bar{\boldsymbol{\nu}}(\boldsymbol{r}'))$ is the weight function to be determined.

In the WDA, one replaces $\bar{g}(\boldsymbol{r},\boldsymbol{r}';[\rho,\boldsymbol{j}_p])$ with that of the homogeneous electron liquid also, but the prefactor is kept the exact density $\rho(\boldsymbol{r}')$. The WDA expression is given by

$$E_{xc}^{WDA}[\rho,\boldsymbol{j}_p] = E_{xc}^{'WDA}[\rho,\boldsymbol{\nu}] \tag{6}$$
$$= \frac{e^2}{2}\iint \frac{\rho(\boldsymbol{r})\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}\left\{\bar{g}^{hom}(|\boldsymbol{r}-\boldsymbol{r}'|,\tilde{\rho}(\boldsymbol{r}),\tilde{\boldsymbol{\nu}}(\boldsymbol{r}))-1\right\}\mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{r}'.$$

The density arguments of $\bar{g}^{hom}(|\boldsymbol{r}-\boldsymbol{r}'|,\rho(\boldsymbol{r}),\boldsymbol{\nu}(\boldsymbol{r}))$ are replaced by the weighted densities $\tilde{\rho}(\boldsymbol{r})$ and $\tilde{\boldsymbol{\nu}}(\boldsymbol{r})$, which are determined by requiring the following sum rule to be satisfied for each $\boldsymbol{r}$:

$$\int \mathrm{d}\boldsymbol{r}'\rho(\boldsymbol{r}')\left\{\bar{g}^{hom}(|\boldsymbol{r}-\boldsymbol{r}'|,\tilde{\rho}(\boldsymbol{r}),\tilde{\boldsymbol{\nu}}(\boldsymbol{r})-1)\right\} = -1. \tag{7}$$

It must be stressed again that the ADA and WDA schemes as well as the LDA can not be defined until the exchange-correlation energy functional $E_{xc}[\rho,\boldsymbol{j}_p]$ is given in an exact form (1). In the similar way to the LDA calculations, the actual energy-band calculations are feasible in the ADA and WDA because the knowledge of $\bar{g}^{hom}(|\boldsymbol{r}-\boldsymbol{r}'|,\rho(\boldsymbol{r}),\boldsymbol{\nu}(\boldsymbol{r}))$ can also be obtained from the homogeneous electron liquid in the uniform magnetic field. So far, the available form of $\bar{g}^{hom}(|\boldsymbol{r}-\boldsymbol{r}'|,\rho(\boldsymbol{r}),\boldsymbol{\nu}(\boldsymbol{r}))$ has been restricted to the random phase approximation (RPA)[7,8]. It is possible to introduce the STLS theory into the present expression of the CDFT as an effective attempt beyond the RPA.

The LDA expression violates most of sum rules derived from the nonuniform coordinate scalings though it obeys sum rules from the uniform coordinate scaling. On the other hand, the ADA and WDA expressions potentially satisfy more sum rules than the LDA if the averaged densities and the weighted densities are determined appropriately[4]. Judging from not only the nonlocality of the exchange-correlation hole but also the sum rules satisfied, we may expect that the ADA and WDA improve on the LDA as to the accuracy.

At the end of this paper, we have a brief discussion concerning the spatial symmetry of the fictitious system of the CDFT. The magnetic Bloch electrons of the fictitious system have the same symmetry as the real system. The commutative translation operators form a ray group with a factor system which depends on the external magnetic field. Thus, the magnetic Bloch function, which corresponds to the basis function of the irreducible multiplier representation of the ray group, depends on both the direction and strength of the magnetic field[6]. Both the knowledge of the magnetic Bloch function and the approximation schemes proposed here are indispensable for the practical energy-band calculations.

References

[1] G. Vignale, M. Rasolt, Phys. Rev. Lett. **59** (1987) 2360; Phys. Rev. B **37** (1988) 10685.

[2] M. Higuchi, A. Hasegawa, J. Phys. Soc. Jpn. **66** (1997) 149; *ibid.* **67** (1998) 2037.

[3] H. Eschrig, G. Seifert, P. Ziesche, Solid State Commun. **56** (1985) 777.

[4] M. Higuchi, K. Higuchi, to appear in Phys. Rev. B.

[5] K. Higuchi, M. Higuchi, Physica B **312-313** (2002) 534.

[6] K. Higuchi, M. Higuchi, Physica B **284-288** (2000) 1193; K. Higuchi, M. Higuchi, in preparation.

[7] G. Vignale, M. Rasolt, D. J. W. Geldart, Phys. Rev. B **37** (1988) 2502.

[8] P. Skudlarski, G. Vignale, Phys. Rev. B **48** (1993) 8547.