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2008 J. Phys.: Condens. Matter 20 385202

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# Rigorous description of exchange–correlation energy of many-electron systems

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Received 18 May 2008, in final form 31 July 2008

Published 21 August 2008

Online at [stacks.iop.org/JPhysCM/20/385202](http://stacks.iop.org/JPhysCM/20/385202)

## Abstract

With the eigenfunctional theory, we study a general interacting electron system, and give a rigorous expression of its ground state energy, which is composed of two parts: one part is contributed by the non-interacting electrons, and the other one is represented by the correlation functions that are controlled by the electron correlation. Moreover, according to the rigorous expression of the ground state energy, an effective scheme beyond the local density approximation of the density functional theory is proposed. As a simple example for a spin-1/2 XXZ chain, under the linear approximation in solving the equation of the phase field, the ground state energy obtained by the present scheme is quite close to that of the Bethe ansatz.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

The electron correlation plays an important role in the description of quantum many-electron systems. According to the electron correlation strength, the systems are approximately divided into two categories: one is called weakly correlated electron systems, and the other one is called strongly correlated electron systems [1]. The former can be approximately described by the usual quasiparticle schemes [2, 3], while the latter has to be represented by new schemes beyond the usual quasiparticle description.

The Hohenberg–Kohn–Sham (HKS) density functional theory [4, 5] opens a new era in description of the quantum many-electron systems, and it and its generalizations [6] are extensively applied in physics and chemistry. However, the rigorous expression of the exchange–correlation energy in the HKS density functional theory is unknown, and the local density approximation (LDA) of the Kohn–Sham scheme plays a central role in calculating the ground state energy of the systems. In general, for the weakly correlated

systems, the result of the LDA is accurately in agreement with experimental data, but for the strongly correlated systems it is unreliable because of the strong electron correlation.

In contrast to the Kohn–Sham scheme of the density functional theory, we use the eigenfunctional theory to study a general quantum many-electron system [7], and give a rigorous expression of the ground state energy, especially the correlation energy. Moreover, according to this rigorous form of the ground state energy, the correlation energy part can be well defined, and a more effective method beyond the LDA is proposed.

This paper is arranged as follows. In section 2 we describe the general formalism of the eigenfunctional theory for calculating the ground state energy of a quantum many-electron system with the Coulomb interaction in three dimensions. To show the effectiveness of our general method, in section 3 we apply it to the spin- $\frac{1}{2}$  XXZ chain to study its ground state energy and the asymptotic behavior of the Green function and the spin–spin correlation function. We conclude in section 4 with some discussions.

## 2. General formalism

The Hamiltonian of a quantum many-electron system can be generally written down,

$$\hat{H} = \hat{H}_0 + \frac{e^2}{2} \int d^3x d^3x' V(x-x') \hat{\rho}(x) \hat{\rho}(x'), \quad (1)$$

where  $\hat{H}_0 = \sum_{\sigma} \int d^3x \hat{\psi}_{\sigma}^{\dagger}(x) (\frac{\hat{p}^2}{2m} + U(x)) \hat{\psi}_{\sigma}(x)$  is the Hamiltonian of the non-interacting electrons,  $\hat{\psi}_{\sigma}^{\dagger}(x)$  ( $\hat{\psi}_{\sigma}(x)$ ) are the creation (annihilation) operators of the electrons with spin label  $\sigma$  at the coordinate  $\mathbf{x}$ ,  $\hat{\rho}(x) = \sum_{\sigma} \hat{\psi}_{\sigma}^{\dagger}(x) \hat{\psi}_{\sigma}(x)$  is the density operator of the electrons, and  $U(x)$  is an external potential. The last term represents the electron Coulomb interaction, and it induces the electron correlation effect, which makes the problem hard to treat. In the usual mean-field theory [8, 9] the (effective) Coulomb interaction is treated as a perturbation parameter, while in the density functional theory it is incorporated into the exchange–correlation energy. However, if the electron correlation is strong, the results obtained by the mean-field theory and the LDA of the density functional theory are unreliable, and the electron Coulomb interaction has to be accurately treated.

With the eigenfunctional theory, the partition function of the system reads [7]

$$Z = \int D\psi^* D\psi D\rho D\phi e^{\frac{i}{\hbar} S}, \quad (2)$$

$$S = \sum_{\sigma} \int d^3x dt \psi_{\sigma}^*(x, t) \hat{M}(x, t) \psi_{\sigma}(x, t) + W[\rho, \phi],$$

where  $W[\rho, \phi] = \int d^3x dt \phi(x, t) \rho(x, t) - \frac{e^2}{2} \int d^3x d^3x' V(x-x') \rho(x, t) \rho(x', t)$ ,  $\hat{M}(x, t) = i\hbar \partial_t + \mu - \frac{\hat{p}^2}{2m} - U(x) - \phi(x, t)$  is the electron propagator operator in the new Hilbert space, and  $\mu$  is the chemical potential. The Lagrange multiplier field  $\phi(x, t)$  is introduced to decouple the electron interaction; in the meantime the original Hilbert space is mapped into a new Hilbert space, in which the electrons are non-interacting, and moving in a fluctuating potential produced by  $\phi(x, t)$ .

In general, the eigenequation of the electron propagator operator reads [10, 7]

$$\hat{M}(x, t) \Psi_{\sigma k \omega}(x, t; [\phi]) = E_{\sigma k \omega}[\phi] \Psi_{\sigma k \omega}(x, t; [\phi]), \quad (3)$$

and the eigenvalue can be obtained by the Hellmann–Feynman theorem,

$$E_{\sigma k \omega}[\phi] = \hbar\omega - E_k - \Sigma_{\sigma k}[\phi]$$

$$\Sigma_{\sigma k}[\phi] = \int_0^1 d\lambda \int dt d^3x \phi(x, t) |\Psi_{\sigma k \omega}(x, t; [\lambda\phi])|^2$$

where  $\omega$  is the frequency,  $\Sigma_{\sigma k}[\phi]$  is the self-energy of the electrons in the new Hilbert space, and  $E_k$  is the eigenvalue of the non-interacting Hamiltonian of the electrons,

$$H_0 \psi_{\sigma k}(x) = (E_k + \mu) \psi_{\sigma k}(x)$$

where  $H_0 = \frac{\hat{p}^2}{2m} + U(x)$ , and  $k$  labels a set of quantum numbers representing the states of the non-interacting electrons.

According to the expression of the eigenvalue  $E_{\sigma k \omega}[\phi]$ , the eigenfunctional can be generally written down,

$$\Psi_{\sigma k \omega}(x, t; [\phi]) = \frac{1}{\sqrt{T}} \psi_{\sigma k}(x) e^{-i(\omega - \Sigma_{\sigma k}[\phi])t} e^{Q_{\sigma k}(x, t; [\phi])} \quad (4)$$

where  $T \rightarrow \infty$  is the timescale of the system, and the phase field  $Q_{\sigma k}(x, t; [\phi])$  satisfies the eikonal-like equation with the condition  $Q_{\sigma k}(x, t; [\phi = 0]) = 0$ ,

$$\phi(x, t) = \left( i\hbar \partial_t - \frac{\hat{p}^2}{2m} - \frac{1}{m} [\hat{p} \ln(\psi_{\sigma k}(x))] \cdot \hat{p} \right) \times Q_{\sigma k}(x, t; [\phi]) - \frac{[\hat{p} Q_{\sigma k}(x, t; [\phi])]^2}{2m}. \quad (5)$$

For the homogeneous case, this equation can be easily solved after neglecting the non-linear term, which in general is a small quantity<sup>3</sup>. It is worth noting that the difference between the eigenfunctional  $\Psi_{\sigma k \omega}(x, t; [\phi])$  of the electrons in the new Hilbert space and the wavefunction  $\psi_{\sigma k}(x)$  of the non-interacting electrons is the functional  $e^{Q_{\sigma k}(x, t; [\phi])}$  but with a pure phase factor  $e^{-i(\omega - \Sigma_{\sigma k}[\phi])t}$ , thus the physical meaning of the phase field  $Q_{\sigma k}(x, t; [\phi])$  is clear: the electron correlation effect can be completely represented by the phase field; i.e., the phase field is a correlation parameter of the electrons.

In terms of the eigenfunctionals  $\Psi_{\sigma k \omega}(x, t; [\phi])$ , the second quantization representation of the electrons in the new Hilbert space can be written down,

$$\hat{\psi}_{\sigma}(x, t) = \sum_{k\omega} \Psi_{\sigma k \omega}(x, t; [\phi]) \hat{c}_{\sigma k \omega}$$

$$\hat{\psi}_{\sigma}^{\dagger}(x, t) = \sum_{k\omega} \Psi_{\sigma k \omega}^*(x, t; [\phi]) \hat{c}_{\sigma k \omega}^{\dagger}, \quad (6)$$

where  $\hat{c}_{\sigma k \omega}$  ( $\hat{c}_{\sigma k \omega}^{\dagger}$ ) is the annihilation (creation) operator of the electrons with the spin index and the quantum number  $k$  and  $\omega$ . Using the orthogonality and the completeness of the eigenfunctionals  $\Psi_{\sigma k \omega}(x, t; [\phi])$ , it can be easily proved that the above electron operators satisfy the standard electron anti-commutation relations. These expressions play a central role in calculating the ground state energy and a variety of correlation functions of the system.

After integrating out the electron fields, and using the mathematical formula

$$\text{Tr} \ln (\hat{A} + \hat{B}) = \text{Tr} \ln (\hat{A}) + \text{Tr} \int_0^1 d\lambda \hat{B} \frac{1}{\hat{A} + \lambda \hat{B}}$$

the partition function can be written down [9],

$$Z = \int D\rho D\phi e^{\frac{i}{\hbar} S[\rho, \phi]},$$

$$S[\rho, \phi] = -i \text{Tr} \ln (\hat{M}_0) + W[\rho, \phi] \quad (7)$$

$$+ i \sum_{\sigma} \int_0^1 d\lambda \int dt d^3x \phi(x, t) G_{\sigma}(x, t; x, t; [\lambda\phi]),$$

<sup>3</sup> This can be easily understood for the lattice case, where the non-linear term originates from the phase difference between the nearest-neighbor sites. In general, the phase field produced by the quantum fluctuation of the Lagrange multiplier field is a smooth function, thus the non-linear term is a small quantity.

where  $\widehat{M}_0 = i\hbar\partial_t + \mu - \frac{\hbar^2}{2m} - U(x)$  is the non-interacting electron propagator operator. The electron Green function  $G_\sigma(x, t; x', t'; [\phi])$  in the new Hilbert space can be written down,

$$G_\sigma(x, t; x', t'; [\phi]) = \sum_{k\omega} \frac{\Psi_{\sigma k\omega}(x, t; [\phi])\Psi_{\sigma k\omega}^*(x', t'; [\phi])}{\hbar\omega - E_k - \Sigma_{\sigma k}[\phi]}$$

and the electron Green function in the original Hilbert space is  $G_\sigma(x, t; x', t') = \langle G_\sigma(x, t; x', t'; [\phi]) \rangle_{\rho\phi}$ , where  $\langle A[\phi] \rangle_{\rho\phi} = \frac{1}{Z} \int D\rho D\phi e^{\frac{i}{\hbar}S[\rho, \phi]} A[\phi]$ . The action  $S[\rho, \phi]$  is used to calculate the functional average over the auxiliary fields  $\phi(x, t)$  and  $\rho(x, t)$ .

According to the expressions of the electron operators, the ground state energy  $E_g = \langle H(t) \rangle$  of the system reads

$$E_g = K_0 + V_{\text{HF}} + \delta K + E_{\text{Hc}} + E_{\text{Fc}}, \quad (8)$$

where  $K_0 = 2 \sum_k n_k (E_k + \mu)$  is the kinetic energy of the non-interacting electrons, and  $n_k = \theta(-E_k)$  is the occupation number of the  $k$ th state of the non-interacting electrons. The term  $V_{\text{HF}}$  is the usual Hartree–Fock potential energy [11],

$$\begin{aligned} V_{\text{HF}} &= \frac{e^2}{2} \int d^3x d^3x' V(x-x') \rho_0(x) \rho_0(x') \\ &\quad - \frac{e^2}{2} \sum_{\sigma k k'} n_k n_{k'} \int d^3x d^3x' V(x-x') \\ &\quad \times \psi_{\sigma k}^*(x) \psi_{\sigma k'}(x) \psi_{\sigma k'}^*(x') \psi_{\sigma k}(x'), \end{aligned} \quad (9)$$

where  $\rho_0(x) = \sum_{\sigma k} n_k |\psi_{\sigma k}(x)|^2$  is the density of the non-interacting electrons. The first two terms in the expression of the ground state energy are similar to those in the LDA of the density functional theory, which can be rigorously represented by the single-particle wavefunctions.

The term  $\delta K$  is a modification of the kinetic energy of the electrons by the Coulomb interaction [12],

$$\delta K = \sum_{\sigma k} \int d^3x \rho_{\sigma k}(x) g_{\sigma k}(x, [\rho_0]), \quad (10)$$

where  $\rho_{\sigma k}(x) = n_k |\psi_{\sigma k}(x)|^2$ , and  $g_{\sigma k}(x, [\rho_0]) = \langle |e^{\mathcal{Q}_{\sigma k}(x, t; [\phi])}|^2 (i\hbar\partial_t \mathcal{Q}_{\sigma k}(x, t; [\phi]) - \phi(x, t)) \rangle_{\rho\phi}$  is the functional of the density  $\rho_0(x)$ , and independent of the time coordinate  $t$  because of the time translation symmetry of the system. For a homogeneous electron system, the function  $g_{\sigma k}(x, [\rho_0]) = g_{\sigma k}[\rho_0]$  is equivalent to the self-energy under the random-phase approximation, and it is a functional of the density  $\rho_0(x)$ . Thus, the term  $\delta K$  can be treated approximately under the LDA.

The correlation energies  $E_{\text{Hc}}$  and  $E_{\text{Fc}}$  can be written down [13–15],

$$\begin{aligned} E_{\text{Hc}} &= \frac{e^2}{2} \int d^3x d^3x' V(x-x') \rho(x, x'), \\ E_{\text{Fc}} &= -\frac{e^2}{2} \int d^3x d^3x' V(x-x') \Gamma(x, x'), \end{aligned} \quad (11)$$

where the functions  $\rho(x, x')$  and  $\Gamma(x, x')$  are defined as

$$\begin{aligned} \rho(x, x') &= \sum_{\sigma\beta k k'} n_k n_{k'} |\psi_{\sigma k}(x)|^2 |\psi_{\beta k'}(x')|^2 \\ &\quad \times \langle |e^{\mathcal{Q}_{\sigma k}(x, t; [\phi])}|^2 |e^{\mathcal{Q}_{\beta k'}(x', t; [\phi])}|^2 - 1 \rangle_{\rho\phi} \\ \Gamma(x, x') &= \sum_{\sigma k k'} n_k n_{k'} \psi_{\sigma k}^*(x) \psi_{\sigma k'}(x) \psi_{\sigma k'}^*(x') \psi_{\sigma k}(x') \\ &\quad \times \langle \exp\{\mathcal{Q}_{\sigma k}^*(x, t; [\phi]) + \mathcal{Q}_{\sigma k}(x', t; [\phi]) \\ &\quad + \mathcal{Q}_{\sigma k'}^*(x', t; [\phi]) + \mathcal{Q}_{\sigma k'}(x, t; [\phi])\} - 1 \rangle_{\rho\phi}. \end{aligned}$$

Obviously,  $E_{\text{Hc}}$  is the Hartree-like correlation energy, while  $E_{\text{Fc}}$  represents the Fock-like correlation energy. The former shows the local behavior, and the latter has the non-local property. It could be demonstrated that the main errors of the LDA of the density functional theory originate from the correlation energy  $E_{\text{Hc}}$  and  $E_{\text{Fc}}$  terms.

For a homogeneous interacting electron system, according to the experience in studying the one-dimensional interacting electron systems<sup>4</sup>, the electron correlation strength is controlled by the imaginary part of the phase field  $\mathcal{Q}_{\sigma k}(x, t; [\phi])$ , and it can be shown that  $\langle |e^{\mathcal{Q}_{\sigma k}(x, t; [\phi])}|^2 |e^{\mathcal{Q}_{\beta k'}(x', t; [\phi])}|^2 \rangle_{\rho\phi} = e^{F_{\sigma\beta k k'}(x-x'; [\rho_0])}$ , where the function  $F_{\sigma\beta k k'}(x-x'; [\rho_0])$  is a small quantity, thus it is reasonable to take the approximation<sup>5</sup>  $e^F \simeq 1 + F$ . Therefore, the function  $\rho(x, x')$  can be approximately represented by the density function,

$$\rho(x, x') \simeq \sum_{\sigma\beta k k'} F_{\sigma\beta k k'}(x-x'; [\rho_0]) \rho_{\sigma k}(x) \rho_{\beta k'}(x'), \quad (12)$$

where  $F_{\sigma\beta k k'}(x-x'; [\rho_0])$  is the functional of the non-interacting electron density  $\rho_0(x)$ . Thus, the correlation energy  $E_{\text{Hc}}$  can be treated approximately under the LDA.

It can be shown that for the homogeneous case  $\langle \exp\{\mathcal{Q}_{\sigma k}^*(x, t; [\phi]) + \mathcal{Q}_{\sigma k}(x', t; [\phi]) + \mathcal{Q}_{\sigma k'}^*(x', t; [\phi]) + \mathcal{Q}_{\sigma k'}(x, t; [\phi])\} \rangle_{\rho\phi} = e^{P_{\sigma k k'}(x-x'; [\rho_0])}$ , while the function  $P_{\sigma k k'}(x-x'; [\rho_0])$  is not a small quantity for the systems with strong electron correlation. For example, for a one-dimensional interacting electron gas, the function  $e^{P_{\sigma k k'}(x-x'; [\rho_0])}$  has a power-law asymptotic behavior [17],

$$e^{P_{\sigma k k'}^{\text{1D}}(x-x'; [\rho_0])} \sim \frac{1}{|x-x'|^\gamma} \quad (13)$$

where  $\gamma > 1$  is a dimensionless coupling constant which depends upon the electron interaction strength and the Fermi velocity. In this case, the function  $\Gamma(x, x')$  shows completely different behavior from that of the function  $\rho(x, x')$ , and the correlation energy  $E_{\text{Fc}}$  cannot be treated approximately under the LDA. In general, it is expected that the correlation energy  $E_{\text{Fc}}$  is important for the systems with strong electron correlation, thus a method beyond the LDA is needed.

The above expression of the ground state energy is obviously different from that of the density functional theory in the LDA (Kohn–Sham scheme), where the ground state energy is represented by the quantity of the non-interacting electrons. The ground state energy in equation (8) is composed

<sup>4</sup> In the usual bosonization method, the phase field is a pure imaginary function.

<sup>5</sup> According to the normalization of the eigenfunctional, we have the relation:  $\langle |e^{\mathcal{Q}_{\sigma k}(x, t)}|^2 \rangle_{\rho\phi} = 1$ .

of two parts: one part corresponds to the non-interacting electrons, and the other one is represented by the correlation functions, that are controlled by the electron correlation, which describes the quantum many-electron effect. In principle, the expression of the ground state energy is independent of the choice of the Hamiltonian  $\widehat{H}_0$  of the non-interacting electrons. A different choice of the Hamiltonian  $\widehat{H}_0$  can give a different non-interacting part, while for the correlation part it will only change the action  $S[\rho, \phi]$  and the wavefunction  $\psi_{\sigma k}(x)$  of the non-interacting electrons.

The method described above is a general approach for calculating the correlation energy in the ground state of quantum many-electron systems, and it is valid in any spacial dimensions. In the following we will apply this general method to one simple but nontrivial example: the one-dimensional spin- $\frac{1}{2}$  XXZ model.

### 3. One-dimensional XXZ model

The Hamiltonian of a spin- $\frac{1}{2}$  XXZ chain with nearest-neighbor (n.n.) interaction is

$$H_{\text{XXZ}} = -J_{\perp} \sum_{\langle ij \rangle} [S_i^x S_j^x + S_i^y S_j^y] + J_z \sum_{\langle ij \rangle} S_i^z S_j^z.$$

We take  $J_{\perp}$  as the unit of energy, i.e.  $J_{\perp} = 1$ , and define the anisotropic parameter  $\Delta \equiv J_z/J_{\perp}$ . Then, the Hamiltonian after the Jordan–Wigner (JW) transformation reads

$$H_{\text{XXZ}} = -\frac{1}{2} \sum_{ij} \widehat{f}_i^{\dagger} \gamma_{ij} \widehat{f}_j - \Delta \sum_i \widehat{n}_i + \frac{1}{4} \Delta L + \frac{1}{2} \Delta \sum_{ij} \widehat{n}_i \gamma_{ij} \widehat{n}_j, \quad (14)$$

where  $\widehat{f}_i^{\dagger}$  ( $\widehat{f}_i$ ) is the creation (annihilation) operator of the spinless fermions,  $\widehat{n}_i = \widehat{f}_i^{\dagger} \widehat{f}_i$ ,

$$\gamma_{ij} = \begin{cases} 1 & \text{if } |i - j| = 1 \\ 0 & \text{otherwise,} \end{cases}$$

and  $L$  is the total number of lattice sites.

The eigenfunctional of equation (3) can be written as

$$\Psi_{k\omega}(x_i, t; [\phi]) = \frac{1}{\sqrt{TL}} e^{ikx_i - i\omega t - \sum_k [\phi]} e^{Q_k(x_i, t; [\phi])}, \quad (15)$$

where  $T \rightarrow \infty$  is the timescale of the system,  $L \rightarrow \infty$  the total number of lattice sites, and the phase field  $Q_k(x_i, t; [\phi])$  satisfies the equation

$$i \partial_t Q_k(x_i, t; [\phi]) - \phi_i(t) + \varepsilon_k = -\frac{1}{2} \sum_j e^{-ikx_j - Q_k(x_j, t; [\phi])} \gamma_{ij} e^{ikx_j + Q_k(x_j, t; [\phi])}, \quad (16)$$

where  $\varepsilon_k = -\cos k$ . It is worthwhile to note that, in calculating the ground state energy, this functional should be normalized to ensure the conservation of the total particle number.

The auxiliary field  $\phi$  can be separated into two parts, a mean-field part  $\phi_i^c$  and a quantum fluctuation part  $\eta_i(t)$ :  $\phi_i(t) = \phi_i^c + \eta_i(t)$ . The former should be obtained self-consistently, which generally gives a renormalization of the chemical potential and possibly a change of the energy band.

It can be shown that in the present model the mean-field effect would lead to a renormalization of the dispersion relation:  $\varepsilon_k \rightarrow \varepsilon_k = -J^* \cos k$ , where  $J^* = 1 + \Delta/\pi$ . The latter part would lead to a phase field  $Q_k(x_i, t; [\eta])$ , which is usually a small quantity (see footnote 3) and hence can be approximated by  $e^{Q_k} \approx 1 + Q_k$ . Then the solution of equation (16) reads

$$Q_k(x_i, t; [\eta]) = \frac{1}{TL} \sum_{q\Omega} e^{iqx_i - i\Omega t} \frac{\eta(q, \Omega)}{\Omega + \varepsilon_k - \varepsilon_{k+q}}, \quad (17)$$

where  $\eta(q, \Omega) = \int dt \sum_i e^{-ikx_i + i\Omega t} \eta_i(t)$  are Fourier components of the fluctuation field  $\eta_i(t)$ . Using this expression for the phase field, and integrating out the  $\rho$  field, the effective action for  $\eta$  reads

$$S_{\text{eff}}[\eta] \approx \text{const.} + \frac{1}{2\Delta} \frac{1}{TL} \sum_{q\Omega} \frac{1}{\gamma^*(q, \Omega)} |\eta(q, \Omega)|^2, \quad (18)$$

where  $|\eta(q, \Omega)|^2 \equiv \eta(q, \Omega)\eta(-q, -\Omega)$ , and

$$\gamma^*(q, \Omega) = \frac{\gamma(q)}{1 - \Delta \gamma(q) \Pi^c(q, \Omega)}, \quad (19)$$

where  $\gamma(q) = \sum_j \gamma_{ij} e^{-iq(x_i - x_j)} = 2 \cos(q)$ , and  $\Pi^c(q, \Omega)$  is the Lindhard function in the presence of the classical field  $\phi^c$ :

$$\Pi^c(q, \Omega) = \frac{1}{L} \sum_k \frac{f(\varepsilon_k) - f(\varepsilon_{k+q})}{\varepsilon_k - \varepsilon_{k+q} - \Omega},$$

where  $f(\varepsilon)$  is the Fermi–Dirac distribution function.

In the following we will first calculate the ground state energy and then evaluate the correlation exponents of the Green function and the spin–spin correlation function.

#### 3.1. Ground state energy

The ground state energy per site  $E_g \equiv \langle H_{\text{XXZ}} \rangle / L$  can be written as  $E_g = E_{\text{HF}} + E_c$ , where  $E_{\text{HF}}$  is the energy in the Hartree–Fock approximation and  $E_c$  the correlation energy.

The Hartree–Fock term  $E_{\text{HF}} = K_0 + V_{\text{HF}} - \Delta/4$ , where

$$K_0 = -\frac{1}{L} \sum_k e^{-ika} f(\varepsilon_k), \quad (20)$$

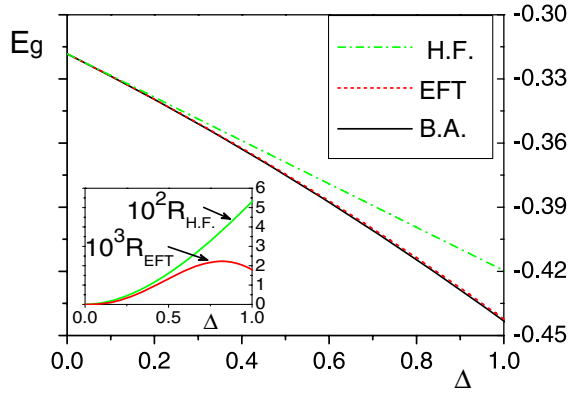
$$V_{\text{HF}} = \frac{\Delta}{L^2} \sum_{k_1 k_2} f(\varepsilon_{k_1}) f(\varepsilon_{k_2}) - \frac{\Delta}{L^2} \sum_{k_1 k_2} e^{-i(k_1 - k_2)a} f(\varepsilon_{k_1}) f(\varepsilon_{k_2}). \quad (21)$$

The correlation energy  $E_c = \delta K + E_{\text{Hc}} + E_{\text{Fc}}$ . The modification of the kinetic energy due to the short-range interaction reads

$$\delta K = -\frac{1}{L} \sum_k e^{-ika} f(\varepsilon_k) [e^{F_k[\Delta]} - 1], \quad (22)$$

where  $a$  is the lattice constant and

$$F_k[\Delta] = i \frac{\Delta}{TL} \sum_{q, \Omega} \frac{\gamma^*(q, \Omega)}{(\Omega + \varepsilon_k - \varepsilon_{k+q})^2} [e^{-iqa} - 1]. \quad (23)$$



**Figure 1.** Dependence of the ground state energy per site on  $\Delta$ , which is numerically evaluated in the eigenfunctional theory (EFT), in comparison with the Bethe ansatz (BA) solution and the Hartree–Fock (HF) approximation. The inset shows the two relative errors  $R_{\text{HF}}$  and  $R_{\text{EFT}}$ , which are defined in the text.

The Hartree-like correlation energy is

$$E_{\text{Hc}} = \frac{\Delta}{L^2} \sum_{k_1 k_2} f(\epsilon_{k_1}) f(\epsilon_{k_2}) [e^{R_{k_1 k_2} + F_{k_1 k_2}} - 1], \quad (24)$$

where

$$R_{k_1 k_2} = i \frac{\Delta}{TL} \sum_{q, \Omega} \frac{\gamma^*(q, \Omega) [2 \cos(qa)]}{(\epsilon_{k_1} - \epsilon_{k_1+q} + \Omega)(\epsilon_{k_2} - \epsilon_{k_2-q} - \Omega)}, \quad (25)$$

$$F_{k_1 k_2} = i \frac{\Delta}{TL} \sum_{q, \Omega} \frac{\gamma^*(q, \Omega) [2 \cos(qa)]}{(\Omega + \epsilon_{k_1} - \epsilon_{k_1+q})(\Omega + \epsilon_{k_2} - \epsilon_{k_2+q})}. \quad (26)$$

The Fock-like interaction energy is

$$E_{\text{Fc}} = -\frac{\Delta}{L^2} \sum_{k_1 k_2} e^{-i(k_1 - k_2)a} f(\epsilon_{k_1}) f(\epsilon_{k_2}) \times [e^{F_{k_1 k_2}^{\text{ex}} + F_{k_1 k_2}^{\text{ex}} + R_{k_1 k_2}^{\text{ex}} + F_{k_1 k_2}^{\text{ex}}} - 1], \quad (27)$$

where

$$R_{k_1 k_2}^{\text{ex}} = i \frac{\Delta}{TL} \sum_{q, \Omega} \frac{[2 \exp(iqa)] \gamma^*(q, \Omega)}{(\epsilon_{k_1} - \epsilon_{k_1+q} + \Omega)(\epsilon_{k_2} - \epsilon_{k_2-q} - \Omega)}, \quad (28)$$

$$F_{k_1 k_2}^{\text{ex}} = i \frac{\Delta}{TL} \sum_{q, \Omega} \frac{2\gamma^*(q, \Omega)}{(\Omega + \epsilon_{k_1} - \epsilon_{k_1+q})(\Omega + \epsilon_{k_2} - \epsilon_{k_2+q})}. \quad (29)$$

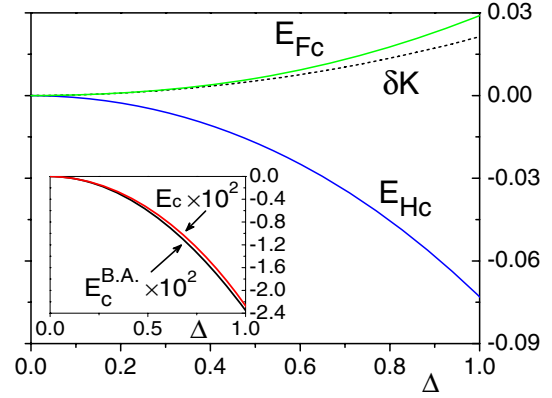
It is well known that the one-dimensional XXZ model can be solved exactly by the Bethe ansatz (BA) [18, 19], which gives the ground state energy for  $0 \leq \Delta \leq 1$  as

$$E_{\text{g}}^{\text{BA}}(\Delta) = \frac{\cos \lambda}{4} - \frac{\sin \lambda}{\lambda} Y(\lambda),$$

$$Y(\lambda) = \int_{-\infty}^{\infty} dx \frac{\lambda \sin \lambda}{2[\cosh(\pi x)][\cosh(2\lambda x) - \cos \lambda]},$$

where  $\lambda \equiv \arccos \Delta$ . This solution gives an exact expression of the correlation energy:  $E_{\text{c}}^{\text{BA}} \equiv E_{\text{g}}^{\text{BA}} - E_{\text{HF}}$ .

The numerical evaluation of the ground state energy per site evaluated in our eigenfunctional (EFT) scheme is plotted in



**Figure 2.** Dependence of  $\delta K$ ,  $E_{\text{Hc}}$  and  $E_{\text{Fc}}$  on  $\Delta$ . The inset shows the total correlation energy  $E_{\text{c}} = \delta K + E_{\text{Hc}} + E_{\text{Fc}}$ , in comparison with the exact one:  $E_{\text{c}}^{\text{BA}} = E_{\text{g}}^{\text{BA}} - E_{\text{HF}}$ .

figure 1, in comparison with the Bethe ansatz solution and the Hartree–Fock approximation. The modification of the kinetic energy  $\delta K$ , the Hartree-like correlation energy  $E_{\text{Hc}}$ , the Fock-like correlation energy  $E_{\text{Fc}}$  and the total correlation energy  $E_{\text{c}}$  are plotted in figure 2. We see that the EFT result is quite close to the exact solution, reflecting the fact that correlation effects can be captured quite effectively in our EFT scheme. To see more clearly, we also plot the two relative errors:  $R_{\text{HF}} \equiv |E_{\text{HF}} - E_{\text{g}}^{\text{BA}}|/|E_{\text{g}}^{\text{BA}}|$  and  $R_{\text{EFT}} \equiv |E_{\text{g}} - E_{\text{g}}^{\text{BA}}|/|E_{\text{g}}^{\text{BA}}|$ . One can see that  $R_{\text{EFT}}$  is smaller than  $R_{\text{HF}}$  by one order or even more.

### 3.2. Correlation exponent

In the same formalism one can also study the asymptotic behavior of the correlation functions. It is straightforward to show that the fermion’s Green function and the transverse spin–spin correlation function all have power-law behavior, the exponents of which depend on the coupling constant  $\Delta$  and can be evaluated quite precisely in the EFT formalism.

We are interested in the long-range behavior of the following two kinds of equal-time correlation function:

$$G_{ij}(t, t) = \langle f_j^\dagger(t) f_i(t) \rangle,$$

$$\langle S_i^-(t) S_j^+(t) \rangle = \langle f_i(t) f_j^\dagger(t') e^{-i \sum_l \int dt_l n_l(t_l) V_{ij}(x_l, t_l; t, t')} \rangle,$$

where  $V_{ij}(x_l, t_l; t, t') = \pi[\Theta(x_i - x_l)\delta(t_1 - t) - \Theta(x_j - x_l)\delta(t_1 - t')]$ .

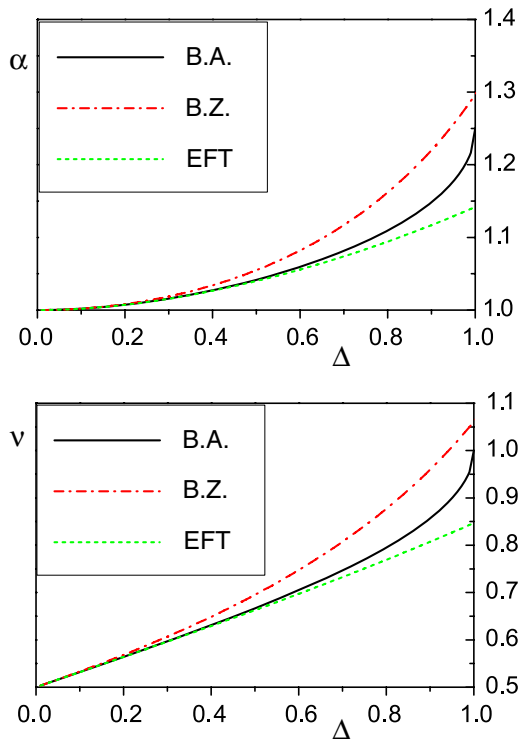
In the limit of  $|x| = |x_i - x_j| \rightarrow \infty$ , these two correlation functions have power-law behavior:

$$G_{ij}(t, t) \sim \frac{1}{|x_i - x_j|^\alpha}, \quad (30)$$

$$\langle S_i^-(t) S_j^+(t) \rangle \sim \frac{1}{|x - x'|^\nu}, \quad (31)$$

where  $\alpha = (g + 1/g)/2$ ,  $\nu = 1/(2g)$ , and

$$g = \sqrt{\frac{1 - \Delta/\pi}{1 + 3\Delta/\pi}}. \quad (32)$$



**Figure 3.** Dependence of the correlation exponents  $\alpha$  and  $\nu$  on  $\Delta$  in the eigenfunctional formalism (EFT), in comparison with the Bethe ansatz (BA) and bosonization (BZ) results.

The dependences of the correlation exponents  $\alpha$  and  $\nu$  are plotted in figure 3 in comparison with the Bethe ansatz and bosonization results.

#### 4. Conclusion and discussion

Based upon the above discussions, a more effective method for calculating the ground state energy  $E_g$  is that, by suitably choosing the non-interacting Hamiltonian  $\hat{H}_0$ , the terms  $K_0$  and  $V_{\text{HF}}$  can be calculated with the usual LDA scheme, then the terms  $\Delta T$ ,  $E_{\text{Hc}}$  and  $E_{\text{Fc}}$  can be calculated by the quantum Monte Carlo method (QMCM) [20], where the action  $S[\rho, \phi]$  can be obtained by solving equation (5) of the phase field. By more accurately treating the correlation energy  $E_c$ , the results of the usual LDA will be heavily modified for the systems with strong electron correlation.

On the other hand, for a suitable LDA, if the contribution of the correlation energy  $E_c$  to the ground state energy is small, this LDA is reliable. If its contribution is important, the LDA will be unreliable and some extension or a new approach is needed. The method suggested in this article is a possible choice and it treats the two cases in a unified way. Of course, corresponding to the local spin density approximation (LSDA) [15, 16] of the density functional theory, it needs to introduce the Lagrange multiplier fields  $\phi_\sigma(x, t)$ , in which case there are four auxiliary fields  $\phi_\sigma(x, t)$  and  $\rho_\sigma(x, t)$ , while the ground state energy has a similar expression to that in equation (8).

In summary, with the eigenfunctional theory, we have studied a general interacting electron system, and given a

rigorous expression of its ground state energy, which is composed of two parts: one part is contributed by the non-interacting electrons, and the other one is represented by the correlation functions that are controlled by the electron correlation. Moreover, according to the rigorous expression of the ground state energy, an effective method beyond the LDA may be the LDA plus the QMCM. The LDA is used to treat the non-interacting electron part, while the correlation part is generally treated by the QMCM. However, as a simple example for a spin- $\frac{1}{2}$  XXZ chain, without the QMCM and only under the linear approximation in solving the equation of the phase field, the ground state energy obtained by the present scheme is quite close to that of the Bethe ansatz.

#### Acknowledgments

This work is partially supported by the National Natural Science Foundation of China, Nos 10547002, 90403015 and 10774188, and by the National Basic Research Program of China, No 2007CB925001.

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