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Gutzwiller approximation in the Fermi hypernetted-chain theory

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We present a general formalism for the variational calculation of the one-body density-matrix and correlation functions for strongly correlated lattice electrons in terms of the Fermi hypernetted-chain (FHNC) diagrammatic expansion. It is shown that, in the limit of infinite spatial dimensions, the local-field-approximate FHNC scheme yields the exact solution for the Gutzwiller wave function, which is equivalent to the result of the Gutzwiller approximation.

The quantitative understanding of correlation effects in strongly interacting electron systems is a challenging issue in many-body physics. In most cases of interest such effects can hardly be handled by means of conventional perturbation theories built upon independent-particle basis functions. The variational approaches based on Fermi hypernetted-chain (FHNC) analysis have been very useful in the study of strongly correlated electrons such as nuclear matter,[1] liquid ^{3}He,[2] atomic systems,[3] and fermionic lattice models (e.g., the Hubbard model).[4] The Hubbard model and related models for interacting lattice electrons are employed in the study of itinerant magnetism,[5] the metal-insulator transition,[6] and high-T_c superconductivity.[7]

The FHNC theory uses a variational ansatz for a trial wave function of the ground state. Most notable and commonly used is the Jastrow ansatz.[8] This type of wave function can be optimized either in a parametrized form in terms of its variational parameters,[4] or by an Euler-Lagrange equation based on the paired-phonon analysis (PPA).[3,8] The FHNC diagrammatic expansion[3,9,10] provides a powerful tool to treat both short- and long-range correlations correctly. However, this linked-cluster expansion cannot be expressed in a fully closed form, and thus requires approximate solutions. The widely used FHNC//0 scheme[3,10] in the minimal approximation permits a derivation of a properly behaved Euler-Lagrange equation for the optimization of Jastrow correlation functions.

In the context of strongly correlated lattice fermion systems, the Gutzwiller variational wave function has been studied extensively.[11–21] The Gutzwiller wave function consists of a correlation operator $\hat{G}$ acting on the Fermi sea of noninteracting particles. The Gutzwiller correlation operator given by

$$\hat{G} = \prod_i [1 - (1-g)\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}], \tag{1}$$

incorporates the local on-site correlations through a variational parameter g. The limiting value $g = 0$ corresponds to completely projecting out configurations with doubly occupied sites. The exact evaluation of the energy[12] and correlation functions[13] with the Gutzwiller wave function was carried out in one dimension for the Hubbard model. It was also shown that the Gutzwiller wave function is the exact ground state of the one-dimensional Heisenberg model with $1/r^2$ exchange.[14,15]

For dimensions higher than one, no complete analytical solution has been obtained thus far. However, numerical calculations based on stochastic methods (e.g., variational Monte Carlo[11,16]) and the FHNC scheme[4,17] have provided valuable insight into the physics described by the Gutzwiller wave function. Moreover, the FHNC scheme has produced useful insights into the role played by certain other types of correlations.[4,18] Since FHNC calculations are done in the thermodynamic limit, they avoid the problems associated with the finite-size effects which may be serious in dimensions higher than one. Furthermore, it makes it possible to apply the full machinery of the correlated-basis-function (CBF) theory to go beyond the variational estimates.[4] An important motivation for the present work has been to assess the applicability of the FHNC//0 theory, and to provide insight into the physics behind approximations intrinsic in such a calculation scheme.

Gutzwiller[19] proposed an approximation to study the Gutzwiller wave function. This *Gutzwiller approximation* was then applied to several physical systems, e.g., the metal-insulator transition[6] and ^{3}He.[5] Recently, Metzner and Vollhardt[12,20] introduced the limit of high spatial dimensions which may play a key role for analytical investigations of strongly correlated electron systems. Remarkably, they showed that the Gutzwiller approximation yields the exact result for the Gutzwiller wave function in infinite dimensions.[20] Moreover, the Gutzwiller approximation was shown to be equivalent to the slave-boson approach for strongly correlated electron models.[21]

In this paper, we first present a general formalism based on chain propagators of the Jastrow correlation operators for the calculation of the correlation functions and one-body density matrix. Then we show that for the Gutzwiller wave function, the FHNC//0 approximation becomes exact in infinite dimensions. This implies that the FHNC//0 method for the Gutzwiller wave function yields the well-known results of the Gutzwiller approximation. The corresponding correlation functions, one-body density matrix, and the ground-state energy for the Hubbard model are calculated. Finally, we discuss the consequences of our studies in developing a generic variational-CBF scheme for lattice fermions.

We begin with a derivation of the chain propagators for the FHNC equations. For a trial wave function consisting of a state-dependent Jastrow correlation operator of the form

$$\hat{G} = \exp\left(\tfrac{1}{2}\sum_{i,j} u_{ij}^{\uparrow\downarrow}\hat{n}_{i\uparrow}\hat{n}_{j\downarrow} + \tfrac{1}{2}\sum_{i,j} u_{ij}^{\sigma\sigma}\hat{n}_{i\sigma}\hat{n}_{j\sigma}\right), \tag{2}$$

acting on the reference Hartree-Fock (HF) state $|\Psi_0\rangle$, the FHNC scheme consists of a linked-cluster expansion in terms of dynamical correlations [$\exp(u_{ij}^{\uparrow\downarrow}) - 1$, $\exp(u_{ij}^{\sigma\sigma}) - 1$ for density and spin correlation functions, and $\exp(\frac{1}{2}u_{ij}^{\uparrow\downarrow})-1$, $\exp(\frac{1}{2}u_{ij}^{\sigma\sigma})-1$ for the one-body density matrix], and statistical correlation which corresponds to the HF one-body density matrix,

$$P_\sigma^0(i,j) = \langle\Psi_0|\hat{c}_{i\sigma}^\dagger\hat{c}_{j\sigma}|\Psi_0\rangle/\langle\Psi_0|\Psi_0\rangle, \tag{3}$$

with the density given by $n_\sigma = P_\sigma^0(i,i)$.

In the hypernetted-chain (HNC) scheme, the linked-cluster expansion diagrams can be classified into nodal (N), composite (X), and elementary (E) diagrams. Composite diagrams comprise the diagrams forming parallel connections between external points, while nodal diagrams consist of chain connections between composite and composite-nodal functions. The resultant convolution equations, along with definitions for composite functions, constitute the exact HNC integral equations. These equations can be readily solved in terms of the Fourier transforms of various functions. Various levels of approximation can be chosen, depending upon the order of elementary diagrams that are included. In the case of fermions, the FHNC method amounts to solving a system of seven coupled nonlinear equations. We refer to the original papers[4,22,23] for the explicit expressions of various composite functions.

The one-body density matrix can be evaluated as[23]

$$P_\sigma(i,j) = n_{0,\sigma}e^{-Q_\sigma(i,j)}[P_\sigma^0(i,j) + Y_\sigma(i,j)], \tag{4}$$

where

$$n_{0,\sigma} = e^{Q_\sigma(i,i)}, \tag{5}$$

which measures the strength of the electron correlations. $Y_\sigma(i,j)$ and $Q_\sigma(i,j)$ are composed of nodal and elementary functions. The Fourier transform of $Y_\sigma(i,j)$ is given by

$$\begin{aligned} Y_\sigma(\mathbf{k}) = {} & E_{\xi c\xi c,\sigma} + (2X_{\xi cc,\sigma} - X_{cc,\sigma})l_\sigma \\ & - X_{\xi cc,\sigma}^2(1-l_\sigma)/(1-X_{cc,\sigma}), \end{aligned} \tag{6}$$

where $l_\sigma(\mathbf{k})$ is the HF momentum distribution function, i.e., the Fourier transform of $P_\sigma^0(i,j)$, $E_{\xi c\xi c,\sigma}(\mathbf{k})$ is an elementary function, and the "cyclic-cyclic" (cc) functions, $X_{cc,\sigma}(\mathbf{k})$ and $X_{\xi cc,\sigma}(\mathbf{k})$, correspond to diagrams with one statistical correlation joining the two external points.

The density-density and spin-spin correlation functions, $C^{NN}(\mathbf{k})$ and $C^{SS}(\mathbf{k})$, can be expressed in the form

$$C^{\alpha\alpha}(\mathbf{k}) = [1 + X_{ee}^{(\alpha)}(\mathbf{k})]/[1 - P^{(\alpha)}(\mathbf{k})], \tag{7}$$

where $\alpha = N, S$ referring to the density and spin indices, respectively, with $A^{(N)} = A^{\sigma\sigma} + A^{\uparrow\downarrow}$, and $A^{(S)} = A^{\sigma\sigma} - A^{\uparrow\downarrow}$. The chain propagator is expressed in terms of composite quantities,

$$P^{(\alpha)} = X_{dd}^{(\alpha)}(1 + X_{ee}^{(\alpha)}) + 2X_{de}^{(\alpha)} - (X_{de}^{(\alpha)})^2, \tag{8}$$

where the labels dd, de, and ee refer to the particular statistical character of the correlation functions considered. The "direct-direct" (dd) diagrams have only dynamical correlations ending at both external points i and j, whereas the label e indicates that the diagrams have two statistical correlations ending at the corresponding external point.

The FHNC equations for the one-body density matrix and correlation functions discussed above can be rather easily solved, once the various elementary functions are known. However, the numeric evaluation of elementary functions is rather involved. Eventually one needs to use approximate schemes such as the scaling approximation[24] or the interpolation equation method.[25] In this regard, it is interesting to note that the FHNC//0 approximation of Krotscheck and Ristig[10] amounts to setting $X_{de}^{(\alpha)} = 0$ and $X_{ee}^{(\alpha)} = X_{ee}^0$, where X_{ee}^0 is the HF result for the "exchange-exchange" (ee) function. With use of this approximation, all the terms of the dd type are summed together with the terms which guarantee the Pauli principle in intermediate states and ensure a correct behavior of correlation functions at long distances. The resulting scheme contains only two integral equations, which makes it possible to proceed with a PPA.

As discussed by Metzner and Vollhardt,[12,20] in infinite dimensions diagrammatic calculations are greatly simplified by the fundamental property that for $i \neq j$, $P_\sigma^0(i,j)$ scales as $d^{-1/2}$, where d is the dimensionality, and is thus negligible in $d = \infty$. The Gutzwiller correlation operator (1) is a special form of the Jastrow correlation operator (2), corresponding to the choice $u_{ij}^{\uparrow\downarrow} = 2\ln g\delta_{ij}$ and

$u_{ij}^{\sigma\sigma} = 0$. As a result for the Gutzwiller wave function, of all diagrams appearing in the FHNC scheme—nodal, composite, and elementary diagrams—only on-site terms survive in $d = \infty$. In other words, in this case the Fourier transform of various functions is a $\mathbf{k}$-independent constant.

In connection with the requirement of satisfying the Pauli principle in intermediate state during the cluster expansion, the composite functions $X_{de}^{(\alpha)}$ and $X_{ee}^{(\alpha)} - X_{ee}^{0}$ should equal zero in the limit of $\mathbf{k} = 0$. This was first studied by Krotscheck in the context of homogeneous systems.[26] Recent calculations for lattice fermions based on cluster expansions also revealed this property,[4] which is important for obtaining the correct long-distance behavior for the correlation functions. As a consequence for the Gutzwiller correlation function at $d = \infty$, the FHNC//0 approximation becomes exact. In view of the fact that the $d = \infty$ solution for the Gutzwiller wave function reduces to the results of the Gutzwiller approximation, we conclude that the FHNC//0 calculation should yield the same results.

To verify this conclusion, we proceed to calculate the corresponding correlation functions, one-body density matrix, and the ground-state energy for the Hubbard model,

$$H = -t \sum_{\langle i,j\rangle,\sigma} \hat{c}_{i\sigma}^{\dagger}\hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \tag{9}$$

where $\langle i,j\rangle$ denotes summation over nearest neighbors, t is the electron hopping integral, and U is the on-site repulsive Coulomb potential. The main scope of this exercise is not to uncover any new physics of this particular situation, which is rather well studied. On the contrary, we wish to use this calculation to assess the applicability and limitations of the FHNC method, and to obtain precise indications which will serve for the future applications.

(1) Correlation functions. As the FHNC//0 approximation is applied, the resulting expressions for density-density and spin-spin correlation functions are particularly simple if we introduce the Hartree-Fock spin and density correlation functions

$$C^{0}(\mathbf{k}) = C_{\mathrm{HF}}^{NN}(\mathbf{k}) = C_{\mathrm{HF}}^{SS}(\mathbf{k}) = 1 + X_{ee}^{0}(\mathbf{k}). \tag{10}$$

The final result has a structure familiar from the ring approximation,

$$C^{\alpha\alpha}(\mathbf{k}) = C^{0}(\mathbf{k})/[1 - X_{dd}^{(\alpha)}C^{0}(\mathbf{k})]. \tag{11}$$

To simplify our discussion, we consider the case $n_{\uparrow} = n_{\downarrow} = n$. $X_{dd}^{(N)}$ and $X_{dd}^{(S)}$ can be determined using sum rules valid at $\mathbf{k} = 0$, yielding

$$X_{dd}^{(N)} = 1/(n - n^2 + 2\eta) - 1/(n - n^2/2),$$
$$X_{dd}^{(S)} = 1/(n - 2\eta) - 1/(n - n^2/2), \tag{12}$$

where η is the probability of double occupancy. It is seen that these expressions coincide with those obtained by van Dongen, Gebhard, and Vollhardt[27] for the Gutzwiller approximation.

(2) One-body density matrix. In the FHNC//0 approximation, the statistical correlation function is replaced by the corresponding dressed quantity. As a result, the one-body density matrix is determined by the renormalization factor which is the "Luttinger jump" at the Fermi surface for the momentum distribution. This jump can be evaluated as

$$q_{\sigma} = 1 - X_{cc,\sigma} + 2X_{\xi cc,\sigma} + X_{\xi cc,\sigma}^{2}/(1 - X_{cc,\sigma}). \tag{13}$$

Noting that for the Gutzwiller wave function, the dynamic correlation function for correlation functions is $g^2 - 1$, while for the one-body density matrix is $g - 1$, we have a simple relation between the two cc functions,

$$X_{cc,\sigma}(\mathbf{k}) = (1 + g)X_{\xi cc,\sigma}(\mathbf{k}). \tag{14}$$

Substituting this relation into (13), and noticing the relationship between $X_{cc,\sigma}$ and the proper self-energy s_{σ}^{*},[22]

$$X_{cc,\sigma} = -s_{\sigma}^{*}/(1 - s_{\sigma}^{*}), \tag{15}$$

we finally arrive at the result

$$q_{\sigma} = 1 + [s_{\sigma}^{*}/(1 + g)^2][-1 + g^2/(1 - s_{\sigma}^{*})], \tag{16}$$

where s_{σ}^{*} is determined by sum rules associated with the conservation of particle number,[20]

$$s_{\sigma}^{*} = (1 - (1 - g^2)(n_{\sigma} - n_{-\sigma}) - \{[1 - (1 - g^2)(n_{\sigma} - n_{-\sigma})]^2 - 4(1 - g^2)(1 - n_{\sigma})n_{-\sigma}\}^{1/2})/2(1 - n_{\sigma}). \tag{17}$$

Equations (16) and (17) are of the same form as those obtained by Metzner and Vollhardt.[20] The double occupancy can be expressed in terms of the on-site self-energy s_{σ}^{*},

$$\eta = g^2 n_{\sigma} s_{\sigma}^{*}/[(1 - g^2)(1 - s_{\sigma}^{*})]. \tag{18}$$

(3) Ground-state energy for the Hubbard model. The ground-state energy in the Gutzwiller approximation for the Hubbard Hamiltonian (9) can be variationally calculated by using the expressions for q_{σ} and η. The resulting ground-state energy turns out to be a good approximation even for one- and two-dimensional systems, indicating that this approximation provides a good starting point for a systematic study.

A few remarks are in order. The FHNC//0 approximation in the FHNC theory neglects diagrams involving higher-order statistical exchange functions. It is therefore easy to understand its relationship to the slave-boson approach in view of the similar underlying physics. Our study indicates that the FHNC//0 approximation is a controlled approximation. It is seen that the cc functions associated with the proper self-energy s_{σ}^{*} are $\mathbf{k}$ independent, which is peculiar for $d = \infty$ systems.[28] To go beyond the Gutzwiller approximation, the FHNC theory permits the evaluation of $1/d$ corrections for the Gutzwiller wave function.[4] More important, the FHNC method is capable of handling more complicated dynamical and statistical correlations. It is worth noting that the Gutzwiller approximation amounts to the inclusion of infinite-order elementary diagrams, which indicates that the FHNC approximation scheme based upon truncation to certain order of elementary diagrams (FHNC/n

scheme) has to be improved for dealing with strongly correlated electrons. To this end, the understanding of the Gutzwiller approximation is a useful step towards the development of a generic variational-CBF scheme for the lattice fermion models.

In summary, we have used the FHNC method for the Gutzwiller wave function to show that the results from the FHNC//0 calculation coincide with those of the Gutzwiller approximation. Our calculation is useful for future applications of the FHNC method to the study of strongly correlated electron systems.

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[1] J. W. Clark, L. R. Mead, E. Krotscheck, K. E. Kürten, and M. L. Ristig, Nucl. Phys. A **328**, 45 (1979).
[2] E. Krotscheck, R. A. Smith, J. W. Clark, and R. Panoff, Phys. Rev. B **24**, 6383 (1981); M. Viviani, A. Buendia, S. Fantoni, and S. Rosati, *ibid.* **38**, 4523 (1988).
[3] T. Pang, C. E. Campbell, and E. Krotscheck, Chem. Phys. Lett. **163**, 537 (1989); C. E. Campbell, E. Krotscheck, and T. Pang, Phys. Rep. **223**, 1 (1992).
[4] X. Q. Wang, S. Fantoni, E. Tosatti, L. Yu, and M. Viviani, Phys. Rev. B **41**, 11 479 (1990).
[5] D. Vollhardt, Rev. Mod. Phys. **56**, 99 (1984).
[6] W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302 (1970).
[7] P. W. Anderson, Science **235**, 1196 (1987).
[8] E. Feenberg, *Theory of Quantum Fluids* (Academic, New York, 1969); C. E. Campbell and E. Feenberg, Phys. Rev. **188**, 396 (1969); C. C. Chang and C. E. Campbell, Phys. Rev. B **15**, 4238 (1977).
[9] S. Fantoni and S. Rosati, Nuovo Cimento A **20**, 179 (1974).
[10] E. Krotscheck and M. L. Ristig, Phys. Lett. **48A**, 17 (1974); Nucl. Phys. A **242**, 389 (1975); E. Krotscheck, Ann. Phys. **155**, 1 (1984).
[11] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **56**, 1490 (1987); **56**, 3570 (1987); **56**, 3582 (1987).
[12] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **59**, 121 (1987); Phys. Rev. **37**, 7382 (1988).
[13] F. Gebhard and D. Vollhardt, Phys. Rev. Lett. **59**, 1472 (1987); Phys. Rev. B **38**, 6911 (1988).
[14] B. S. Shastry, Phys. Rev. Lett. **60**, 639 (1988); **69**, 164 (1992).
[15] F. D. M. Haldane, Phys. Rev. Lett. **60**, 635 (1988).
[16] C. Gros, R. Joynt, and T. M. Rice, Phys. Rev. B **36**, 381 (1987).
[17] M. L. Ristig, Z. Phys. B **79**, 351 (1990).
[18] T. A. Kaplan, P. Horsh, and P. Fulde, Phys. Rev. Lett. **49**, 889 (1982); P. Fazekas and K. Penc, Int. J. Mod. Phys. B **1**, 1021 (1988).
[19] M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963); Phys. Rev. **134**, A293 (1964); **137**, A1726 (1965).
[20] W. Metzner, Z. Phys. B **77**, 253 (1989); W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
[21] G. Kotliar and A. E. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986).
[22] E. Krotscheck, Phys. Rev. B **31**, 4267 (1985).
[23] J. W. Clark and M. L. Ristig, in *Momentum Distributions*, edited by R. N. Silver and P. E. Sokol (Plenum, New York, 1989).
[24] E. Krotscheck, Phys. Rev. A **15**, 397 (1977).
[25] Q. N. Usmani, B. Friedman, and V. R. Pandharipande, Phys. Rev. B **25**, 4502 (1982).
[26] M. Viviani, A. Buendia, A. Fabrocini, and S. Rosati, Nuovo Cimento D **8** 561 (1986).
[27] P. G. J. van Dongen, F. Gebhard, and D. Vollhardt, Z. Phys. B **76**, 199 (1989).
[28] E. Müller-Hartmann, Z. Phys. B **74**, 507 (1989).