COMMENTS

Comments are short papers which criticize or correct papers of other authors previously published in **Physical Review B**. *Each Comment should state clearly to which paper it refers and must be accompanied by a brief abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

Comment on "Gutzwiller approximation in the Fermi hypernetted-chain theory"

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The "local-field approximation" Fermi hypernetted-chain scheme is regarded by Wang and Campbell [Phys. Rev. B **47**, 15 984 (1993)] to be equivalent to the Gutzwiller approximation, i.e., to be exact in the infinite dimensional case. We point out that their conclusion is not valid.

Recently, Metzner and Vollhardt[1] have shown that the Gutzwiller approximation (GA) (Ref. 2) becomes an exact solution to the Gutzwiller wave function[3] (GWF) in the infinite dimensions. In the well-known Fermi hypernetted-chain (FHNC) theory,[6,5] unfortunately, there is no closed form for evaluating the elementary diagrams ($E_{\alpha\beta}$) (we adopt the notations for the FHNC quantities and the numbering of equations as used in Ref. 4), which makes the FHNC theory intrinsically approximate in usual cases (e.g., see Refs. 5 and 7 and references therein). However, in the application of the FHNC theory to the lattice Hubbard model, especially with the Gutzwiller ansatz, the exact solutions can be achieved within the FHNC theory in the one dimensional, as well as in the infinite dimensional case.[7,8] Recently, Wang and Campbell (WC) claimed[4] that the "local-field-approximation" (LFA) FHNC scheme yields an exact solution in the infinite dimensional case, which is equivalent to the result of the GA on the GWF. This conclusion is not valid for the following three reasons.

First, the LFA is based on the long wavelength limit, by keeping the most divergent contributions, as caused by the long range correlation tail, in the summation of cluster diagrams. Therefore, the long range correlation effect and Fermi statistics are properly kept in the small momentum limit in the LFA.[5] On the contrary, the GA is based on the conservation of the particle number by neglecting the spatial correlation of particles involved in the particle configurations, which are formed by the on-site Gutzwiller operator acting on the Fermi sea in the paramagnetic case.[9] Consequently, the LFA is still an approximation in $d \to \infty$ (details as seen in the next reason and d is dimensionality), while the GA becomes exact in this limit, since it neglects correlation effects to *higher orders than* $1/\sqrt{d}$. This treatment is carried out only with the statistical operator rather than the dynamical correlation operator in the summation of all the cluster diagrams. It is an incorrect argument in WC's paper that "in infinite dimensions, diagrammatic calculations are greatly simplified by the fundamental property that for $i \neq j$, $P^0_\sigma(i,j)$ scales as $d^{-1/2}$, where d is the dimensionality, and *is thus negligible* in $d = \infty$." In fact, the statistical correlation proportional to $1/\sqrt{d}$ at $r = a$ (a lattice spacing) is essentially kept to evaluate the kinetic energy.[1]

In addition, WC claimed that "of all the diagrams appearing in the FHNC scheme, ..., only on-site terms survive in $d = \infty$," which turns out that they are all $\mathbf{k}$ independent in $\mathbf{k}$ space. Nevertheless, this is only true for two-particle irreducible parts of diagrams. In fact, the bubble diagram $X^0_{ee}(i,j)$, as a basic ingredient for the evaluation of various correlation functions at $d = \infty$, is only one-particle irreducible. In $\mathbf{k}$ space, $X^0_{ee}(\mathbf{k})$ like $P^0_\sigma(\mathbf{k})$ is not $\mathbf{k}$ independent, which originates from the off-site diagonal contributions of $X^0_{ee}(i,j)$. A systematic study on the $\mathbf{k}$ independence at $d = \infty$ has been given by van Dongen *et al.* in Ref. 10.

On the other hand, the GA only includes the $\mathbf{k}_F$ singularity, and the contributions from $3\mathbf{k}_F$ singularity, being of the order of $1/d^{3/2}$, are neglected in the evaluation of the momentum distribution and the kinetic energy, while the modified HNC iterations in the LFA actually go beyond the mean field approximation, i.e., the $3\mathbf{k}_F$ singularity still exists in X_{cc} at $d \neq \infty$, for the momentum distribution function. A corresponding feature associated with $2\mathbf{k}_F$ also occurs for other correlation functions in those two approximations. Therefore, the LFA is intrinsically different from the GA on the basis of physical reasoning. The former is particularly related to the $\mathbf{r} \to \infty$ (or $\mathbf{k} \to 0$) limit, while the later is to the $d \to \infty$ limit.

Second, in the Gutzwiller approximation or in the infinite dimensional case for Gutzwiller wave function,[1,10] one is just faced with the summation over all bubble and bubble chain diagrams owing to the "collapse" of the *proper self energy* and *various vertex functions* in the evaluation of various correlation functions. Setting $X_{de} = 0$ and $X_{ee} = X^0_{ee}$ in WC's paper leads to an incomplete summation over all bubble and bubble chain diagrams in the evaluation of correlation functions. This point is illustrated below.

In the standard FHNC theory as used by WC, one has the following cluster expansion for X_{de}:

$$X_{de}(\mathbf{r}_{12}) = \sum_{n\geq 2} \text{diagrams}(h(\mathbf{r}_{i_1j_1}), \ldots, h(\mathbf{r}_{i_nj_n})),$$

where for each n, all the diagrams having n dynamical correlation factors are summed up. Therefore, *any exact statement related to X_{de} must be valid up to any order of n in the above expression.* More explicitly, for Gutzwiller wave function, one gets,

$$X_{de}(\mathbf{r}_{12}) = \sum_{n\geq 2} \mathcal{C}^n_{de}(\mathbf{r}_{12})(g^2-1)^n,$$

since one can easily integrate out all the dynamical correlation functions $h(\mathbf{r}_{ij}) = (g^2-1)\delta(\mathbf{r}_{ij})$, and $\mathcal{C}^n_{de}$ gives rise to a set of corresponding reduced diagrams one by one (in which dashed lines have been integrated in the original FHNC diagrams) at nth order. $X_{de} = 0$ implies that $\mathcal{C}^n_{de} = 0$, which is not allowed at an exact summation of bubble structure diagrams. For instance, at $n = 2$, there are two X_{de} ($\mathcal{C}^2_{de}$) diagrams as given by two terms in the following equation:

$$\begin{aligned} X_{de}(\mathbf{r}_{12}) &= \sum_{\mathbf{r}_i} h(\mathbf{r}_{12})h(\mathbf{r}_{1i})X^0_{ee}(\mathbf{r}_{i2}) - 2\sum_{\mathbf{r}_i,\mathbf{r}_j} h(\mathbf{r}_{1i})h(\mathbf{r}_{1j})\left(-\frac{1}{2}l(\mathbf{r}_{2i})\right)\left(-\frac{1}{2}l(\mathbf{r}_{ij})\right)\left(-\frac{1}{2}l(\mathbf{r}_{j2})\right) \\ &= \left[-\frac{1}{2}l(0)^2\rho\delta(\mathbf{r}_{12}) - \frac{1}{2}l(0)\rho^2X^0_{ee}(\mathbf{r}_{12})\right](g^2-1)^2. \end{aligned}$$

The second diagram is reduced to a bubble diagram $X^0_{ee}(\mathbf{r}_{12})$, as given by the second term in the last square bracket, the coefficient of which is $-l(0)\rho^2/2$ stemming from the collapse of the corresponding vertex. Therefore, since X^0_{ee} is kept by WC in their chain summation for obtaining density and spin correlation functions, the second diagram must be taken into account in the summation over bubble diagrams, which means that one cannot obtain X_{de} (or $\mathcal{C}^2_{de}$) $= 0$ at $\mathbf{k} \neq 0$, because otherwise the summation of diagrams for the correlation functions is not carried out in an exact sense.

The same fact exists for X_{ee}, where one cannot simply put $X_{ee} = X^0_{ee}$ in the evaluation of the correlation functions. Explicitly, one has, for example, three diagrams at $n = 1$ as follows:

$$X_{ee}(\mathbf{r}_{12}) = \left[-\frac{1}{2}l(0)^2\delta(\mathbf{r}_{12}) - l(0)\rho X^0_{ee}(\mathbf{r}_{12}) - \frac{1}{2}\rho^2\sum_{\mathbf{r}_j} X^0_{ee}(\mathbf{r}_{1j})X^0_{ee}(\mathbf{r}_{j2})\right](g^2-1),$$

where the second term is a bubble diagram and the last one corresponds to a bubble chain diagram, which certainly contribute to the correlation functions.

Moreover, the necessity of having X_{de} and X_{ee} in the bubble diagram summation for evaluation of the correlation function is also seen in canceling some corresponding unphysical nodal diagrams ($N_{\alpha\beta}$). Therefore, *$X_{de} = 0$ and $X_{ee} = X^0_{ee}$ cannot be valid for achieving an exact solution at the level of a summation over bubble diagrams for the evaluation of the correlation functions.*

Finally, two essential Eqs. (13) and (14), related to the momentum distribution, are found being invalid. In the standard FHNC theory which WC were working with, it is well-known that as one can see from Eqs. (4), (5), and (6) of WC's paper, the momentum distribution consists of two parts: one is continuous at $\mathbf{k}_F$, and another is discontinuous at $\mathbf{k}_F$. The coefficient of this discontinuous part gives rise to the jump at $\mathbf{k} = \mathbf{k}_F$, for the momentum distribution as given exactly by

$$q_\sigma = n_{0,\sigma}\frac{(1 + X_{\xi,cc,\sigma} - X_{cc,\sigma})^2}{1 - X_{cc,\sigma}}.$$

However, *the factor $n_{0,\sigma}$ disappeared in Eq. (13)* without any explanation in a physical or mathematical sense. Moreover, from the exact FHNC expressions,[6,8] which sum $X_{cc,\sigma}$ and $X_{\xi,cc,\sigma}$ diagrams up to all the orders, one cannot conclude that $X_{cc,\sigma} = (1+g)X_{\xi,cc,\sigma}$ even in the LFA,[5] *irrespective of* $h(\mathbf{r}) = (1+g)\xi(\mathbf{r})$.

Using the same way for showing that $X_{de} \neq 0$ and $X_{ee} \neq X^0_{ee}$ for the evaluation of the correlation functions, one can also see why $n_{0,\sigma}$ exists in q_σ and why $X_{cc,\sigma} \neq (1+g)X_{\xi,cc,\sigma}$. In fact, it is seen that q_σ, $X_{cc,\sigma}$, and $X_{\xi,cc,\sigma}$ all contain not only physical diagrams, but also unphysical diagrams, which are proportional to $\delta(\mathbf{r}_{12})^n$ ($n \geq 2$). Nevertheless, q_σ, like any other physical quantity, globally does not include any unphysical contribution. In other word, the unphysical diagrams involved in q_σ, $X_{cc,\sigma}$, and $X_{\xi,cc,\sigma}$ are essentially canceled among themselves in the evaluation of q_σ. Consequently, the consistency between the two sides of Eq. (15) is also necessarily questioned.

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