Effects of two-site correlations in the Hubbard model

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Abstract

We propose a theoretical approach, within the framework of the Composite Operator Method, to include the effects of finite cluster correlations into the self-energy of strongly correlated systems. The Hubbard model is analyzed as significant example. The self-energy is rewritten in terms of two-site composite-operator propagators, which are computed by means of a two-site approximation preserving relevant symmetries (e.g., particle-hole symmetry). The involved composite operators describe charge, spin and pair nearest-neighbor correlations and the excitations related to the induced exchange coupling ($J = 4t^2/U$). The procedure results in a very rich band structure going well beyond the results of the two-pole approximation.

Key words: Hubbard model; Composite Operator Method; two-site correlations

Since the discovery of cuprate high-T_c superconductors, many new theoretical approaches have been proposed to describe electronic states subject to the strong correlations present in these materials. In general, the difficulties come from the treatment of the composite excitations emerging in these systems. They cannot be simply expanded in terms of the original electronic fields, especially near the Mott-Hubbard Transition. In this paper, we study the electronic states of the Hubbard model beyond the two-pole approximation within the Composite Operator Method [1,2], which has shown to be capable to describe the physics of strongly correlated systems in a proper way.

The d-dimensional Hubbard Hamiltonian reads as follows,

$$H = \sum_{ij\sigma}(t_{ij} - \mu\delta_{ij})c^\dagger_\sigma(i)c_\sigma(j) + U\sum_i n_\uparrow(i)n_\downarrow(i), \quad (1)$$

where $c^\dagger_\sigma(i)$ and $c_\sigma(i)$ are the creations and annihilation operators of electrons with spin σ at the site i, respectively, $n_\sigma(i) = c^\dagger_\sigma(i)c_\sigma(i)$, μ is the chemical potential, $t_{ij} = -2dt\alpha_{ij}$ with $\mathcal{F}[\alpha_{ij}] = \frac{1}{2}\left[\cos(k_x a) + \cos(k_y a)\right]$, a is the lattice constant, $\mathcal{F}$ is the Fourier transform, U is the on-site Coulomb repulsion. We define the following basis operator,

$$\psi_\sigma(i) = \begin{pmatrix} \xi_\sigma(i) \\ \eta_\sigma(i) \end{pmatrix} = \begin{pmatrix} c_\sigma(i)\left(1 - n_{-\sigma}(i)\right) \\ c_\sigma(i)n_{-\sigma}(i) \end{pmatrix}, \quad (2)$$

where $\xi_\sigma(i)$ and $\eta_\sigma(i)$ describe the transitions $n(i) = 0 \leftrightarrow 1$ and $1 \leftrightarrow 2$, respectively. Its equation of motion reads as

$$i\frac{\partial}{\partial t}\psi_\sigma(i) = \begin{pmatrix} -\mu\xi_\sigma(i) - dtc^\alpha_\sigma(i) - 2dt\pi_\sigma(i) \\ (-\mu + U)\eta_\sigma(i) - dtc^\alpha_\sigma(i) + 2dt\pi_\sigma(i) \end{pmatrix}, \quad (3)$$

where $\pi_\sigma(i) = \left(\frac{1}{2} - n_{-\sigma}(i)\right)c^\alpha_\sigma(i) + c^\dagger_{-\sigma}(i)c_\sigma(i)c^\alpha_{-\sigma}(i) + c_\sigma(i)c^{\alpha\dagger}_{-\sigma}(i)c_{-\sigma}(i)$ with $c^\alpha_\sigma(i) = \sum_j \alpha_{ij}c_\sigma(j)$.

We can rewrite the equation of motion (3) by isolating the term which is linear in the basis as

$$i\frac{\partial}{\partial t}\psi = E\psi + \delta j, \quad (4)$$

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where $E(\mathbf{k}) = m(\mathbf{k})I^{-1}(\mathbf{k})$ with $I(\mathbf{k}) = \mathcal{F}\langle\{\psi,\psi^\dagger\}\rangle$ and $m(\mathbf{k}) = \mathcal{F}\langle\{i\frac{\partial}{\partial t}\psi,\psi^\dagger\}\rangle$. In the paramagnetic and translational invariant state, $I(\mathbf{k})$ is diagonal and uniform: $I_{11} = 1-\langle n\rangle/2$ and $I_{22} = \langle n\rangle/2$. $m(\mathbf{k})$ is symmetric and has the following entries

$$\begin{aligned} m_{11}(\mathbf{k}) &= -\mu I_{11} - 2dt\left[\Delta + \alpha(\mathbf{k})\left(1-\langle n\rangle + p\right)\right] \\ m_{12}(\mathbf{k}) &= m_{21}(\mathbf{k}) = 2dt\left[\Delta - \alpha(\mathbf{k})\left(I_{22} - p\right)\right] \\ m_{22}(\mathbf{k}) &= \left[-\mu + U\right] I_{22} - 2dt\left[\Delta + \alpha(\mathbf{k})p\right], \end{aligned} \tag{5}$$

with

$$\Delta = \langle \xi^\alpha_\uparrow(i)\xi^\dagger_\uparrow(i)\rangle - \langle \eta^\alpha_\uparrow(i)\eta^\dagger_\uparrow(i)\rangle \tag{6}$$

$$p = \frac{1}{4}\langle n_\nu(i) n^\alpha_\nu(i)\rangle - \langle (c_\uparrow(i)c_\downarrow(i))^\alpha c^\dagger_\downarrow(i)c^\dagger_\uparrow(i)\rangle, \tag{7}$$

where $n_\nu(i)$ is the charge ($\nu = 0$) and spin ($\nu = 1,2,3$) density operator. δj is the residual term as it is orthogonal, in the sense of the averaged anticommutators, to the basic field ψ; it contains the two-site composite excitations. The thermal retarded Green's function $G(\mathbf{k},\omega) = \mathcal{F}\langle\mathcal{R}[\psi(i),\psi^\dagger(j)]\rangle$ has the structure,

$$G(\mathbf{k},\omega) = \frac{1}{\omega - E(\mathbf{k}) - \Sigma(\mathbf{k},\omega)} I. \tag{8}$$

where the self-energy $\Sigma(\mathbf{k},\omega)$ reads as,

$$\Sigma(\mathbf{k},\omega) = \frac{1}{I + A(\mathbf{k},\omega)} B(\mathbf{k},\omega) I^{-1}, \tag{9}$$

with $A(\mathbf{k},\omega) = \mathcal{F}\langle\mathcal{R}[\delta j,\psi^\dagger]\rangle$ and $B(\mathbf{k},\omega) = \mathcal{F}\langle\mathcal{R}[\delta j,\delta j^\dagger]\rangle$. By neglecting δj (i.e., by setting $\Sigma(\mathbf{k},\omega) = 0$) we obtain a generalized mean field approximation in terms of the Hubbard operators, which shows a two-band structure [2]. To improve the solution beyond the two-pole approximation, we need to take into account the self-energy contribution.

In order to do this, we introduce a 6-component basis φ which reads as: $\varphi_1(i) = \xi(i)$, $\varphi_2(i) = \eta(i)$ and

$$\varphi_3(i) = \xi_{s\sigma}(i) = \sum_j \alpha_{ij}\bar{\xi}_{s\sigma}(ij) \tag{10}$$

$$\varphi_4(i) = \eta_{s\sigma}(i) = \pi_\sigma(i) - \xi_{s\sigma}(i) = \sum_j \alpha_{ij}\bar{\eta}_{s\sigma}(ij) \tag{11}$$

$$\varphi_5(i) = \tilde{\xi}_{s\sigma}(i) = \sum_j \alpha_{ij}\bar{\xi}_{s\sigma}(ji) \tag{12}$$

$$\varphi_6(i) = \tilde{\eta}_{s\sigma}(i) = \sum_j \alpha_{ij}\bar{\eta}_{s\sigma}(ji) \tag{13}$$

with

$$\begin{aligned} \bar{\xi}_{s\sigma}(ij) &= (1/2 - n_{-\sigma}(i))\xi_\sigma(j) + c^\dagger_{-\sigma}(i)c_\sigma(i)\xi_{-\sigma}(j) \\ &\quad - \eta^\dagger_{-\sigma}(j)c_\sigma(i)c_{-\sigma}(i) \\ \bar{\eta}_{s\sigma}(ij) &= (1/2 - n_{-\sigma}(i))\eta_\sigma(j) + c^\dagger_{-\sigma}(i)c_\sigma(i)\eta_{-\sigma}(j) \\ &\quad - \xi^\dagger_{-\sigma}(j)c_\sigma(i)c_{-\sigma}(i). \end{aligned} \tag{14, 15}$$

φ_1 to φ_4 will permit us to exactly rewrite

$$\delta j(i) = \begin{pmatrix} \Delta j(i) \\ -\Delta j(i) \end{pmatrix} \tag{16}$$

$$\Delta j(i) = \sum_{n=1}^{4}\sum_j \lambda_n(i,j)\varphi_n(j) \tag{17}$$

where $\lambda(\mathbf{k}) = \mathcal{F}[\lambda(i,j)]$ has the following expression

$$\lambda_1(\mathbf{k}) = 2dt\left[\Delta + \alpha(\mathbf{k})(p + I_{11}/2 - I_{22})\right]/I_{11} \tag{18}$$

$$\lambda_2(\mathbf{k}) = -2dt\left[\Delta + \alpha(\mathbf{k})(p - I_{22}/2)\right]/I_{22} \tag{19}$$

$$\lambda_3(\mathbf{k}) = \lambda_4(\mathbf{k}) = -2dt \tag{20}$$

Accordingly, $A(\mathbf{k},\omega)$ and $B(\mathbf{k},\omega)$ can be exactly rewritten in terms of $S(\mathbf{k},\omega) = \mathcal{F}\langle\mathcal{R}[\varphi(i),\varphi^\dagger(j)]\rangle$.

Then, we linearize the equation of motion of φ by means of a two-site approximation reducing any higher-order field to its two-site component and explicitly preserving the particle-hole symmetry. This latter requirement forced the introduction of φ_5 and φ_6 [3]. It is worth mentioning that the four fields ξ, η, ξ_s and η_s are a complete fermionic set of eigenoperators for the two-site Hubbard model [4] and exactly describe its two relevant scales of energy U and $J = 4t^2/U$. Then, with the approximate expression of the propagator $S(\mathbf{k},\omega)$ we can finally compute the self-energy $\Sigma(\mathbf{k},\omega)$ and the thermal retarded Green's function $G(\mathbf{k},\omega)$.

We are left with the problem of fixing the parameters Δ, p and μ. Δ can be computed, through its definition, directly from the Green's function. p and μ will be computed self-consistently from the constraint $\langle\xi^\dagger(i)\eta(i)\rangle = 0$ required by the Pauli principle and the equation defining the electron number density $\langle n\rangle$ as a function of the Green's function elements.

The presented procedure will give us a solution with a very rich band structure which is well beyond the one obtained by the two-pole approximation. The details of the formula and the computational implementation will be presented elsewhere.

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