A 4-pole approach to the Hubbard model within the Composite Operator Method

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Abstract. The Hubbard model is studied within the Composite Operator Method framework in a 4-pole approximation. The operatorial basis is chosen according to both the hierarchy of equations of motion and the exact solution of the model reduced to the minimal cluster (2 sites) where all Hamiltonian terms are still active. Such a recipe amounts to include into the basis not only the two Hubbard operators, which usually take care of the scale of energy related to the on-site Coulomb repulsion \( U \), but also two other non-local operators describing the Hubbard operators dressed by charge, spin and pair fluctuations on the nearest-neighboring sites and addressing the dynamically generated scale of energy related to the exchange \( J = 4t^2/U \). The calculation framework is outlined and a very first comparison to numerical simulations, showing very good qualitative and quantitative agreement, is reported. As reference, the results in the 2-pole approximation are also reported and the differences discussed.

1. Introduction

Strongly correlated systems in solid state physics and condensed matter theory pose such a difficult, but inspiring, challenge to be by far one of the research fields with the higher number of active scholars. Among all other open quests in the field, the one for an analytical calculation framework capable to catch the most relevant features of the many model Hamiltonians proposed in the literature is surely very exciting and fundamental to any advancement in the understanding of these systems. The Composite Operator Method (COM) \cite{1, 2} has proved to be quite efficient in capturing the anomalous unconventional features \cite{3, 4} of the Hubbard model \cite{5, 6}, which is the prototype of all strongly correlated systems in absence of extrinsic magnetic defects. COM is based on three main ingredients: the use of a basis, for the relevant Green’s functions, consisting of composite fields (that is, fields obtained by the composition of canonical electronic fields) embedding as much as possible of the interactions under study; the use of Algebra Constraints \cite{1, 2} to impose relevant symmetries - secure the correct Hilbert space as well as to determine the unknowns of the theory; the choice of an appropriate (with respect to the specific case under study) treatment of the residual self-energy \cite{1, 2} in order to describe the interactions among the composite field adopted in the basis.

In this short manuscript, we outline a calculation framework where the Composite Operator Method is applied to the two-dimensional Hubbard model: a basis of four composite fields is chosen, the unknowns of the theory are fixed by means of Algebra Constraints as well as by
exploiting the knowledge of the exact solution on two sites, the residual self-energy is neglected so that the approximation used falls into the 4-pole class. A very first comparison to numerical simulation data (specifically quantum Monte Carlo ones) for the double occupancy is reported and analysed. 2-pole approximation results, obtained within the same COM framework, are also reported in order to establish the main differences and the quantitative and qualitative improvements obtained by augmenting the number of poles.

2. Formulation

2.1. The Hamiltonian

The Hamiltonian of the 2-dimensional Hubbard model reads as

$$H = \sum_{ij} (-4t \alpha_{ij} - \mu \delta_{ij}) c_i^\dagger c_j + U \sum_i n_i^\dagger n_i (1)$$

where $i$ is a vector of the lattice; $t$ is the hopping and the energy unit; $\alpha_{ij}$ is the projector on the nearest-neighbour sites; $\mu$ is the chemical potential; $U$ is the strength of the on-site Coulomb repulsion; the electronic operators $c(i)$ and $c^\dagger(i)$, as well as all other fermionic operators, are expressed in the spinorial notation and in the Heisenberg picture ($i = (i, t)$); $n_\sigma(i) = c^{\dagger}_\sigma(i)c_\sigma(i)$ is the electronic number operator of an electron of spin $\sigma$.

2.2. The equations of motion

The electronic operator $c(i)$ obeys the following equation of motion

$$i \frac{\partial}{\partial t} c(i) = -\mu c(i) - 4tc^\alpha(i) + U \eta(i) (2)$$

Hereafter, given a generic operator $\Phi(t)$, we will use the notation $\Phi^{\kappa}(i) = \sum_{\gamma} \kappa_{ij} \Phi(j, t)$ for any projector $\kappa$ (e.g. $\kappa = \alpha, \alpha^2, ...$).

The Hubbard operators $\xi(i) = c(i) - \eta(i)$ and $\eta(i) = n(i)c(i)$ ($n(i) = c^\dagger(i)c(i)$) satisfy the following equations of motion

$$i \frac{\partial}{\partial t} \xi(i) = -\mu \xi(i) - 4tc^\alpha(i) - 4t (\xi_s(i) + \eta_\sigma(i)) (3)$$

$$i \frac{\partial}{\partial t} \eta(i) = (U - \mu) \eta(i) + 4t (\xi_s(i) + \eta_\sigma(i)) (4)$$

Keeping only the 2-site terms ($\delta_{ij}$ and $\alpha_{ij}$) and forcing a particle-hole symmetric closure, the operators $\xi_s(i) = \frac{1}{2} \sigma^\mu n_\mu(i) \xi^\sigma(i) + \eta^\sigma(i) c(i)c(i)$ and $\eta_\sigma(i) = \frac{1}{2} \sigma^\mu n_\mu(i) \eta^\sigma(i) + \xi^\sigma(i) c(i)c(i)$ enter the following approximated equations of motion

$$i \frac{\partial}{\partial t} \xi_s(i) \approx -\mu \xi_s(i) + 8t \eta^2 \xi_s(i) + 4t \xi^\sigma(i) + 8t \eta^\sigma(i) \approx (U - \mu) \eta_\sigma(i) + 4t \xi^\sigma(i) (5)$$

$$i \frac{\partial}{\partial t} \eta_\sigma(i) \approx (U - \mu) \eta_\sigma(i) + 4t \eta^\sigma(i) + 4t \xi^\sigma(i) \approx (U - \mu) \eta_\sigma(i) + 4t \xi^\sigma(i) (6)$$

where $n_\mu(i) = c^\dagger(i)\sigma_\mu c(i)$, $\sigma^\mu = (-1, \vec{\sigma})$ and $\sigma_\mu = (1, \vec{\sigma})$, where $\vec{\sigma}$ are the Pauli matrices.

2.3. The basis

Given the above reported equations (3-6) of motion and the full knowledge of the exact solution, within the COM framework [7], of the corresponding two-site system, we have chosen as
operatorial basis for our fermionic retarded Green’s function $G^R(i, j) = \langle \mathcal{R}\{\psi(i), \psi^\dagger(j)\}\rangle$ the following one

$$\psi(i) = \left(\begin{array}{c}
\xi(i) \\
\eta(i) \\
\xi_s(i) \\
\eta_s(i)
\end{array}\right)$$

(7)

The first two fields describe the Hubbard subbands and, consequently, the scale of energy of $U$. The second two fields, together with the first two, give a fermionic closed basis [2] for the Hubbard model on two sites [7] and, in such a case, they open up the possibility to access and exactly describe the virtual exchange energy $J = 4t^2/U$.

This basis, once the equations (5-6) are enforced, closes the following equation of motion

$$\frac{i}{\hbar}\frac{\partial}{\partial t} \psi(i) = [\psi(i), H] \cong \sum_j \varepsilon(i,j)\psi(j,t)$$

(8)

where $\varepsilon(i,j)$, named energy matrix, has entries that can be just read in equations (3-6). Following this route, we have neglected residual terms in the current ($i\frac{\partial}{\partial t}\psi(i)$) of the chosen basis that would lead to the appearance of higher-order composite operators.

2.4. The normalization matrix

The equation of motion (8) leads to the following expression of the Green’s function $G^R(i, j)$

$$G^R(k, \omega) = \frac{1}{\omega - \varepsilon(k) + i\delta} I(k)$$

(9)

where $I(i,j) = \langle \{\psi(i,t), \psi^\dagger(j,t)\}\rangle$ is the normalization matrix, whose entries have the following expressions

$$I_{\xi\xi}(k) = 1 - \frac{n}{2}$$

(10)

$$I_{\eta\eta}(k) = 0$$

(11)

$$I_{\xi\eta}(k) = \frac{n}{2}$$

(12)

$$I_{\xi,\xi}(k) = \Delta + \alpha(k) \left(p - \frac{n}{2}\right)$$

(13)

$$I_{\eta,\eta}(k) = 0$$

(14)

$$I_{\eta,\xi}(k) = 0$$

(15)

$$I_{\eta,\eta}(k) = -\Delta - \alpha(k)p$$

(16)

$$I_{\xi,\eta}(k) = I_{\eta,\xi}(k)$$

(17)

$$I_{\xi,\eta}(k) = I_{\eta,\xi}(k)$$

(18)

$$I_{\eta,\eta}(k) = I_{\eta,\eta}(k)$$

(19)

where $\Delta = C_{11}^\alpha - C_{22}^\alpha$, $p = \frac{1}{4}\langle n_{\alpha}(i)n_{\beta}(i) \rangle - \langle |c_{\uparrow}(i)c_{\downarrow}(i)|^\alpha c_{\downarrow}^\dagger(i)c_{\uparrow}^\dagger(i) \rangle$ and $C_{ab}^\alpha = \langle \psi_{\alpha}^a(i)\psi_{\beta}^b(i) \rangle$.

$\beta(k)$ and $\eta(k)$ are the projectors on the second-neighbour sites along the diagonals and the main directions of the lattice, respectively.

$I_{\xi,\xi}(k)$, $I_{\xi,\xi}(k)$, $I_{\xi,\eta}(k)$, $I_{\xi,\eta}(k)$, $I_{\eta,\eta}(k)$, $I_{\eta,\eta}(k)$, $I_{\eta,\eta}(k)$, and $I_{\eta,\eta}(k)$ have so lengthy and complex forms (very many correlation functions of higher-order appear) that we were forced to reduce them to treatable expressions (where no new higher-order correlation functions are present) by selecting only two-site correlation functions and mode-coupling non-nearest-neighbor charge, spin, and pair correlations function.
2.5. Self-consistency

The only self-consistent parameters not connected to correlation functions straightforwardly attainable by the Green’s function exploiting the fluctuation-dissipation theorem in a self-consistent manner are $\mu$ and $p$. They will be fixed by the following two equations

$$n = 2(1 - C_{11} - C_{22})$$

$$C_{12} = 0$$

where $C_{ab} = \langle \psi_a(i) \psi_b^\dagger(i) \rangle$. These two equations should be added to all others coming from the fluctuation-dissipation theorem. The first equation trivially fixes the number of particles in a self-consistent way and directly springs from the definition of the chemical potential. The second equation is an Algebra Constraint [1, 2] coming from the Pauli exclusion principle and can be easily traced back to $c_\sigma(i)c_\sigma(i) = 0$. Such a constraint will ensure that no spurious same-spin double-occupancy of any site can take place securing the fundamental connection between charge configurations and spin ones at the basis of the exchange processes that rule low-energy physics of the model.

3. Results

In fig. 1, we present the double occupancy $D = \langle n_\uparrow(i)n_\downarrow(i) \rangle = I_{nn} - C_{22}$ for $T = 1/6$ as function of doping $n$ for two different values of the Coulomb repulsion $U$ ($U = 1, 2$). The quantum Monte Carlo (qMC) data refer to a 12 $\times$ 12 cluster [8]. The COM results in the 2-pole approximation for both $p < 0$ and $p > 0$ solutions are also reported for reference and comparison. We can see that the 4-pole approximation results improve upon the 2-pole ones as they better reproduce the numerical data both quantitatively and qualitatively. In particular, the 4-pole approximation results are closer to the numerical points in average and, much more relevant, they manage to interpolate between the $p < 0$ and $p > 0$ 2-pole solutions. As a matter of fact, the 4-pole solution avoids the extended zero-double-occupancy region in filling featured by the 2-pole $p > 0$ solution, but not by the $p < 0$ one, but also the sudden down-turn featured by the 2-pole $p < 0$ solution, but not by the $p > 0$ one. Accordingly, the 4-pole solution seems to capture the best of both 2-pole solutions.
4. Conclusions
In this very short manuscript, we have outlined a 4-pole approximation for the two-dimensional Hubbard model within the Composite Operator Method framework. The choices related to the basis, the closure of the equations of motion, the determination of the normalization matrix and of the energy matrix have been discussed and their main aspects illustrated in some detail. The results of such a 4-pole approximation, as regards a very fundamental local quantity, the double occupancy, have been compared with those of numerical simulation, i.e. quantum Monte Carlo, and of the corresponding 2-pole approximation [1] (for both flavours available: $p < 0$ and $p > 0$). The 4-pole approximation performs better than both 2-pole ones and seems to nicely interpolate between them retaining only the better aspects of both. This result is quite encouraging and we are planning to extend the present 4-pole analysis to the study of single-particle and thermodynamics properties of the Hubbard model.

Acknowledgments
A. A. thanks the Max-Planck-Institut FKF Stuttgart for hospitality and financial support.

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