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Variational cluster approximation and exact diagonalization for calculation of Hubbard models

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Abstract. The numerical method was developed that combines the variational cluster approximation and the exact diagonalization techniques to solve Hubbard models of various dimensionality, number of orbitals, and lattice geometry. The developed method was tested on the one-band Hubbard model; antiferromagnetic ordering and the superconducting phase were observed, in accordance with known results obtained by other techniques. The method may be successfully used for studying properties of high-temperature superconductors.

1. Introduction
The Hubbard model, now is 55 years old [1], is one of the most used, simple and at the same time complex models in condensed matter physics. Its history began in 1963 [2–4], when it was introduced to explain properties of transition-metal monoxides. Since when, the model has had various successful applications, the most remarkable of which were its use for describing cuprate high-temperature superconductors (HTSCs) and systems in optical lattices [5, 6]. Despite it's seeming simplicity, the model is a hard mathematical problem and has no analytical solution in general case; therefore, a great number of analytical approximation methods, as well as numerical techniques, were developed for Hubbard model for specific systems.

After the discovery of high-temperature superconductivity in iron-based compounds [7], the question of the nature of this phenomenon arose with a new importance, since, on the one hand, new compounds possessed a layered crystal structure similar to cuprate HTSCs, and, on the other hand, they had a more complex electronic subsystem with several orbitals. The corresponding multi-orbital Hubbard model is much more complicated [8]. Numerical methods are required to solve it, which are able to take into account the dynamics and nonlocality of the correlation properties of the system and to correctly describe its phase states under changing of external parameters (e.g., doping or temperature).

Variational cluster approximation (VCA), introduced in [9], applies to models with local interactions and accounts for both short-range correlations and long-range order by means of exact diagonalization of finite clusters and variational optimization of a symmetry-breaking fields. It may be used for zero or finite temperature calculations, is free of the sign problem, which is characteristic of Monte Carlo algorithms for Fermi systems, and is numerically less demanding compared with methods based on dynamical mean-field theory (DMFT).

The aim of this work is to develop a numerical technique that implements the VCA for solving the Hubbard model and its extensions to the cases of multiple orbitals, various dimensionality and various lattice geometries, with the possibility of taking into account the change in the external parameters of
the model and potential future application for studying correlation properties of HTSCs. The developed method was tested on the one-band Hubbard model; antiferromagnetic ordering and the superconducting phase were observed, in accordance with known results obtained by other techniques.

2. Method

Variational cluster approximation is based on the Potthoff functional \[10\] defined for many-body Hamiltonian \( H = T + V \) with one-particle part \( T \) and two-particle part \( V \):

\[
\Omega[\Sigma] = F_V[\Sigma] - \text{Tr} \ln (G_0^{-1} - \Sigma).
\] (1)

Here \( F_V[\Sigma] \) is the Legendre transform of the Luttinger-Ward functional; \( G_0 \) is the Green’s function of the system without interaction; \( \Sigma \) is the self-energy. The functional \( \Omega[\Sigma] \) is stationary at the physical self-energy of the system, and at this point it has the meaning of the grand potential of the system. Therefore, the problem reduces to the search for stationary points of the functional \( \Omega[\Sigma] \).

The functional \( F_V[\Sigma] \) has the property of universality, i.e. it depends only on the interaction \( V \), and not on \( T \). This property allows one to associate the functional of the whole system with the functional of a reference system described by a Hamiltonian \( H' = T' + V \) which differs from \( H \) only by its one-particle part:

\[
\Omega[\Sigma] + \text{Tr} \ln (G_0^{-1} - \Sigma) = \Omega'[\Sigma] + \text{Tr} \ln (G_0'^{-1} - \Sigma),
\] (2)

and, therefore,

\[
\Omega[\Sigma] = \Omega'[\Sigma] - \text{Tr} \ln (1 + (G_0^{-1} - G_0'^{-1}) G').
\] (3)

The reference system is chosen in such a way that it is accessible to exact evaluation by numerical methods. The above equation is exact; however, it cannot be solved in this form, as the dependence \( \Omega[\Sigma] \) is unknown. The idea of VCA is to replace the dependencies \( \Omega[\Sigma] \) and \( \Omega'[\Sigma] \) by approximated ones \( \Omega[\Sigma'] \) and \( \Omega'[\Sigma'] \), where \( \Sigma' \) is the self-energy of the reference system. This approximation becomes exact in the limit of infinite size of the reference system and is based on the assumption that the self-energy, in most general cases, is much more local quantity compared with, e.g., the Green’s function.

Since the size of the reference system is usually small enough because of the restrictions associated with the exponential growth of the dimension of the Hilbert space with the system size, it is not possible to observe directly the symmetry breaking corresponding to a phase transition by searching for the stationary point of \( \Omega[\Sigma'] \). Instead, one introduces fictitious one-particle Weiss fields \( W \),

\[
H = (T + W) + (V - W)
\] (4)

that are local to each reference system and represent the effect of the rest of the system. For example, the Weiss field associated with the AFM ordering has the form

\[
W_{AFM} = M \sum_i e^{iQr_i}(n_{i\uparrow} - n_{i\downarrow}),
\] (5)

where \( Q \) is AFM form factor, and the Weiss field associated with the superconducting phase is

\[
W_{SC} = D \sum_{ij} (\Delta_{ij} c_{i\uparrow} c_{j\downarrow} + h.c.),
\] (6)

where \( \Delta_{ij} \) is the superconducting order parameter. If the stationary point obtained by varying of \( \Omega \) with respect to the amplitude of the Weiss field (\( M \) or \( D \) in the above-mentioned examples) corresponds to a non-zero value of the amplitude, then the system has the corresponding symmetry.

The realization of VCA, therefore, consists of the following steps:

a) to construct the Hamiltonian of the reference system in the Fock basis;
b) to diagonalize the Hamiltonian of the reference system and to obtain the energy and the wave functions of the eigenstates;
c) to calculate the Green's function of the reference system;
d) to calculate the value of the Potthoff functional;
e) to find stationary points of the Potthoff functional;
f) to calculate the Green's function of the whole system and its spectral characteristics.

3. Implementation

The first step in the practical implementation of the VCA algorithm is the construction of the Hamilton matrix in the Fock basis $|n_1^{\uparrow}n_1^{\downarrow}n_2^{\uparrow}n_2^{\downarrow} \ldots \rangle$. The basis states may be conveniently represented in a 32-bit ‘unsigned integer’-type encoding in the form of a binary array of the length equal to the number of states in the system. For a given basis, a set of matrices corresponding to annihilation operators $c_{i\sigma}$ is assembled; the matrices of creation operators $c_{i\sigma}^+$ are constructed by complex conjugation. The whole Hamiltonian is obtained by a sequence of multiplying and adding matrices of creation and annihilation operators (Figure 1). This approach allows one to quickly compile the Hamiltonian of the system taking into account any admixture of the Weiss field.

![Figure 1](image1.png)

**Figure 1.** Construction of the Hamilton matrix for an 8-sites Hubbard cluster (65536 states). Non-zero matrix elements are shown in blue.

The energy and the wave function of the ground state of the system are determined with the help of Lanczos algorithm. This algorithm is extremely widely used in the field of studying strong-correlated systems [11] since it usually convergences fast (about 100-300 iterations for a 12-sites Hubbard cluster). In our VCA implementation, the standard Lanczos algorithm was taken from the ARPACK library.

To calculate the Green’s function, the block Lanczos algorithm is used. This algorithm is the fastest one in calculating off-diagonal correlators of the Hubbard model. The convergence time of this algorithm approximately equals the convergence time of the standard Lanczos algorithm. The resulting Green’s function is obtained in Lehmann representation.

The calculation of the Potthoff functional

$$
\Omega[\Sigma] = \Omega'[\Sigma] - \text{Tr} \ln(1 + (G_0^{-1} - G_0^{-1}) G') = \Omega' - \int_0^\infty \frac{d\omega}{\pi} \int_{BZ} \ln |\det \left( (1 + V(k)) G'(i\omega) \right)|
$$

is implemented with the use of QUADPACK software. Integration is performed according to the following scheme. First, the integration over the Brillouin zone is performed for each value of the frequency. The integration over frequencies is carried out by dividing the frequency domain into three segments: from zero to the energy of the minimum one-particle excitation obtained by the block Lanczos algorithm, then from the minimum to the maximum one-particle excitation, and from the maximum one-particle excitation to infinity. This partition allows correctly to take into account each type of excitation in the system, both low-energy and high-energy ones.

The determination of the stationary point of the Potthoff functional is carried out by widely used Newton method. The main advantage of this method is a small number of calculations of $\Omega$, which are extremely time-consuming.
4. Results

The developed software package was used to study the two-dimensional Hubbard model of the type

$$H = -\sum_{\langle ij \rangle} t (c_{i\sigma}^+ c_{j\sigma} + h. c.) - \sum_{\langle\langle ij \rangle\rangle} t' (c_{i\sigma}^+ c_{j\sigma} + h. c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_i n_{i\sigma}. \tag{8}$$

Here operator $c_{i\sigma}^+$ ($c_{i\sigma}$) creates (annihilates) an electron with spin $\sigma$ on site $i$; $U$ is on-site Coulomb interaction; $\mu$ is the chemical potential; $t$ and $t'$ describe nearest-neighbor and next-nearest-neighbor hoppings, respectively. The following values were chosen:

$$U = 8; \quad t = -1; \quad t' = -0.3t. \tag{9}$$

At the half-filling, the dependence of the Potthoff functional on the amplitude of the AFM Weiss field has a non-trivial stationary point for the form-factor $Q = (\pi, \pi)$ (Figure 2), which corresponds to the presence of ‘chess’-like AFM ordering and spontaneous symmetry breaking phase. The band structure in this phase has typical flat bands (Figure 3) which match magnetic ordering in the system.

At low electron doping $\delta = 0.04$, both AFM ordering and the superconducting phase are present in the system. The band structure in this case is shown in Figure 4. It has not only flat bands because of AFM, but also a superconducting gap near $K$ point. The Fermi surface, which is also located near $K$ point, is shown in Figure 5. This result is in a good agreement with ARPES experiment on cuprate HTSCs [12].

![Figure 2. Non-trivial stationary point of the Potthoff functional corresponding to AFM ordering.](image)

![Figure 3. The band structure at half-filling. Flat bands correspond to AFM ordering.](image)

![Figure 4. The band structure at electron doping. Both AFM and SC gaps are present.](image)

![Figure 5. The Fermi surface at electron doping.](image)
At hole-doping, AFM ordering ceases to exist, and the corresponding band structure has no flat bands, but the superconducting gap is still present between \( \Gamma \) and \( X \) points (Figure 6). The Fermi surface (Figure 7) is located in the same region of the reciprocal space. Even in this case, despite the smallness of the cluster used in VCA, a good agreement with the experimental ARPES data on cuprate HTSCs is observed [13].

![Figure 6](image6.png)

**Figure 6.** The band structure at hole doping. The system is in SC state.

![Figure 7](image7.png)

**Figure 7.** The Fermi surface at hole doping.

### 5. Conclusions

In this work, we have developed the numerical technique that realizes the variational cluster approximation for solving the Hubbard model and its generalizations taking into account systems of various dimensionality, with multiple orbitals, and various lattice geometries. The method was successfully tested on the one-band Hubbard model; antiferromagnetic ordering and the superconducting phase were observed, in accordance with known results obtained by other experimental and numerical techniques. The method may be used for studying properties of high-temperature superconductors.

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