Charge Ordering in Extended Hubbard Models: Variational Cluster Approach

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Introduction

In recent years an increasing number of theoretical and experimental studies in condensed matter physics have focused on the description and understanding of quasi one and two dimensional strongly correlated electronic systems. Several fascinating properties of these materials are due to the competition between different phases with long-range order. For many theoretical investigations of strongly correlated materials the Hubbard model is used, which consist of nearest neighbor hopping and Coulomb interaction U locally on each site. Although this model was used with great success for the description of a wide class of materials, there are interesting physical questions which require an extension. The inclusion of the nearest-neighbor Coulomb interaction, for example, is necessary for the study of inhomogeneous phases, such as the charge-density wave (CDW). This leads to the so called extended Hubbard model (EHM).

Here we present a generalization of the recently proposed variational cluster perturbation theory to extended Hubbard models at half filling with repulsive nearest neighbor interaction.[1] The method takes into account short-range correlations correctly by the exact diagonalisation of clusters of finite size, whereas long-range order beyond the size of the clusters is treated on a mean-field level.

Cluster Perturbation Theory (CPT)

First the original lattice is decoupled into clusters of finite size yielding the Hamiltonian

$$H = \sum_{\mathbf{R}} \left[H_0^{(\mathrm{c})}(\mathbf{R}) + H_1(\mathbf{R}) \right] + \sum_{\mathbf{R},\mathbf{R}'} H_0^{(\mathrm{i})}(\mathbf{R},\mathbf{R}'), \qquad (1)$$

where $\mathbf{R}$ labels the individual clusters, $H_1(\mathbf{R})$ is the interacting part, $H_0^{(\mathrm{c})}(\mathbf{R})$ the intra-cluster single-particle part, and $H_0^{(\mathrm{i})}(\mathbf{R},\mathbf{R}')$ the single-particle inter-cluster coupling, given by

$$H_0^{(\mathrm{i})}(\mathbf{R},\mathbf{R}') = \sum_{a,b} T_{a,b}^{\mathbf{R},\mathbf{R}'} c^\dagger_{\mathbf{R},a} c_{\mathbf{R}',b}. \qquad (2)$$

The indices a and b are general quantum numbers within a cluster. The CPT approximation[2] for the Green's function is expressed in terms of the cluster Green's function $\mathbf{G}'(\omega) = G'_{a,b}(\omega)$

$$\mathbf{G}_{\mathbf{Q}}(\omega) = \left[\mathbf{G}'(\omega)^{-1} - \mathbf{T}_{\mathbf{Q}} \right]^{-1}, \qquad (3)$$

with $T_{\mathbf{Q},a,b}$ the super-cluster Fourier transformed hopping matrix. The approximation Eq. (3) is exact in the limits $t \to 0$ and $U \to 0$.

Variational Cluster Perturbation Theory (V-CPT)

Observation underlying V-CPT:[3] Perturbation term $H_0^{(\mathrm{i})}(\mathbf{R},\mathbf{R}')$ need not be fixed to inter-cluster hopping. It is easy to see that the Hamiltonian is invariant under the transformation

$$\begin{aligned} H_0^{(\mathrm{c})}(\mathbf{R}) &\to H_0^{(\mathrm{c})}(\mathbf{R}) + \mathcal{O}(\mathbf{R}) \\ H_0^{(\mathrm{i})}(\mathbf{R},\mathbf{R}') &\to H_0^{(\mathrm{i})}(\mathbf{R},\mathbf{R}') - \delta_{\mathbf{R},\mathbf{R}'}\mathcal{O}(\mathbf{R}), \end{aligned} \qquad (4)$$

with an arbitrary intra-cluster single-particle operator

$$\mathcal{O}(\mathbf{R}) = \sum_{a,b} \Delta_{a,b}\, c^\dagger_{\mathbf{R},a} c_{\mathbf{R},b}, \qquad (5)$$

$\mathcal{O}(\mathbf{R})$ can consist of any single-particle operator of the original Hamiltonian, and of additional single-particle operators like a staggered chemical potential or staggered magnetic field.

For free fermions the result is independent of the transformation Eq. (4), since in this case Eq. (3) is exact. In the interacting case the result depends on the particular choice of $\mathcal{O}(\mathbf{R})$. The optimal choice for $\mathbf{\Delta} = \Delta_{a,b}$ can be answered by the Self-Energy-Functional Approach (SFA):[4] The best choice for the variational parameters $\mathbf{\Delta}$ is given by the stationary point of the grand potential

$$\begin{aligned} \Omega(\mathbf{\Delta}) = \Omega'(\mathbf{\Delta}) &\\ + T \sum_{\omega_n,\mathbf{Q}} \mathrm{tr}\, \ln \frac{-\mathbf{1}}{\mathbf{G}^{(0)}_{\mathbf{Q}}(i\omega_n)^{-1} - \mathbf{\Sigma}(\mathbf{\Delta}, i\omega_n)} &\\ - LT \sum_{\omega_n} \mathrm{tr}\, \ln(-\mathbf{G}'(\mathbf{\Delta}, i\omega_n)). & \end{aligned} \qquad (6)$$

$\Omega'(\mathbf{\Delta})$, $\mathbf{\Sigma}(\mathbf{\Delta}, i\omega_n)$, and $\mathbf{G}'(\mathbf{\Delta}, i\omega_n)$ are the grand potential, self energy, and Green's function on the cluster obtained by the Lanczos procedure, and L is the number of clusters ($\mathbf{Q}$ points). In the following the grand potential is evaluated by analytic continuation to the real frequency axis and frequency integration.

V-CPT for Extended Hubbard models

The perturbation term, which couples the individual clusters, must be of single-particle type. Thus we perform a Mean-Field decoupling of the Coulomb interaction on inter-cluster bonds, yielding external mean-field parameters λ_i. We propose two procedures to determine the λ_i:

1. Self-consistent determination on an isolated cluster. Only suitable for first-order transitions.
2. From the SFA grand potential: Here we have $\Omega = \Omega(\mathbf{\Delta}, \lambda_i)$, which reduces after SFA-optimization to a function $\Omega = \Omega(\lambda_i)$. The proper values for the λ_i are given by the minimum of this function.

1D – Phase transition

We study the 1D EHM at half-filling, which means that we have only one mean-field parameter δ and the average densities on sublattices A and B are $n_A = 1 - \delta$ and $n_B = 1 + \delta$.

Variational parameter: staggered field $\Delta_{a,b} = \varepsilon \delta_{a,b} e^{i\mathbf{Q}\mathbf{R}_a}$

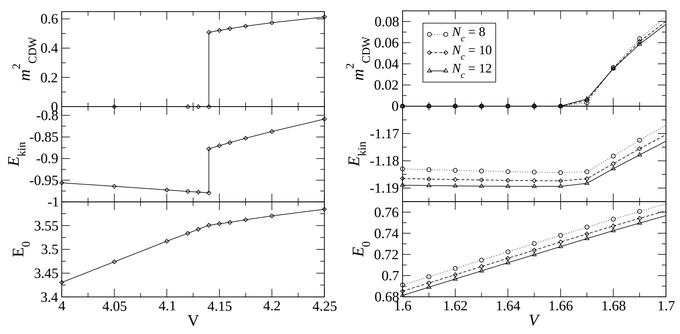


Fig. 1: Charge order parameter m^2_{CDW}, kinetic energy E_{kin}, and ground state energy E_0 for $U = 8$ (left) and $U = 3$ (right).

Fig. 1 shows, that at $U = 8$ the transition is of first order, whereas at $U = 3$ it is continuous. The transition points predicted by our method are $V_c = 4.14$ at $U = 8$, and $V_c = 1.66$ at $U = 8$, in good agreement with other methods.[5]

1D – Spectral functions

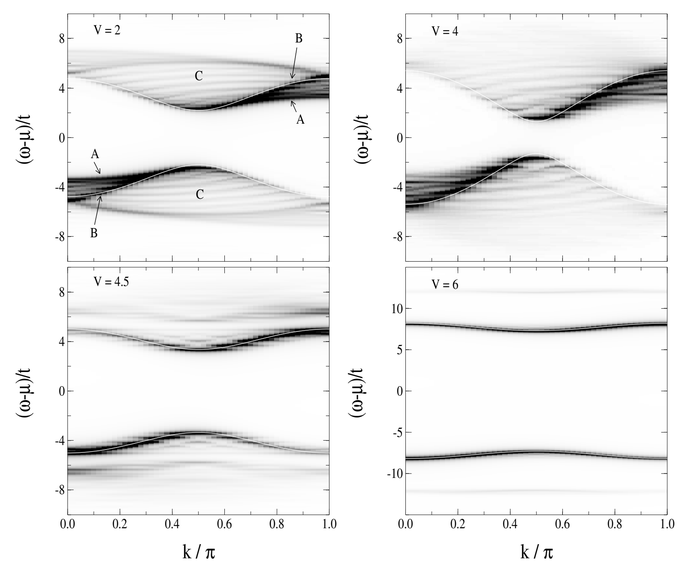
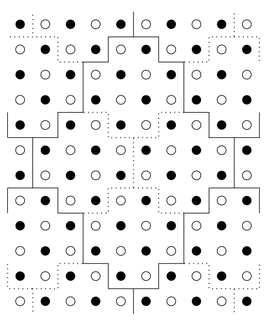


Fig. 2: Spectral function of the 1D EHM at $U = 8$ at selected values of V. A and B denote the spinon and holon bands, respectively.

In Fig. 2 it is clearly visible, that there is evidence for spin-charge separation in the SDW phase, but not in the CDW phase. The white lines are fits to a Hartree-Fock dispersion.

2D – Possible cluster tilings

In two dimensions one has to be careful when dividing the lattice into clusters of finite size. Whereas for small and intermediate cluster sizes ($N_c = 8$ and $N_c = 10$, not shown) the order pattern fits into cluster, some other tilings are not commensurate with the charge ordering. In such cases a super cluster has to be constructed, as shown on the right side. In this study we used this $N_c = 4 \times 12$ super cluster, which is in fact the largest treatable cluster size, because for smaller cluster sizes the ratio between decoupled bonds and bonds treated exactly is larger, which increases the mean-field and finite-size effects.



2D – Phase transition

Similar calculation to 1D, but different variational parameters:

SDW: staggered magnetic field + hopping inside the cluster

CDW: staggered chemical potential (like in 1D)

Mean-field parameters are calculated self-consistently on an isolated cluster (first order transition, see figure below).

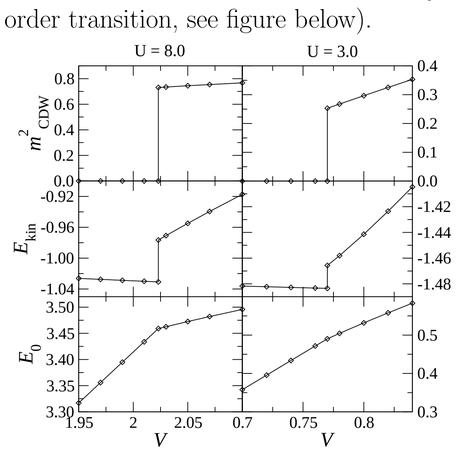


Fig. 3: Charge order parameter m^2_{CDW}, kinetic energy E_{kin}, and ground state energy E_0 for $U = 8$ (left) and $U = 3$ (right).

Different to 1D, we found at both $U = 8$ and $U = 3$ first order phase transitions with transition points $V_c = 2.023(1)$ at $U = 8$ and $V_c = 0.770(3)$ at $U = 3$ at the $N_c = 4 \times 12$ cluster.

2D – Spectral functions

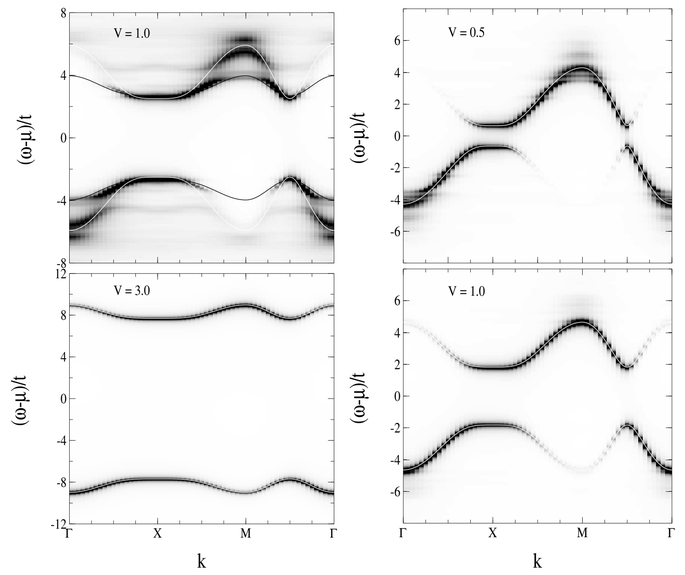


Fig. 4: Spectral function of the 2D EHM at $U = 8$ (left) and $U = 3$ (right). White lines: Hartree-Fock fit. Black lines: fit to magnetic dispersion, bandwidth J.

The low energy excitations have magnetic origin only in the SDW phase, not in the charge ordered CDW phase. The Hartree-Fock dispersion in the SDW phase (white lines) do not account for the splitting into low energy quasi-particle bands and high energy Hubbard bands. In the CDW phase the agreement between fitted and numerically calculated dispersions is much better.

Conclusion

- Mean-field decoupling provides consistent cluster approach to extended Hubbard models.
- Results in 1D in good agreement with other methods. Spectral functions show spin-charge separation only in the SDW phase.
- In 2D no continuous transitions for onsite interactions $U \geq 3$. Magnetic excitations only in the SDW phase

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