Exact bounds on the ground-state energy of the infinite-\( U \) Hubbard model

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(March 21, 2022)

We give upper and lower bounds for the ground-state energy of the infinite-\( U \) Hubbard model. In two dimensions, using these bounds we are able to rule out the possibility of phase separation between the undoped-insulating state and an hole-rich state.

74.25.Jb, 71.10.Fd, 71.27.+a

The problem of phase separation (PS) in strongly correlated systems is one of the most debated subject, especially after the seminal paper by Emery and co-workers [1], who also pointed out its relevance in the framework of high-temperature superconductivity. However, after several years of intensive numerical and analytical investigation, there is no general consensus even for the qualitative features of the possible instability in the Hubbard and \( t-J \) models [2–7].

In this work we focus on the Hubbard model on a square lattice of \( L \) sites in the infinite-\( U \) limit, and prove that there is no PS in the low doping limit: our result being one of the few rigorous statements in this field. The Hamiltonian is defined by

\[
\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} \mathcal{P}_G c_{i,\sigma}^\dagger c_{j,\sigma} \mathcal{P}_G,
\]

where the \( \langle i,j \rangle \) denotes nearest neighbor sites, and the Gutzwiller projector \( \mathcal{P}_G \) enforces the constraint of no double occupancy on each site.

An upper bound on the ground-state (GS) energy can be easily obtained by use of a variational wavefunction. A very simple choice is given by the fully polarized ferromagnetic (FM) state of energy \( E_{FM} = 2t \sum_{R} \sum_{\sigma} \cos k_i \), where \( d \) is the dimensionality of the lattice and the sum over \( k \) is restricted to the lowest hole energy orbitals.

A lower bound to the GS energy is instead more involved and can be derived as follows. The GS of the Hamiltonian \( \mathcal{H} \) with \( M \) holes can be generally written as

\[
|\psi\rangle = \sum_{\mathbf{R}_1 \ldots \mathbf{R}_M} \Psi(\mathbf{R}_1 \ldots \mathbf{R}_M)|\mathbf{R}_1 \ldots \mathbf{R}_M\rangle,
\]

where \( |\mathbf{R}_1 \ldots \mathbf{R}_M\rangle \) are normalized states representing suitable superpositions of spin states with the constraint of having the holes placed in the sites labeled by \( (\mathbf{R}_1 \ldots \mathbf{R}_M) \). The sum is over all distinct hole configurations. The matrix elements \( K_{ij} \) of the hopping operator \( \hat{K} \) on the reduced Hilbert space defined by the hole configurations are non vanishing only if a single hole hops at nearest neighbor distance. Therefore, \( K_{ij} \) has no diagonal elements. For instance, the element corresponding to the hopping \( \mathbf{R}_1 \rightarrow \mathbf{R}_1' \) is \( (\mathbf{R}_1' \ldots \mathbf{R}_M\rangle |\hat{K}| \mathbf{R}_1 \ldots \mathbf{R}_M\rangle \) and its modulus is always smaller or equal than \( t \). By construction, the lowest eigenvalue \( E_0 \) of this matrix is the GS energy of the infinite-\( U \) Hubbard model.

Now we prove that a lower bound of the GS energy is obtained by considering the matrix with all the non vanishing entries equal to \( -t \). In fact, for the hermitian matrix with only non diagonal elements \( K_{ij} \), GS energy \( E_0 < 0 \) and with components \( \psi_i = \Psi(\mathbf{R}_1 \ldots \mathbf{R}_M) \) we have:

\[
E_0 = -\sum_{i,j} |\psi^*_i K_{ij} \psi_j| \geq -\sum_{i,j} |K_{ij}| |\psi_i| |\psi_j| \\
\geq \sum_{i,j} B_{ij} |\psi_i| |\psi_j| \geq E_B \tag{3}
\]

Here, the matrix \( B \) describes a gas of \( M \) hard-core bosons (HCB) with nearest neighbor hopping \( B_{ij} = -t \) for the non zero entries, which satisfies \( |B_{ij}| \geq |K_{ij}| \). The last inequality in (3) follows from the Perron-Frobenius theorem [8] and \( E_B \) is the lowest eigenvalue of \( B \). This proves that a lower bound on the energy of the infinite-\( U \) Hubbard model is given by the GS energy of an HCB gas with density equal to the doping of the infinite-\( U \) Hubbard model: \( E_B \leq E_0 \leq E_{FM} \). These bounds clearly hold in any dimension \( d \).

It is worth noting that the lower bound is not at all trivial, indeed \( i) \) the Hilbert space for a system of \( M \) HCB is much smaller than the Hilbert space of a system of spin-1/2 with \( M \) holes, \( ii) \) in general it is not true that for a given Hamiltonian \( \mathcal{H} \), the energy of the bosonic GS is lower than the energy of the fermionic GS. This is actually the case for the spin-1/2 infinite-\( U \) Hubbard model but it does not hold in general (it is true if all the off-diagonal matrix elements of \( \mathcal{H} \) for the bosonic model are negative). For example let us consider the two-dimensional \( t-J \) model

\[
\mathcal{H}_{t-J} = -t \sum_{\langle i,j \rangle, \sigma} \mathcal{P}_G c_{i,\sigma}^\dagger c_{j,\sigma} \mathcal{P}_G
\]
where \( S_i = \frac{1}{2} \sum_{\sigma,\sigma'} c_{i,\sigma}^\dagger \tau_{\sigma,\sigma'} c_{i,\sigma'} \), being \( \tau_{\sigma,\sigma'} \) the Pauli matrices, and \( \xi_i = \sum_{\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} \). If we consider \( L = 16 \) and 2 holes, the fermionic GS has an energy lower than the corresponding bosonic GS \([9]\) for \( J \geq 0.2t \). Indeed for this Hamiltonian, even for bosons, the off-diagonal terms are not all negative definite. In Table I we report the GS energies of the \( t - J \) model for different values of \( J \) both for fermions and bosons. Remarkably Lanczos diagonalizations on finite clusters show that, even at finite density or at finite \( U > 0 \), the hole-hole correlations in the \( t - J \) model are quite similar to the corresponding HCB results \([10]\).

In conclusion we have obtained a rigorous result that rules out PS in the infinite-\( U \) Hubbard model starting from the zero doping limit. Of course our findings do not exclude that PS could take place between two finite densities or at finite \( U > 0 \).

This work has been partially supported by INFN and MURST (COFIN99).

### Table I. GS energies \( E_f \) and \( E_b \) for 2 holes on \( L = 16 \) sites for the fermionic and bosonic \( t - J \) model respectively.

| \( J/t \) | \( E_f/t \)  | \( E_b/t \)  |
|--------|----------|----------|
| 0.1    | -7.7348  | -7.7695  |
| 0.2    | -8.2118  | -8.1967  |
| 0.3    | -9.4199  | -9.3755  |
| 0.4    | -10.6839 | -10.6056 |
| 0.5    | -11.9843 | -11.8897 |

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