ULDF-TH-1/4/99

Maximal Stability Regions for Superconducting Ground States of Generalized Hubbard Models

Matteo Beccaria
matteo.beccaria@le.infn.it
Dipartimento di Fisica, Università di Lecce, Via Arnesano, 73100 Lecce, Italy
(submitted to Physical Review Letters, April 9, 1999)

For a class of generalized Hubbard models, we determine the maximal stability region for the superconducting η-pairing ground state. We exploit the Optimized Ground State (OGS) approach and the Lanczos diagonalization procedure to derive a sequence of improved bounds. We show that some pieces of the stability boundary are asymptotic, namely independent on the OGS cluster size. In this way, necessary and sufficient conditions are obtained to realize superconductivity in terms of an η-pairing ground state. The phenomenon is explained by studying the properties of certain exact eigenstates of the OGS hamiltonians.

Generalized Hubbard models are important theoretical frameworks for the study of superconductivity. Apart from special cases, they are not solvable and rigorous results on their physical properties are quite valuable.

The inclusion of nearest neighbour extra couplings beyond the on site Coulomb interaction has a long history and is still an interesting issue. Indeed, the qualitative effects of these interactions is not definitely understood and examples can be provided where they are not negligible at all.

As is well known, a good marker for superconductivity is off-diagonal long-range order (ODLRO) [1], a property that makes sense in any number of dimensions and implies both Meissner effect and flux quantization. Ground state ODLRO can be detected by studying the asymptotic behaviour of fermion correlation functions [2]. Of course, if the ground state is analitically known, it can be checked explicitely. This is the case of the so-called η-pairing [3] states that exhibit ODLRO and, under some constraints, can be the ground states of certain generalized Hubbard models.

When an η-pairing state is discovered to be an exact eigenstate, the next problem is to determine the region in the coupling space where it is also the ground state. To answer this question many analytical methods have been developed to establish rigorous bounds for the superconducting region. Among them, we recall the positive semidefinite operator approach [5,6] and the bounds derived by application of Gerschgorin's theorem [7]. The algorithm which however appears to be the simplest and most powerful is the Optimal Ground State (OGS) scheme proposed for generalized Hubbard models [8] and recently applied to the case of next to nearest neighbour couplings [9]. The method is based on the exact diagonalization of a certain local hamiltonian defined over a cluster of sites. If the cluster is made larger, the superconducting region is generally expected to expand. In the limit of an infinite cluster we obtain exact bounds.

For simplicity, in the following we shall call superconducting (SC) region, the subset of coupling space where the η-pairing state is the ground state. In this Letter, we apply the OGS algorithm to study the stability of the superconducting η-pairing state with momentum π. We discuss the behaviour of the OGS bounds as a function of the cluster size using the Lanczos algorithm to diagonalize the cluster hamiltonian. We obtain an improved SC region that can be considered *numerically* asymptotic and discuss in details the inclusion problem by stating the conditions under which larger clusters are expected to give better bounds. Another interesting result is that some pieces of the boundary between the SC and non SC regions are independent on the cluster size and determine necessary and sufficient conditions for η-pairing superconductivity. We explain these stable boundaries by means of certain exact eigenstates of the OGS hamiltonians whose properties are crucial in this respect.

Let us consider the Hamiltonian of a one dimensional generalized Hubbard model (we denote by $\langle i,j\rangle$ the sum over nearest neighbour sites)

$$
\begin{aligned}
H = & -t \sum_{\langle i,j\rangle,\sigma=\uparrow,\downarrow} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + \\
& + X \sum_{\langle i,j\rangle,\sigma=\uparrow,\downarrow} (n_{i,-\sigma} + n_{j,-\sigma})(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + \\
& + U \sum_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right) + \\
& + V \sum_{\langle i,j\rangle} (n_i - 1)(n_j - 1) + Y \sum_{\langle i,j,\rangle} (p^\dagger_i p_j + p^\dagger_j p_i) + \\
& + \frac{1}{2} J_{xy}(S^+_i S^-_j + S^+_j S^-_i) + J_z S^Z_i S^Z_j, \qquad (1)
\end{aligned}
$$

where $c_{i\sigma}$ and $c_{i\sigma}^\dagger$ are canonical Fermi operators obeying $\{c_{i\sigma}^\dagger, c_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}$ and $\{c_{i\sigma}, c_{j\sigma'}\} = \{c_{i\sigma}^\dagger, c_{j\sigma'}^\dagger\} = 0$. The number operators are defined as usual: $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ and $n_i = n_{i\downarrow} + n_{i\uparrow}$. The operator ${p_i}^\dagger$ creates pairs $p_i^\dagger = c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$. The Heisenberg exchange interaction is written as usual in terms of $su(2)$ operators $S_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow}$, $S^- = (S^+)^\dagger$ and $S^Z = \frac{1}{2}(n_\uparrow - n_\downarrow)$.

The Hamiltonian in (1) contains many couplings: X parametrizes the bond-charge repulsion interaction which has been related to high-T_c materials [10]; U is the usual on site Coulomb interaction; V is the nearest neighbour charge-charge coupling; Y controls the pair hopping term as in the Penson-Kolb-Hubbard models [11]. Finally, J_{xy} and J_z are the $t-J$ like Heisenberg exchange couplings.

We introduce the η-pairing operator

$$\eta^\dagger = \sum_n (-1)^n p_n^\dagger, \tag{2}$$

from which we build the state

$$|\eta\rangle = (\eta^\dagger)^{N/2}|0\rangle, \tag{3}$$

where $|0\rangle$ is the empty state and N is the number of lattice sites. The state $|\eta\rangle$ is an eigenstate of H provided $V + 2Y = 0$. In this case it describes a half-filled state with energy

$$E_+ = \frac{1}{4}(U + 4V), \tag{4}$$

and can be shown to possess ODLRO. Since E_+ is an upper bound for the ground state energy, a strategy to proof that $|\eta\rangle$ is the ground state is to find a lower bound E_- and a region in the coupling space where $E_- = E_+$. The same procedure applies also to other exact eigenstates like, for instance, the η-pairing state with zero momentum. Also, if $V = Y = J_{xy} = J_z = 0$ and $t = X$, exact eigenstates can be built by applying $\eta^\dagger$ to eigenstates of the $U = +\infty$ standard Hubbard model due to the fact that $t = X$ implies a conserved number of doubly occupied sites. However, we remark that the state $|\eta\rangle$ is particularly interesting from a methodological point of view as can be seen by the complete failure of the naive Gerschgorin approach [12].

Lower bounds for the ground state of H may be obtained following the OGS approach [8]. The Hamiltonian (1) is written as

$$H = \sum_{n=-\infty}^{\infty} (h_n^{(1)} + h_{n,n+1}^{(2)}), \tag{5}$$

where $h_n^{(1)}$ contains operators acting only on site n and $h_{n,n+1}^{(2)}$ links site n to site $n+1$ and depends on operators acting on both. To recast (5), we introduce extended operators

$$\tilde{h}_n^{(k)} = \frac{1}{2}h_n^{(1)} + \sum_{m=n}^{n+k-2} h_{m,m+1}^{(2)} + \\ + \sum_{m=n+1}^{n+k-2} h_m^{(1)} + \frac{1}{2}h_{n+k-1}^{(1)}, \tag{6}$$

for any integer $k \geq 2$. The local hamiltonian $\tilde{h}^{(k)}$ describes a cluster of k sites. Like H, also $\tilde{h}^{(k)}$ is symmetric under $\eta^\dagger$. All the states

$$(\eta^\dagger)^p|\underbrace{0\cdots0}_{\text{k sites}}\rangle, \quad p \text{ integer} \tag{7}$$

are degenerate with energy E_+ and are precisely those needed to build the $|\eta\rangle$ state on the infinite lattice (see [8] for a complete discussion of the $k = 2$ case). The Hamiltonian can be written in terms of $\tilde{h}^{(k)}$ as

$$H = \sum_{n=-\infty}^{\infty} \tilde{h}_n^{(k)}. \tag{8}$$

If we denote by $E_0(N)$ the ground state energy for a system of N sites, the asymptotic ground energy per site is by definition

$$\mathcal{E}_0 = \lim_{N\to\infty} \frac{E_0(N)}{N}, \tag{9}$$

and, for each k, satisfies the rigorous bound

$$\mathcal{E}_0 \geq \frac{1}{k-1} \min \sigma(\tilde{h}^{(k)}) \stackrel{def}{=} \mathcal{E}_0^{(k)}, \tag{10}$$

where $\sigma(A)$ denotes the spectrum of the operator A. The normalization factor $1/(k-1)$ takes into account the number of terms in Eq. (8) which contain a given site. The right hand side of Eq. (10) depends on the cluster size k and a better bound is expected as k increases. However, strictly speaking, this is false. Let us write a cluster of k sites in terms of smaller clusters

$$\tilde{h}_n^{(k)} = \tilde{h}_n^{(k-l)} + \tilde{h}_{n+k-l-1}^{(l+1)}, \qquad 1 \leq l \leq k-2. \tag{11}$$

From (11) we obtain the exact inequalities

$$\mathcal{E}_0^{(k)} \geq \frac{k-l-1}{k-1}\mathcal{E}_0^{(k-l)} + \frac{l}{k-1}\mathcal{E}_0^{(l+1)}, \tag{12}$$

and in particular

$$\mathcal{E}_0^{(2k-1)} \geq \mathcal{E}_0^{(k)}. \tag{13}$$

This allows to build sequences of bounds converging to the exact bound in the infinite cluster size limit. In more details, Eq. (13) splits into disjoint sequences of cluster sizes as follows

$$2 \subset 3 \subset 5 \subset \cdots, \\ 4 \subset 7 \subset 13 \subset \cdots, \tag{14}$$

where the notation means that each sequence gives better and better bounds. We notice that in general two sequences are not related at all and, in particular, $3 \subset 4$ may be false as we shall see in explicit examples. What can be stated in full generality is that the minimal choice $k = 2$ is always the worst bound since from

$$\mathcal{E}_0^{(N+1)} \geq \frac{N-1}{N}\mathcal{E}_0^{(N-1)} + \frac{1}{N}\mathcal{E}_0^{(2)}, \tag{15}$$

we proof inductively that $\forall N \geq 2$ we have

$$\mathcal{E}_0^{(N)} \geq \mathcal{E}_0^{(2)}. \tag{16}$$

Keeping these remarks in mind, we study the size dependence of the conditions under which (1) with $Y = -2V$ admits $|\eta\rangle$ as its ground state by explicit diagonalization of $\tilde{h}^{(L)}$ on clusters of increasing sizes. The OGS method requires diagonalization of the local hamiltonian in all sectors of definite up and down electron numbers; for the numerical diagonalization we use the Lanczos algorithm. In the following we shall always assume $t \equiv 1$ and denote by L the cluster size.

Since the couplings constants space is large, we decide to discuss separately what happens with the Heisenberg exchange interaction switched on or off. Let us begin with $J_{xy} = J_z = 0$.

In Fig. 1 we show at $X = 0$ the size dependence of the bounds when $V > -1$. As can be seen, there are regions where the corrections are definitely negligible beyond $L = 3$, i.e. $V > -0.4$. On the other hand, around $V = -0.5$, size effects can be important up to large cluster sizes. We remark that this figure does not show any non trivial relationship among the bounds obtained at different L: they just improve monotonically.

In Fig. 2 we show the best bounds obtained with $L = 6$ at several values of X. In the inset we expand the region around $V = -2$. A remarkable feature of the plot is that an enveloping straight line appears around $V = -1$. Successive corrections are quite small and the region shown can be considered maximal from any practical point of view [13].

In Fig. 3 we plot at four different X the difference $\Delta U(L) = U(L) - U(2)$ between the boundary curves at $L > 2$ and the minimal one at $L = 2$. The inclusion tree (14) is non trivially satisfied and indeed the $L = 4$ bound is not always better than the $L = 3$ one. As a second remark, we observe that at each X there is a piece of the boundary where finite size corrections vanish. This turns out to happen between two of the $L = 2$ boundary points. As shown in [8], the result at $L = 2$ is that a sufficient condition for $|\eta\rangle$ to be the the ground state is

$$V \leq 0, \tag{17}$$
$$U \leq -2 \max\left(2 + 2V, 2|1 - 2X| + 2V, V - \frac{(1-X)^2}{V}\right).$$

For $0 \leq X \leq 1$ (we study this case only), the difference ΔU vanishes between the intersections of the curves $U = -4(1 + V)$ and $U = -2(V - (t - X)^2/V)$, namely for $|V + 1| \leq \sqrt{X(2 - X)}$.

Let us now discuss why this stable boundary subset appears. For each value of L, the normalized cluster Hamiltonian $\frac{1}{L-1}\tilde{h}^{(L)}$ has many eigenstates $|E_i^{(L)}(U, V, X)\rangle$ $(i = 1, \ldots, \dim(\tilde{h}))$ which we label by their eigenvalue.

Let X play the role of a parameter; following the OGS approach, the inequalities $E_i^{(L)} \geq E_+$ determine the superconducting region in the (U, V) plane. Each point of its boundary satisfies $E_i^{(L)} = E_+$ for some index i. Hence, if a subset of the boundary turns out to be L independent, a possible reason can be the existence of an eigenvalue independent on L. A trivial case is provided by the states $(\eta^\dagger)^p|0\rangle$ (p integer) where $|0\rangle$ is the empty state for $\tilde{h}^{(L)}$. However, in this case, the condition $E^{(L)} = E_+$ is identically satisfied for all U, V and X and does not determine any boundary. To find a non trivial eigenstate with eigenvalue independent on L we can consider the one particle sector (i.e. $n_\uparrow = 1$, $n_\downarrow = 0$ or viceversa). The two states

$$|S_\sigma\rangle = \sum_{n=1}^{L} c_{n\sigma}^\dagger |0\rangle, \qquad \sigma = \uparrow, \downarrow, \tag{18}$$

are indeed exact eigenstates of $\frac{1}{L-1}\tilde{h}^{(L)}$ provided $U = -4(1 + V)$ and in this case their eigenvalue is precisely $E_+ = -1$ ($t \equiv 1$). The states $|S_\sigma\rangle$ are thus responsible for the stable boundary. To understand why it is confined to $|V + 1| \leq \sqrt{2X - X^2}$ we introduce additional eigenstates of $\tilde{h}^{(L)}$. Indeed, on the line $U = -4(V + 1)$, the $su(2)$ singlet state ($X \neq 1$)

$$|\gamma\rangle = \left\{ \sum_{i \neq j} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + \rho \sum_i \frac{1 - (-1)^{i+L}}{2} p_i^\dagger \right\} |0\rangle, \tag{19}$$

can be shown to be an exact eigenstates of $\frac{1}{L-1}\tilde{h}^{(L)}$ with eigenvalue E_+ if and only if $\rho = (2 + V)/(1 - X)$ and $V = -1 \pm \sqrt{2X - X^2}$. This is the $L > 2$ generalization of the state $|\psi_\pm\rangle$ discussed in [8] in the $L = 2$ case. It forbids to extend the bounds associated to $|S_\sigma\rangle$ beyond the points $|V + 1| = \sqrt{2X - X^2}$. The case $X = 1$ is singular and must be treated separately; the number of doubly occupied sites is conserved and splitting may occur. For instance, the state $|\gamma_+\rangle$ with $V = 0$ splits into the independent eigenstates $|\gamma_i\rangle = p_i^\dagger|0\rangle$.

The above analytical and numerical results lead us to the conclusion that the inequality $U \leq -4(1+V)$ is a necessary and sufficient condition for $|\eta\rangle$ being the ground state in the subset of the coupling space constrained by the conditions $t \equiv 1$, $Y + 2V = 0$, $0 < X < 1$ and $|V + 1| \leq \sqrt{X(2 - X)}$.

The above facts do not change qualitatively when the Heisenberg exchange interaction is switched on. To simplify the analysis, we consider the special point $J_{xy} = J_z = -2Y$ which allows for a comparison with the results illustrated in [6,8].

The plot of Fig. 4 is analogous to that of Fig. 1; we show the OGS bounds in the (U, V) plane at $X = 0$. A part of the boundary is clearly independent on L. This fact is clearly visible in the left inset and mostly in Fig. 5 where (as in Fig. 3) the asymptotic part of the boundary can be seen as a function of X. In particular, the left edge is at $V = -1$ and is independent on X. These features can be analyzed as in the previous case. The bounds valid at $L = 2$ are

$$V \leq 0, \tag{20}$$
$$U \leq -2 \max\left(0, 2+2V, 2|1-2X|+2V, 4V - \frac{(1-X)^2}{V}\right),$$

and the stable part (with $0 \leq X \leq 1$) is that between the intersections of the lines $U = 0$, $U = -4(1+V)$ and the curve $U = -2(4V-(1-X)^2/V)$. Thus we obtain the following interval for V: $-1 \leq V \leq \frac{1}{2}(1-\sqrt{3-4X+2X^2})$. As before, the line $U = -4(1+V)$ appears at all L since on it the states $|S_\sigma\rangle$ are eigenstates of $\frac{1}{L-1}\tilde{h}^{(L)}$. Moreover, as before, there are two states which forbid to cross the above interval for V. At the right edge, such a state has the form of Eq. (19) with $\rho = 2(1-V)/(1-X)$ and $V = \frac{1}{2}(1-\sqrt{3-4X+2X^2})$. At the left edge, $V = -1$, the exact (X independent) eigenstate is instead

$$|\gamma'\rangle = \left(\sum_{i<j} c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} + \sum_{i>j} c^\dagger_{j\downarrow} c^\dagger_{i\uparrow}\right)|0\rangle. \tag{21}$$

To summarize, in this case, our conclusion is that under the conditions $t = 1$, $Y + 2V = 0$, $0 < X < 1$ and $-1 \leq V \leq \frac{1}{2}(1-\sqrt{3-4X+2X^2})$, a necessary and sufficient condition for $|\eta\rangle$ being the ground state is $U \leq -4(1+V)$.

To conclude, in this Letter we have considered generalized Hubbard models with nearest neighbour couplings and the problem of determining when the ground state is a superconducting η-pairing state. By diagonalizing local hamiltonians associated to clusters of sites with different sizes we studied the convergence of the OGS bounds. As predicted in [8], it may happen that the bounds obtained with the smallest clusters are actually exact. This peculiar situation seems rather typical and indeed we have shown that there exist subsets of the bounding region which are asymptotic and remain unchanged as the cluster size is varied. We clarified the origin of the phenomenon by providing several exact eigenstates which play a crucial role in its derivation.

We thank A. Montorsi for very useful discussions on generalized Hubbard models and η-pairing superconductivity.

[1] C. N. Yang, Rev. Mod. Phys. **34**, 694 (1962); G. L. Sewell, J. Stat. Phys. **61**, 415 (1990).

[2] R. Friedberg and T. D. Lee, Phys. Rev. B **40**, 6745 (1989); H. Q. Lin, E. R. Gagliano, D. K. Campbell, E. H. Fradkin and J. E. Gubernatis, in *The Hubbard Model*, Edited by D. Baeriswyl et al., Plenum Press, New York (1995); G. Bouzerar and G. I. Japaridze, Report No. cond-mat/9605161; R. T. Clay, A. W. Sandvik, D. K. Campbell, Phys. Rev. B**59**, 4665 (1999)

[3] C. N. Yang, Phys. Rev. Lett. **63**, 2144 (1989).

[4] W. O. Putikka, M. U. Luchini and M. Ogata, Phys. Rev. Lett. **69**, 2288 (1992).

[5] U. Brandt and A. Giesekus, Phys. Rev. Lett. **68**, 2648 (1992); R. Strack and D. Vollhardt, Phys. Rev. Lett. **70**, 2637 (1993); R. Strack and D. Vollhardt, Phys. Rev. Lett. **72**, 3425 (1994); R. Strack and D. Vollhardt, in *The Hubbard Model*, Edited by D. Baeriswyl et al., Plenum Press, New York (1995);

[6] A. Montorsi and D. K. Campbell, Phys. Rev. B**53**, 5153 (1996).

[7] A. A. Ovchinnikov, Mod. Phys. Lett. B**7**, 1397 (1993); A. A. Ovchinnikov, J. Phys. C**6**, 11057 (1994); J. de Boer, V. E. Korepin and A. Schadschneider, Phys. Rev. Lett. **74**, 789 (1995).

[8] J. de Boer and A. Schadschneider, Phys. Rev. Lett. **75**, 4298 (1995).

[9] Z. Szabó, Report No. cond-mat/9807083. We point out that due to a different normalization of the Heisenberg couplings, the values of J_{xy} and J_z are doubled with respect to ours and those of [6,8].

[10] J. E. Hirsch, Physica C**158**, 326 (1990); R. Z. Bariev, A. Klümper, A. Schadschneider, J. Zittartz, J. Physics A**26**, 1249 (1993).

[11] K. A. Penson, M. Kolb, Phys. Rev. B**33**, 1663 (1986); K. A. Penson, M. Kolb, J. Stat. Phys. **44**, 129 (1986); I. Affleck, J. B. Marston, J. Physics C**21**, 2511 (1988).

[12] The reason for the failure of the Gerschgorin approach in the case of the $|\eta\rangle$ state is that for the state $s = |\uparrow\downarrow, 0, \uparrow\downarrow, 0, \uparrow\downarrow, 0, \cdots\rangle$ the Gerschgorin lower bound is $E_- = H_{ss} - \sum_{s' \neq s} H_{ss'} < E_+$ and we cannot never impose the equality $E_- = E_+$

[13] The numerical data defining the boundary between the SC and non SC region are available upon request to the author.

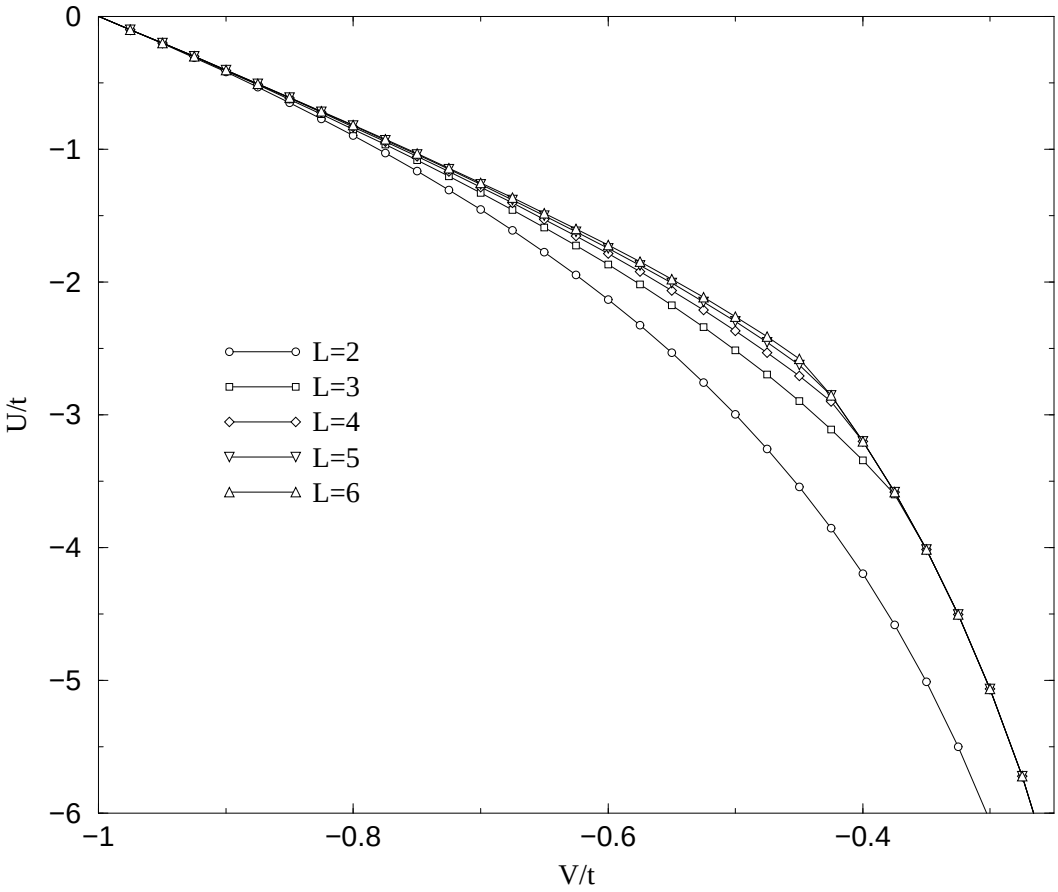

FIG. 1. Size dependence of the OGS bounds in the (U, V) plane at $J_{xy} = J_z = 0$ and $X = 0$.

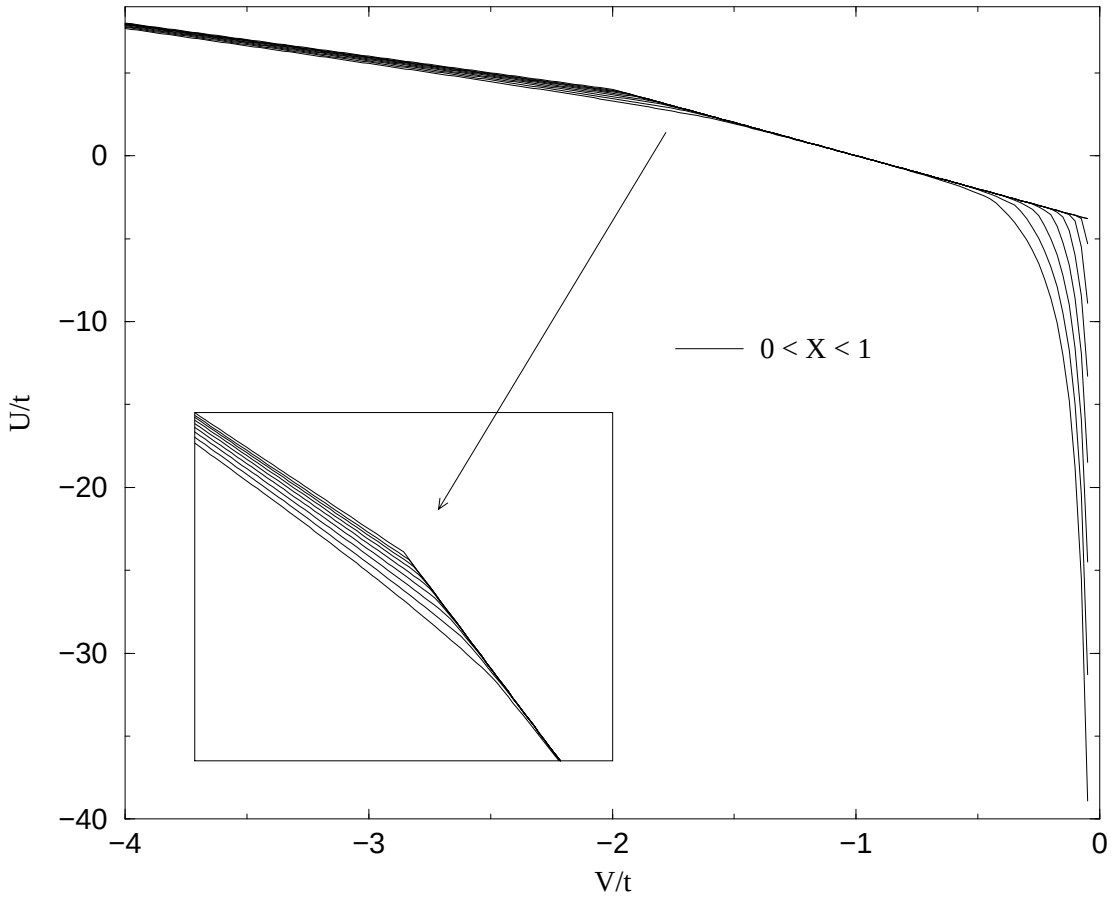

FIG. 2. Best OGS bounds obtained with $L = 6$ clusters. The Heisenberg interactions are switched off $J_{xy} = J_z = 0$. The different curves correspond (from bottom to top) to $X = 0$, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 1.0.

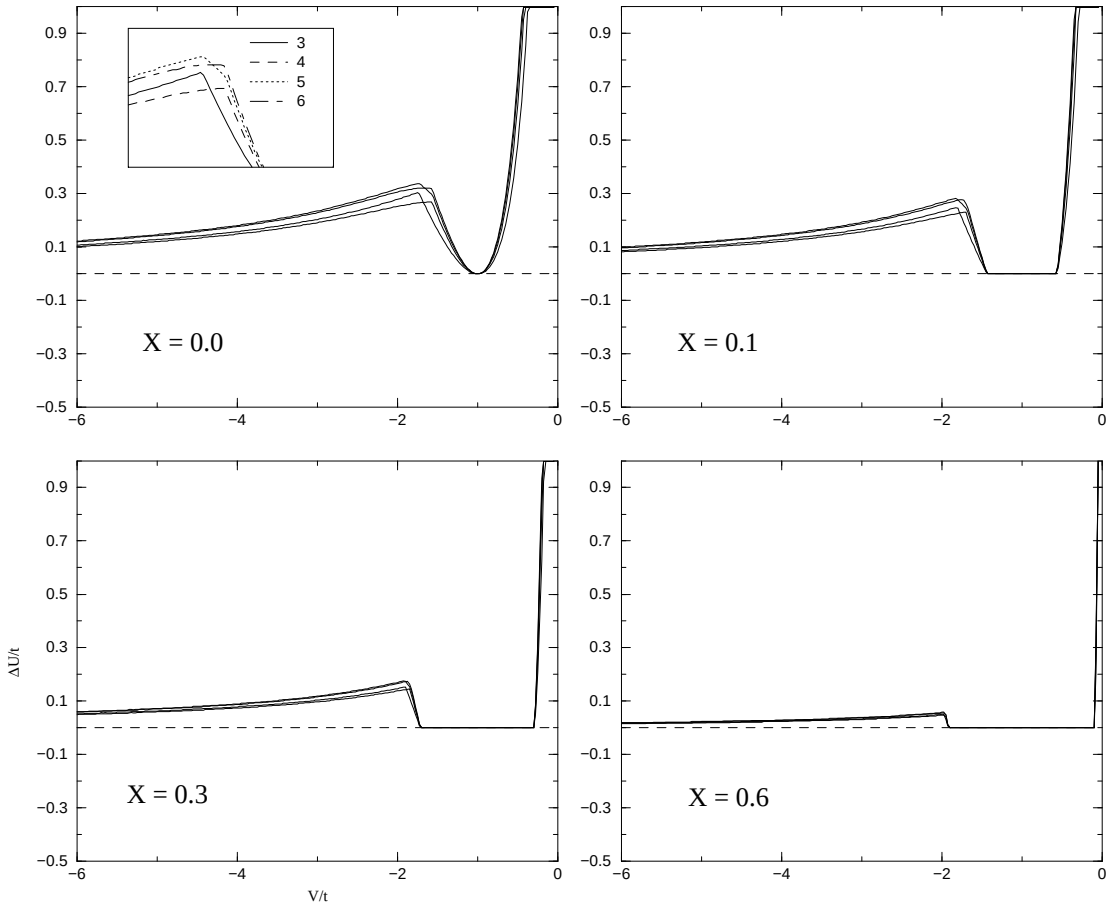

FIG. 3. Existence of an asymptotic boundary. The plots show $U(V;L) - U(V;2)$ as a function of V (always in units of t) for four values of X. The function $U(V;L)$ is the curve obtained from the OGS bounds using clusters of L sites. The inset at $X = 0$ shows a non trivial inclusion tree as the cluster size is increased. See also Fig. 4.

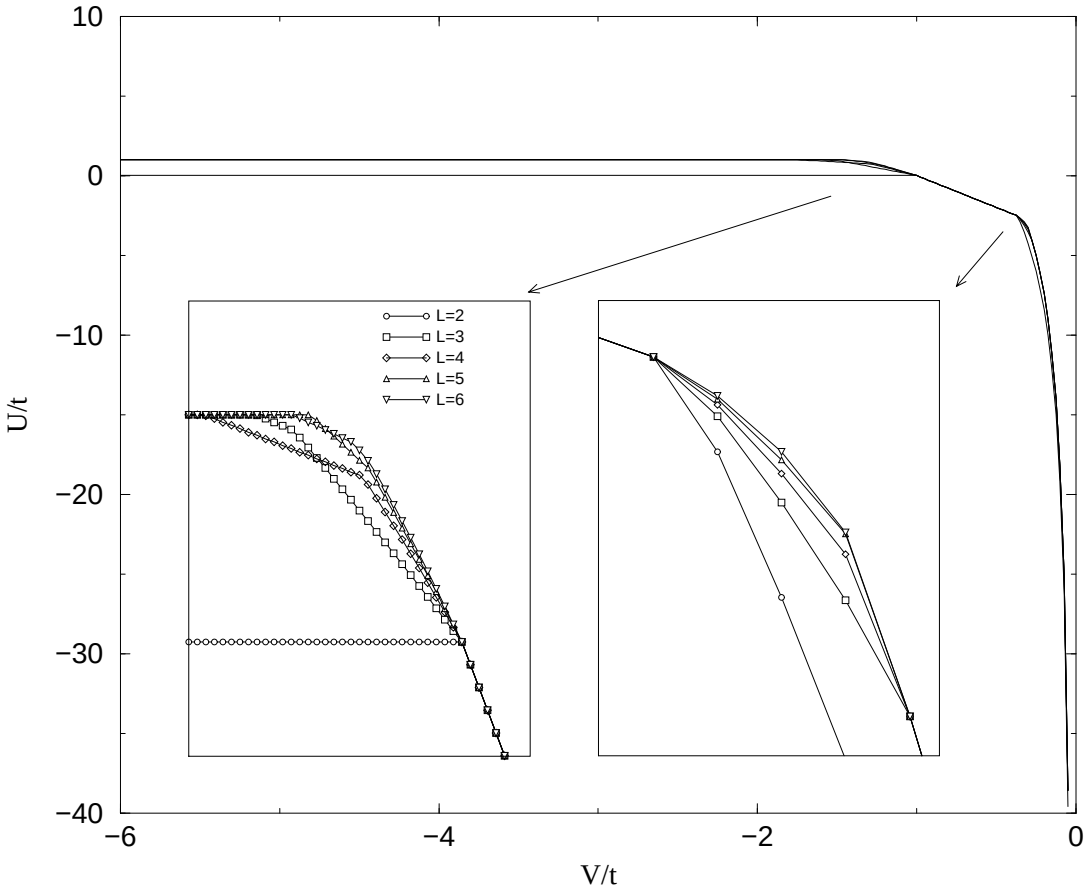

FIG. 4. As Fig. 1, but with $J_{xy} = J_z = -2Y$. The left inset shows a non trivial inclusion tree.

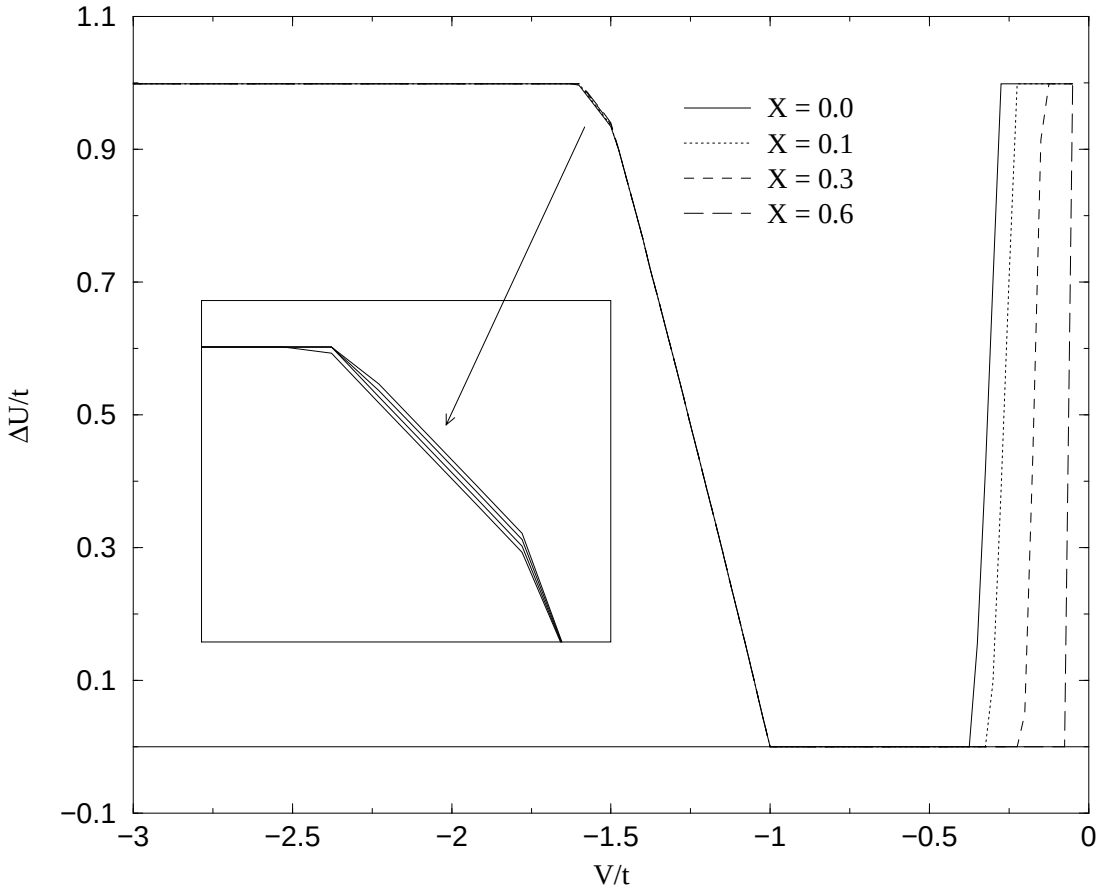

FIG. 5. As Fig. 4, but with $J_{xy} = J_z = -2Y$. The inset magnifies a portion of the curves to confirm that the OGS bound is not asymptotic for $V < -1$.