Eur. Phys. J. B **14**, 523–526 (2000)

THE EUROPEAN PHYSICAL JOURNAL B

EDP Sciences

Hierarchies of stability regions for η-pairing superconducting ground states of generalized Hubbard models

M. Beccaria[a]

Dipartimento di Fisica and INFN, Università di Lecce, Via Arnesano, 73100 Lecce, Italy

Received 27 July 1999 and Received in final form 29 September 1999

Abstract. For a class of generalized one dimensional Hubbard models, we study the stability region for the superconducting η-pairing ground state. We exploit the Optimum 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. The phenomenon is explained by studying the properties of certain exact eigenstates of the OGS Hamiltonians.

PACS. 74.20.-z Theories and models of superconducting state

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.

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 analytically known, it can be checked explicitly. 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 Optimum 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 paper, 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. 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)

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

where $c_{i\sigma}$ and $c^\dagger_{i\sigma}$ are canonical Fermi operators obeying $\{c^\dagger_{i\sigma}, c_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}$ and $\{c_{i\sigma}, c_{j\sigma'}\} = \{c^\dagger_{i\sigma}, c^\dagger_{j\sigma'}\} = 0$. The number operators are defined as usual: $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ and $n_i = n_{i\downarrow} + n_{i\uparrow}$. The operator ${p_i}^\dagger$ creates pairs $p^\dagger_i = c^\dagger_{i\uparrow} c^\dagger_{i\downarrow}$.

[a] e-mail: matteo.beccaria@le.infn.it

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].

We introduce the η-pairing operator with momentum $P = \pi$

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

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 particles. The state $|\eta\rangle$ is an eigenstate of H provided $2V + Y = 0$. In this case it describes a 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.

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 $\tilde{h}^{(k)}$ admits exact eigenstates obtained by acting with $\eta^\dagger$ on the vacuum. All the states

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

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

$$H = \frac{1}{k-1} \sum_{n=-\infty}^{\infty} \tilde{h}_n^{(k)}. \tag{8}$$

The normalization factor $1/(k-1)$ takes into account the number of terms in equation (8) which contain a given site. We remark that other choices of $\tilde{h}_n^{(k)}$ are possible which are associated, for instance, with different splittings of the boundary one site operators. If we denote by $E_0(L)$ the ground state energy for a system of L sites and fixed filling, the asymptotic ground energy per site is by definition

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

and, for each k, satisfies the rigorous bound

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

where $\sigma(A)$ denotes the spectrum of the operator A.

The quantity $\mathcal{E}_0^{(k)}$, the ground state energy of the renormalized cluster Hamiltonian, is a function of the couplings. It must be lower or equal to E_+ since, as we have seen, the local η-pairing states equation (7) have energy E_+. In the region of coupling space where equality holds $\mathcal{E}_0^{(k)} = E_+$ the state $|\eta\rangle$ becomes an *optimal* ground state which can be built in terms of local ground states (for more details, see [8] and the clear discussion in [12])

The right hand side of equation (10) depends also 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

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

The derivation of equations (12, 13) does not require $|\eta\rangle$ to be an OGS. If we now impose the OGS condition, $\mathcal{E}_0^{(k)} = E_+$, then equations (12, 13) allow us to build sequences of bounds converging to the exact bound in the infinite cluster size limit. In more details, equation (13) splits into disjoint sequences of cluster sizes as follows

$$\begin{aligned} &2 \subset 3 \subset 5 \subset \cdots, \\ &4 \subset 7 \subset 13 \subset \cdots, \end{aligned} \tag{14}$$

where the notation means that each sequence gives better and better bounds and the size of the corresponding SC regions increases along the sequence. 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

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

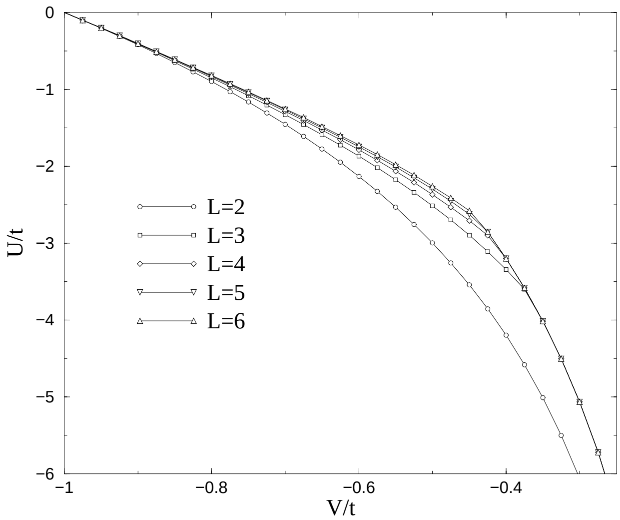

Fig. 1. Size dependence of the OGS bounds in the (U, V) plane at$X = 0$.

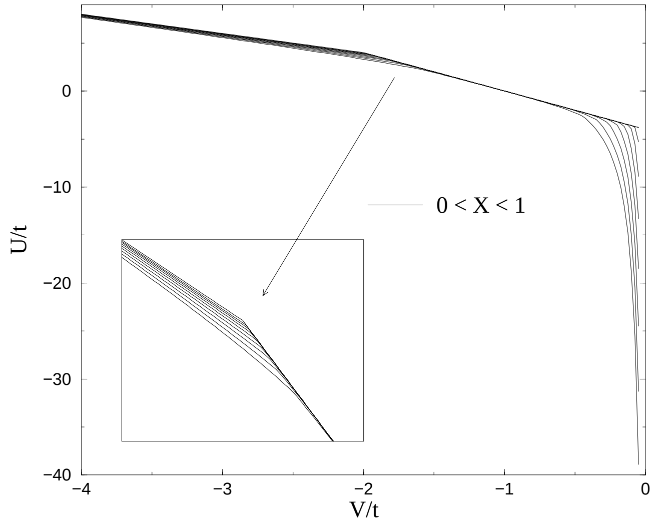

Fig. 2. Best OGS bounds obtained with $L = 6$ clusters. The different curves correspond (from bottom to top) to $X = 0$, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 1.0.

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.

In Figure 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 Figure 2 we show the best bounds obtained with $L = 6$ at several values of X. An enveloping straight line appears around $V = -1$. Successive corrections are quite small and the shown region is effectively asymptotic [13].

In Figure 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 [6,8], the result at $L = 2$ is that a sufficient condition for $|\eta\rangle$ to be the the ground state is

$$V \leq 0, \tag{17}$$

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

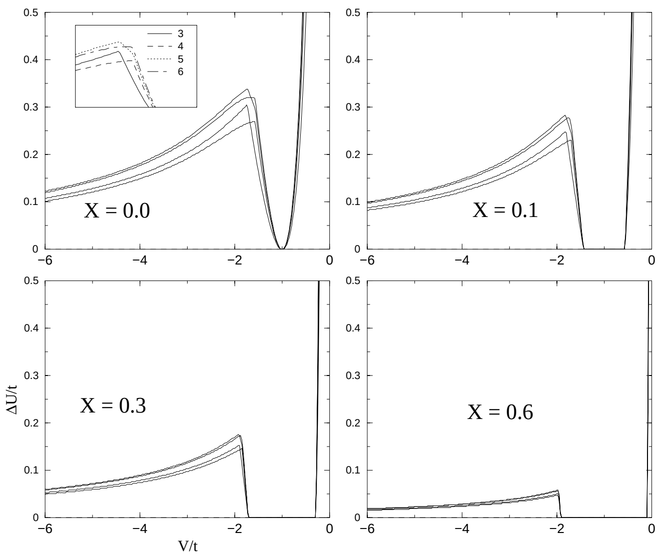

Fig. 3. Existence of an asymptotic boundary. The plots show $U(V; L) - U(V; 2)$ as a function of V (always in units of t) for four values of X. The function $U(V; L)$ is the curve obtained from the OGS bounds using clusters of L sites. The inset at $X = 0$ shows a non trivial inclusion tree as the cluster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

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 *vice versa*). 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. A complete analysis of a general extended Hubbard model will be given elsewhere [14].

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. As predicted in [8], it may happen that the OGS 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.

Finally, I would like to mention [15] where the optimum ground state approach is exploited to analyze *analytically* the 3-sites bounds for the stability domains of ground states of generalized Hubbard models with next-nearest neighbour interaction.

References

1. C.N. Yang, Rev. Mod. Phys. **34**, 694 (1962); G.L. Sewell, J. Stat. Phys. **61**, 415 (1990).
2. R. Friedberg, T.D. Lee, Phys. Rev. B **40**, 6745 (1989); H.Q. Lin, E.R. Gagliano, D.K. Campbell, E.H. Fradkin, J.E. Gubernatis, in *The Hubbard Model*, edited by D. Baeriswyl *et al.* (Plenum Press, New York, 1995); G. Bouzerar, 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, M. Ogata, Phys. Rev. Lett. **69**, 2288 (1992).
5. U. Brandt, A. Giesekus, Phys. Rev. Lett. **68**, 2648 (1992); R. Strack, D. Vollhardt, Phys. Rev. Lett. **70**, 2637 (1993); R. Strack, D. Vollhardt, Phys. Rev. Lett. **72**, 3425 (1994); R. Strack, D. Vollhardt, in *The Hubbard Model*, edited by D. Baeriswyl *et al.* (Plenum Press, New York, 1995).
6. A. Montorsi, 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, A. Schadschneider, Phys. Rev. Lett. **74**, 789 (1995).
8. J. de Boer, A. Schadschneider, Phys. Rev. Lett. **75**, 4298 (1995).
9. Z. Szabó, Phys. Rev. B **59**, 10007 (1999). In this reference the case $L = 4$ is also studied numerically in dimension $d = 2$.
10. J.E. Hirsch, Physica C **158**, 326 (1990); R.Z. Bariev, A. Klümper, A. Schadschneider, J. Zittartz, J. Phys. 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. Phys. C **21**, 2511 (1988).
12. H. Niggemann, J. Zittartz, Z. Phys. B **101**, 289 (1996).
13. The numerical data defining the boundary between the SC and non SC region are available upon request to the author.
14. M. Beccaria, A. Moro, in preparation.
15. C. Dziurzik, A. Schadschneider, J. Zittartz, Eur. Phys. J. B **12**, 209 (1999).