

Superconductivity with *s* and *p* symmetries in an extended Hubbard model with correlated hopping^{*}

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Abstract. We consider a generalized Hubbard model with on-site and nearest-neighbour repulsions U and V respectively, and nearest-neighbour hopping for spin up (down) which depends on the total occupation n_b of spin down (up) electrons on both sites involved. The hopping parameters are t_{AA} , t_{AB} and t_{BB} for $n_b = 0, 1, 2$ respectively. We briefly summarize results which support that the model exhibits *s*-wave superconductivity for certain parameters and extend them by studying the Berry phases. Using a generalized Hartree-Fock(HF) BCS decoupling of the two and three-body terms, we obtain that at half filling, for $t_{AB} < t_{AA} = t_{BB}$ and sufficiently small U and V the model leads to triplet *p*-wave superconductivity for a simple cubic lattice in any dimension. In one dimension, the resulting phase diagram is compared with that obtained numerically using two quantized Berry phases (topological numbers) as order parameters. While this novel method supports the previous results, there are quantitative differences.

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1 Introduction

Since the discovery of high T_c much effort has been devoted to the study of the pairing mechanisms in highly correlated electronic systems. Two very well studied microscopic models for such systems are the Hubbard and $t - J$ models. While the search for superconductivity in the positive- U Hubbard model by numerical methods has failed so far [1–5], $t - J$ -like models exhibit *d*-wave superconductivity for certain parameters [6–10].

Although most of the high T_c superconducting materials have a two-dimensional character, calculations in one dimension (1D) have been very useful. In one dimension the Hubbard and supersymmetric ($J = 2t$) $t - J$ models can be exactly solved using the Bethe ansatz [11,12]. It has been shown that for this particular case of the $t - J$ model, the ground state consists of bound states with a gapless excitation spectrum, but for $J < 2t$ bound states exist for large enough densities [13].

Other strongly correlated models that introduce correlated hopping interactions are subject of current research [14–51]. In 1989, Hirsch [14] proposed a model for the description of oxide superconductors by considering the holes in a nearly filled band as charge carriers.

The Hamiltonian in standard notation reads:

$$H_H = - \sum_{j=1}^L \sum_{\sigma=\pm 1} (c_{j,\sigma}^\dagger c_{j+1,\sigma} + c_{j+1,\sigma}^\dagger c_{j,\sigma}) \times \left(1 - \frac{\Delta t}{2} (n_{j,-\sigma} + n_{j+1,-\sigma}) \right). \quad (1)$$

In contrast to the Hubbard model, the hopping amplitude for single-particle hopping to a nearest-neighbour site depends on the occupancy of one of the sites involved in the process.

A few years ago, a new integrable model of strongly correlated fermionic systems for hole superconductivity has been introduced [15,16]. It is a modified version of Hirsch's model (1) and its Hamiltonian reads:

$$H_B = - \sum_{j=1}^L \sum_{\sigma=\pm 1} (c_{j,\sigma}^\dagger c_{j+1,\sigma} + c_{j+1,\sigma}^\dagger c_{j,\sigma}) \times \left(1 - \Delta t n_{j+(1+\sigma)/2,-\sigma} \right). \quad (2)$$

In 1D, it has been solved using the Bethe ansatz in three parameter regimes: $0 < \Delta t < 1$, $\Delta t < 0$ [15–17] and $\Delta t > 1$ [18]. The two first regimes are related by a particle-hole transformation and present similar behaviour to the Hirsch model (1): there is a good quantitative agreement between the ground state energies, both models show gapless charge excitations and spin excitations with a finite

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gap for all densities and also dominating superconducting correlations for densities larger than a critical value [19]. Instead, for the case with $\Delta t > 1$, both models (1 and 2) behave quite differently: while the spin gap in the Hirsch model vanishes and there are no indications of superconductivity, the gap remains finite and superconducting correlations are present for small doping in the Bariev model (2).

An important interaction that has not been considered in the above models is the Coulomb repulsion. We consider a more complete Hamiltonian that includes on-site U and nearest-neighbour V interactions between the particles, and contains a more general kinetic term with different hopping parameters, depending on the total occupation of the sites involved:

$$\begin{aligned}
H = & - \sum_{\langle ij \rangle \sigma} \Phi_{ij} (c_{i,-\sigma}^\dagger c_{j,-\sigma} + hc) + U \sum_i n_{i\uparrow} n_{i\downarrow} \\
& + V \sum_{\langle ij \rangle} n_i n_j; \\
\Phi_{ij} = & t_{AA}(1 - n_{i\sigma})(1 - n_{j\sigma}) + t_{BB} n_{i\sigma} n_{j\sigma} \\
& + t_{AB}(n_{i\sigma} + n_{j\sigma} - 2n_{i\sigma} n_{j\sigma}). \quad (3)
\end{aligned}$$

The model (1) corresponds to taking $t_{AA} + t_{BB} - 2t_{AB} = 0$, $U = V = 0$ and $\Delta t/2 = 1 - t_{AB}/t_{AA}$, and the Hubbard model is obtained when $V = 0$, $t_{AA} = t_{BB} = t_{AB}$. The case $V = 0$ has been derived as the model that describes the low energy excitations of intermediate-valence systems [20] and ‘‘hole’’ and cuprate superconductors [21,22]. The model with V was obtained for cuprate superconductors [23,24] and proposed to describe the benzene molecule [25,26].

For $t_{AB} = V = 0$ and $|t_{AA}| = |t_{BB}|$ an exact solution of (3) exists in 1D [27–30], but this case is too peculiar, as discussed later. Hamiltonian (3) supplemented by a hopping of pairs of the type $t_p \sum_{\langle ij \rangle} c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger c_{j,\uparrow} c_{j,\downarrow}$ has also been solved in 1D using Bethe ansatz [31–33] for $U = -2t_p$ and $t_{AA} t_{BB} = t_{AB}^2$. Its behaviour is similar to that of the Hubbard model. For negative U the model displays superconductivity. A more general model including this one and that of Bariev for particular parameters has also been solved using Bethe ansatz [34].

For $t_{AB} = 0$, $|t_{AA}| = |t_{BB}| = t$, $U, V \neq 0$ the phase diagram of the model (3) has been investigated previously [26,35–37] and some exact results have been found for the half-filled system (density of particles $n = 1$): a) in any arbitrary lattice in D dimensions with coordination number $z = 2D$ the ground state is a Mott insulator (MI) with all sites singly occupied if $U > z \max(V, |t_{AA}| + |t_{BB}|)$; b) the ground state is a charge density wave (CDW) if $V > \max(U/z, U/2 + |t_{AA}| + |t_{BB}|)/2$ (simple cubic lattices); c) there is a region with mobile carriers which we call metallic (M) between these two phases, the M-MI boundary being at $U_{M-MI} = z(|t_{AA}| + |t_{BB}|)$ (for $D = 1$ this state is a ‘‘non-conducting metal’’ [30,36]); d) for $D = 1$ the M-CDW boundary is at $V_{M-CDW} = (U/2 + |t_{AA}| + |t_{BB}|)/2$.

For $0 < t_{AB} < t_{AA} = t_{BB} = t$, $U, V \neq 0$ the phase diagram at $n = 1$ has been studied numerically in 1D and

2D and within mean-field approximation [37–39]. The high spin degeneracy of the MI phase for $t_{AB} = 0$ is lifted and gives place to a spin density wave (SDW) phase. There exists a metallic phase (the detailed nature of which will be discussed later) for small values of U and V , which shrinks as $t_{AB} \rightarrow t$. When $t_{AB} = t$ (Hubbard limit), several results indicate that there is no M phase, except, eventually, on the second-order transition line between the CDW and SDW phases, that ends at a tricritical point. The position of this point is, to date, not well determined and should be around $U \sim 2V \sim 4t$ [52–56].

The aim of the present work is to study, by numerical and analytical methods, possible existence of superconductivity in the model (3) in regions of parameters for which exact results are not available. Special attention is paid to the occurrence of exotic p -wave triplet superconductivity (TS). In particular, we show strong evidence that the extension to finite t_{AB} of the above mentioned M phase displays TS. Some evidence of triplet superconductivity exists in the extended Hubbard model (Eq. (3) with $t_{AA} = t_{AB} = t_{BB}$) very near the line $U = -2V$ for positive U [56,57].

In Section 2 we briefly review the results which indicate that the model (3) exhibits s -wave superconductivity (or dominant singlet superconducting correlations at large distances in 1D) for certain parameters. At half filling we present evidence of a superconductor-insulator transition. In Section 3 we explain the HF-BCS decoupling scheme and apply it to the electron-hole symmetric case $t_{AB} < t_{AA} = t_{BB}$ at half filling. We obtain a phase diagram separating regions in which the stable phase is a CDW, SDW or triplet p -wave superconductor (TS). The latter is the stable one for sufficiently small U and V in a simple cubic lattice in any dimension. In Section 4 we calculate the phase diagram in 1D by a numerical method recently introduced by two of us [40], which uses topological quantum numbers as order parameters, and compare with the HF-BCS results. Section 5 contains the conclusions.

2 s-wave superconductivity

The model (3) becomes simpler when the three-body part of it vanishes. The coefficient of terms of the form $c_{i,\sigma}^\dagger c_{j,\sigma} n_{i,-\sigma} n_{j,-\sigma}$ is $t_3 = 2t_{AB} - t_{AA} - t_{BB}$.

We concentrate first in the results for $t_3 = 0$. Using a HF-BCS decoupling, it has been shown that the model leads to (extended) s -wave superconductivity for $V = 0$, small enough U and positive (negative) $t_2 = t_{AA} - t_{AB}$ for a more (less) than half-filled band [41]. In 1D Japaridze and Müller-Hartmann have calculated the correlation exponent K_ρ using continuum limit theory and bosonization [43]. They obtained that $K_\rho > 1$ (superconducting correlations dominate at large distances) if

$$U < U_c = 8(t_{AB} - t_{AA}) \cos(\pi n/2) - 6V \quad (4)$$

where n is the number of particles per site.

The particular case $t_2 = t_{AA}$ corresponds to the relation $t_{AA} = -t_{BB}$, $t_{AB} = 0$, and has been exactly solved for $V = 0$ [27–30]. Superconducting η -paired states with off-diagonal long-range order (ODLRO) are part of the highly degenerate ground state. However, as a consequence of this degeneracy, the system does not display anomalous flux quantization (AFQ) for large rings [30]. In other words, the Meissner effect is absent.

Since, due to the rather pathological degeneracy of the ground state, the exact results do not allow to draw definite conclusions for $t_{AB} \neq 0$ while the bosonization results are expected to be valid only for weak interactions, we have carried out a detailed numerical study of the model for $V = 0$ in rings of 10 and 12 sites [42]. For $t_{AA} = 1$, $t_{AB} = 2$, $t_{BB} = 3$, $2/3 < n < 4/5$ and small U , there are clear indications of binding and AFQ (a tendency towards a periodicity of half a flux quantum in the energy as a function of flux). The calculation of the correlation exponent K_ρ indicates that superconducting correlations dominate for $U < U_c$, where $U_c \sim 9, 8$ or 6.5 for $n = 0.4, 0.5$ or 0.6 electrons per site respectively. These values are nearly 1.4 times larger than the corresponding continuum limit results: 6.46, 5.66 and 4.70 respectively, according to equation (4). For $n = 0.8$, $t_{AA} = 1$, $t_{AB} = 1.5$ and $t_{BB} = 2$ we obtain $U_c = 1.6$, while equation (4) gives $U_c = 1.24$.

The qualitative agreement between equation (4) and our numerical results is lost at half filling. While the continuum limit theory predicts that the system is an insulator for all positive values of U [43], we find evidence of a superconductor-insulator transition as a function of U when $t_3 = 2t_{AB} - t_{AA} - t_{BB} = 0$ and any sign of $t_2 = t_{AA} - t_{AB}$ (the sign can be changed using the symmetry properties of the model [30,42]). This agrees with previous numerical work of K_ρ [42,44], a BCS calculation [44] and recent results using slave bosons [45]. For small positive values of U we find in rings of 10 sites that the energy as a function of flux $E(\phi)$ has a form that suggests AFQ for $t_{AA} = 1$, $t_{AB} = 0.5$ and $t_{BB} = 0$. Furthermore, using topological quantum numbers [40] (as explained briefly in Sect. 4), we detect a transition from charge (γ_c) and spin (γ_s) Berry phases $(\gamma_c, \gamma_s) = (0, 0)$ to (π, π) (corresponding to the SDW phase) as U increases. We point out that the topological values $(0, 0)$ are also obtained for the negative- U Hubbard model which displays singlet s -wave superconductivity. The value of U_c separating both phases is small. For 10 sites we obtain $U_c = 0.075$. From the size-dependence we estimate that this actually corresponds to a lower bound. From the results of K_ρ of reference [42] and using symmetry arguments we estimate (remember $n = 1$) $U_c = 0.5$ for $t_{AA} = 1$, $t_{AB} = 3/5$ and $t_{BB} = 1/5$ and $U_c = 0.3$ for $t_{AA} = 1$, $t_{AB} = 2/3$ and $t_{BB} = 1/3$, but careful finite-size scaling is necessary to give accurate values of U_c .

While the values of K_ρ alone cannot distinguish between singlet s -wave (even) and triplet p -wave (odd) superconducting states, the BCS results and the Berry phases $(0, 0)$ are indicative of the former. A demonstration of the s -wave character was provided by the results of stochastic diagonalization by Michielsen and De Raedt

[46] which showed the presence of singlet-singlet quasi ODLRO in 1D for $t_{AA} = 1$, $t_{AB} = 1.4$ and $t_{BB} = 1.8$, $n = 1.5$ and $U < 1$, and also for $t_{AA} = t_{AB} = t_{BB} = 1$, $U = -4$ and $n = 1.5$ (negative- U Hubbard model).

We discuss now the effect of the three-body term $t_3 = 2t_{AB} - t_{AA} - t_{BB}$. When $t_{AA} = t_{BB}$ the model is electron-hole symmetric for bipartite lattices [42]. For the electron-hole symmetric case with $t_3 > 0$, the mean-field HF-BCS decoupling of the two- and three-body terms leads to singlet s -wave (and also d -wave in 2D) superconducting solutions [47]. However, a positive t_3 also favours CDW and SDW instabilities [38]. In 2D, the detailed (mean-field) calculation of the phase diagram for $V = 0$ shows that the SDW is stable for positive U near half filling, while extended s -wave superconductivity is present in the ground state for small U or large doping. The d -wave paramagnetic solution has always larger energy than the other two [47]. The electron-hole symmetric case with $t_3 < 0$ is analyzed in the next section.

3 p -wave superconductivity

In this section we discuss the phase diagram of the model for the electron-hole symmetric case $t_{AB} < t_{AA} = t_{BB}$ and half filling, in simple cubic lattices in arbitrary dimensions using HF-BCS. This decoupling leads naturally to p -wave superconductivity for small U and V . Although a real proof of the existence of this phase is lacking, further arguments given in the next Section support its existence in 1D. For $t_{AB} = 0$, exact results have shown that for small U and V , the CDW and SDW phases become unstable because the system lowers its energy taking advantage of the kinetic energy terms t_{AA} and t_{BB} , which are inactive in the CDW and SDW phases [26,35,36]. As mentioned in the Introduction, a phase diagram valid for several lattices in arbitrary dimensions was constructed [36]. For $t_{AB} = V = 0$, an exact solution exists in 1D [27–30], but these exact results were unable to identify the nature of the third phase for finite t_{AB} . The numerical and mean-field results [37,38] show the presence of mobile carriers and a non-vanishing Drude weight within the M phase in 1D and 2D, suggesting that the system is a Luttinger liquid in 1D and metallic in 2D for small U and V . However, a suggestion that this phase has dominant triplet superconducting correlations at large distances was given only recently [40].

Note that if in the three-body part of the correlated hopping (see Eq. (3)), the operator $c_{i,\sigma}^\dagger c_{j,\sigma}$ is replaced by its expectation value τ (assumed for this argument independent of spin and nearest-neighbour pair, as in the non-interacting case), this term takes the form $t_3 \tau \sum_{\langle ij \rangle} n_{i,-\sigma} n_{j,-\sigma}$, with $t_3 = 2t_{AB} - t_{AA} - t_{BB} < 0$. Thus, the three-body term reduces to an attraction of nearest-neighbour electrons *with the same spin* and triplet pairing is a natural consequence of it.

The HF-BCS decoupling is the most convenient mean-field approximation to reduce the many-body terms of the Hamiltonian to one-body terms. It is a generalization

of the procedure used by Foglio and Falicov for the normal case [20]. A more direct way of obtaining the HF-BCS Hamiltonian (H_{HFBCS}) is to define the vacuum as the (unknown for the moment) Slater determinant that is the ground state of H_{HFBCS} . Then one should normal order the exact Hamiltonian with respect to this vacuum using Wick's theorem [58,59]. Clearly the contractions that appear using this theorem are the HF-BCS expectation values. The exact Hamiltonian takes the form of the HF-BCS ground-state energy plus normal ordered one- and many-body terms. Neglecting the latter, one obtains the HF-BCS Hamiltonian.

Neglecting also for simplicity spin-flip expectation values of the form $\langle c_{i,\sigma}^\dagger c_{j,-\sigma} \rangle$ (related to spiral spin structures), we obtain H_{HFBCS} using the following approximations for the two- and three-body terms of H :

$$n_{i\uparrow}n_{i\downarrow} \simeq \langle n_{i\uparrow} \rangle n_{i\downarrow} + n_{i\uparrow} \langle n_{i\downarrow} \rangle - \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + (c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \langle c_{i\downarrow} c_{i\uparrow} \rangle + h.c.) - |\langle c_{i\downarrow} c_{i\uparrow} \rangle|^2, \quad (5)$$

$$\begin{aligned} (n_{i\uparrow} + n_{i\downarrow})(n_{j\uparrow} + n_{j\downarrow}) &\simeq \langle n_{i\uparrow} + n_{i\downarrow} \rangle (n_{j\uparrow} + n_{j\downarrow}) \\ &+ \langle n_{i\uparrow} + n_{i\downarrow} \rangle \langle n_{j\uparrow} + n_{j\downarrow} \rangle - \langle n_{i\uparrow} + n_{i\downarrow} \rangle \langle n_{j\uparrow} + n_{j\downarrow} \rangle \\ &+ \sum_{\sigma} \{ -(\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle c_{j\sigma}^\dagger c_{i\sigma} + h.c.) + |\langle c_{i\sigma}^\dagger c_{j\sigma} \rangle|^2 \\ &+ \sum_{\sigma'} [(\langle c_{i\sigma}^\dagger c_{j\sigma'}^\dagger \rangle c_{j\sigma'} c_{i\sigma} + h.c.) - |\langle c_{i\sigma}^\dagger c_{j\sigma'} \rangle|^2] \}, \quad (6) \end{aligned}$$

$$\begin{aligned} c_{i\uparrow}^\dagger c_{j\uparrow} (n_{i\downarrow} + n_{j\downarrow}) &\simeq \langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle (n_{i\downarrow} \\ &+ n_{j\downarrow}) + c_{i\uparrow}^\dagger c_{j\uparrow} (\langle n_{i\downarrow} \rangle + \langle n_{j\downarrow} \rangle) \\ &- \langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle (\langle n_{i\downarrow} \rangle + \langle n_{j\downarrow} \rangle) \\ &+ c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \langle c_{j\downarrow} c_{j\uparrow} \rangle + c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \langle c_{i\downarrow} c_{j\uparrow} \rangle \\ &+ \langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle c_{j\downarrow} c_{j\uparrow} + \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle c_{i\downarrow} c_{j\uparrow} \\ &- \langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle \langle c_{j\downarrow} c_{j\uparrow} \rangle - \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle \langle c_{i\downarrow} c_{j\uparrow} \rangle, \quad (7) \end{aligned}$$

and the same interchanging spin up and down. Choosing one spin orientation for the sake of clarity, the three-body terms are replaced as:

$$\begin{aligned} c_{i\uparrow}^\dagger c_{j\uparrow} n_{i\downarrow} n_{j\downarrow} &= c_{i\uparrow}^\dagger c_{j\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} c_{j\downarrow}^\dagger c_{j\downarrow} \\ &\simeq c_{i\uparrow}^\dagger c_{j\uparrow} (\langle n_{i\downarrow} \rangle \langle n_{j\downarrow} \rangle + |\langle c_{i\downarrow}^\dagger c_{j\downarrow}^\dagger \rangle|^2 - |\langle c_{i\downarrow}^\dagger c_{j\downarrow} \rangle|^2) \\ &- c_{i\downarrow}^\dagger c_{j\downarrow}^\dagger (\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle \langle c_{j\downarrow}^\dagger c_{i\downarrow} \rangle + \langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle \langle c_{i\downarrow} c_{j\uparrow} \rangle) \\ &- c_{j\downarrow}^\dagger c_{i\downarrow}^\dagger (\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle \langle c_{i\downarrow}^\dagger c_{j\downarrow} \rangle + \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle \langle c_{j\downarrow} c_{j\uparrow} \rangle) \\ &+ n_{i\downarrow} (\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle \langle n_{j\downarrow} \rangle + \langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle \langle c_{j\downarrow} c_{j\uparrow} \rangle) \\ &+ n_{j\downarrow} (\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle \langle n_{i\downarrow} \rangle + \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle \langle c_{i\downarrow} c_{j\uparrow} \rangle) \\ &+ c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger (\langle c_{i\downarrow} c_{j\uparrow} \rangle \langle n_{j\downarrow} \rangle - \langle c_{j\downarrow} c_{j\uparrow} \rangle \langle c_{j\downarrow}^\dagger c_{i\downarrow} \rangle) \\ &+ c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger (\langle n_{i\downarrow} \rangle \langle c_{j\downarrow} c_{j\uparrow} \rangle - \langle c_{i\downarrow} c_{j\uparrow} \rangle \langle c_{i\downarrow}^\dagger c_{j\downarrow} \rangle) \\ &+ c_{i\downarrow} c_{j\uparrow} (\langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle \langle n_{j\downarrow} \rangle - \langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle \langle c_{i\downarrow}^\dagger c_{j\downarrow} \rangle) \end{aligned}$$

$$\begin{aligned} &+ c_{j\downarrow} c_{j\uparrow} (\langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle \langle n_{i\downarrow} \rangle - \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle \langle c_{j\downarrow}^\dagger c_{i\downarrow} \rangle) \\ &+ (c_{i\downarrow}^\dagger c_{j\downarrow}^\dagger \langle c_{j\downarrow} c_{i\downarrow} \rangle + c_{j\downarrow} c_{i\downarrow} \langle c_{i\downarrow}^\dagger c_{j\downarrow}^\dagger \rangle) \langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle \\ &+ 2[\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle (|\langle c_{i\downarrow}^\dagger c_{j\downarrow} \rangle|^2 - \langle n_{i\downarrow} \rangle \langle n_{j\downarrow} \rangle) \\ &+ \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle (\langle c_{j\downarrow} c_{j\uparrow} \rangle \langle c_{j\downarrow}^\dagger c_{i\downarrow} \rangle - \langle c_{i\downarrow} c_{j\uparrow} \rangle \langle n_{j\downarrow} \rangle) \\ &+ \langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle (\langle c_{i\downarrow} c_{j\uparrow} \rangle \langle c_{i\downarrow}^\dagger c_{j\downarrow} \rangle - \langle c_{j\downarrow} c_{j\uparrow} \rangle \langle n_{i\downarrow} \rangle) \\ &- \langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle |\langle c_{i\downarrow}^\dagger c_{j\downarrow}^\dagger \rangle|^2]. \quad (8) \end{aligned}$$

Each thermodynamic phase of the model in the HF-BCS approximation is characterized by a different symmetry breaking of the expectation values entering equations (5-8) with respect to the unperturbed system. Since singlet s - and d -wave solutions do not exist for $t_{AB} < 0$ [47], we have looked for triplet p -wave superconductivity (TS). Based on symmetry properties expected for the ground state in 1D (explained at the end of the next section), we assumed that only the $S_z = \pm 1$ components of the triplet order parameter do not vanish like in the Anderson-Brinkman-Morel phase of superfluid ^3He [60]. For this case we have $\langle c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle = 0$ for all i, j in one lattice direction and a vector δ connecting nearest-neighbours $\langle c_{i+\delta,\sigma}^\dagger c_{i,\sigma}^\dagger \rangle = -\langle c_{i-\delta,\sigma}^\dagger c_{i,\sigma}^\dagger \rangle = \psi \neq 0$, while in other directions $\langle c_{i+\delta,\sigma}^\dagger c_{i,\sigma}^\dagger \rangle = 0$. As a consequence also $\langle c_{i+\delta,\sigma}^\dagger c_{i,\sigma} \rangle$ depends on direction. We also considered the usual CDW and SDW phases for which the cubic lattice in D dimensions is divided into two equal interpenetrating sublattices A and B, in such a way that the nearest-neighbours of any site of A lie in B. In this case, for the SDW $\langle n_{i,\sigma} \rangle = (1 + m\sigma e^{i\mathbf{Q}\cdot\mathbf{R}_i})/2$ while for the CDW $\langle n_{i,\sigma} \rangle = (1 + \Delta e^{i\mathbf{Q}\cdot\mathbf{R}_i})/2$ with $\mathbf{Q} = (\pi, \pi, \dots, \pi)$ and m and Δ order parameters. The resulting one-particle Hamiltonian has the form of the non-interacting one with a renormalized effective hopping t_{eff} , plus a symmetry breaking perturbation which, at half filling, depends on two or three parameters to be determined selfconsistently. These parameters are the corresponding order parameter (ψ, m or Δ) and the different values of $\langle c_{i+\delta,\sigma}^\dagger c_{i,\sigma} \rangle$: one for CDW, SDW, or TS in 1D, two for TS in more than 1D (for TS in more than 1D t_{eff} becomes anisotropic).

The phase diagram has a natural energy scale which we call E : the absolute value of the energy of the half-filled non-interacting case for hopping $|t_3| = t_{AA} + t_{BB} - 2t_{AB}$, counting both spins. The ratio $E/|t_3|$ depends only on the dimension of the simple cubic lattice and is $4/\pi = 1.273$ in 1D, $16/\pi^2 = 1.621$ in 2D, 2.005 in 3D [61] and 0.798 in ∞D [61]. The only point in the $U - V$ phase diagram for which the paramagnetic solution is stable is the triple point $(U_t, V_t) = (E, E/z)$ where $z = 2D$ is the coordination number. If and only if $V < V_t$, for any U , the paramagnetic solution is unstable against the TS phase; if and only if $U > U_t = E$, it is unstable against SDW; and if and only if $V > (E + U)/2z$ it is unstable against the CDW. These boundaries allow us to establish that, in any dimension, inside the region bounded by the dashed line in Figure 1, the TS is the stable phase. Also the CDW-TS boundary lies between the dashed and dot-dashed lines of Figure 1. With an adequate change of variables, it can

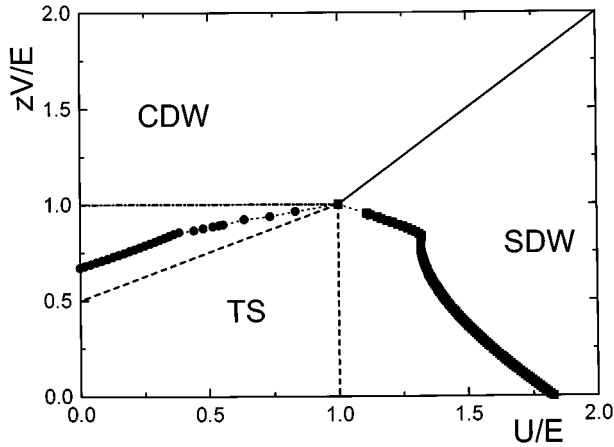


Fig. 1. Mean-field (HF BCS) phase diagram of the model (3) for one particle per site and $t_{AA} = t_{BB} > t_{AB}$. The full line is the CDW-SDW boundary in any dimension. Inside the region bounded by the dashed lines, the triplet superconducting (TS) phase is the stable one. The CDW-TS boundary lies between the dashed and dot-dashed lines. $E/2(t_{AA} - t_{AB})$ is a number of order one which depends on dimension (see text). Solid circles (squares) are points on the CDW-TS (SDW-TS) boundary in 1D for $t_{AA} = t_{BB} = 1$ and $t_{AB} = 0.2$.

be shown that the self-consistency problems for the CDW and SDW take the same form on the line $U = zV$. Thus, in any dimension, for $U \geq E$, $U = zV$ is the boundary of the CDW-SDW first-order transition, independently of the other parameters of the model.

The above results are quite general and valid in any dimension. The region of stability of the TS extends always beyond the dashed lines of Figure 1 and the precise location of the boundaries of the TS depends on t_{AB} and the dimension. In Figure 1, the specific case of 1D and $t_{AA} = t_{BB} = 1$, $t_{AB} = 0.2$ is shown. The change in slope of the SDW-TS boundary is due to a metamagnetic first-order transition inside the SDW from large to small order parameter as V increases. A similar situation occurs in the CDW-TS boundary. Near the triple point, and particularly for $t_{AB} \sim 1$, all order parameters become very small, and the numerical method used to solve the self-consistency equations breaks down. Similarly, in 1D, for $V = 0$ and $t_{AB} = 0.097$, the effective hopping vanishes in the paramagnetic phase and the HF-BCS approximation becomes invalid for $t_{AB} \sim 0.1$ or smaller.

One expects that the HF-BCS results are reliable for small values of the interactions (small U , V and $1 - t_{AB}$, with $t_{AA} = t_{BB} = 1$) and $D \gg 1$, supporting the existence of the p -wave TS for these parameters. In 1D there is no true LRO and the HF-BCS results only have qualitative validity. A comparison with more accurate methods in 1D is made in the next section.

4 Phase diagram obtained from topological transitions

In recent years, the concept of Berry phase was a subject of great interest in a variety of fields in physics. Zak has shown that it can be used for labeling energy band in solids [62], and subsequent work showed that changes of polarization are proportional to the corresponding change in a Berry phase [63]. Ortiz and Martin have generalized these concepts to a many-body ground state [64], and Resta and Sorella used this concept to identify a ferroelectric transition [65]. This many-body Berry phase is simply the phase captured by the ground state in a ring of L sites as the boundary conditions $c_{i+L,\sigma}^\dagger = e^{i\phi} c_{i,\sigma}^\dagger$, complete a cycle from a flux $\phi = 0$ to $\phi = 2\pi$ [40, 64–66]. We call this phase the charge Berry phase γ_c .

While previous work assumed always that the ground state is non-degenerate for all ϕ (except at isolated points of the parameter space at which γ_c is indefinite), two of us have recently generalized this concept for the case in which there is a crossing of levels in the ground state as a function of ϕ [40]. This is the case of the superconducting phases, for which there is AFQ as a consequence of the crossing energy levels. Furthermore, a “spin” Berry phase γ_s was defined as that captured by the ground state in the cycle $0 \leq \phi \leq 2\pi$ varying the boundary conditions as $c_{i+L,\sigma}^\dagger = e^{i\sigma\phi} c_{i,\sigma}^\dagger$ with $\sigma = 1$ (-1) for spin up (down) [40]. Due to the inversion symmetry of the model (3), the Berry phases are quantized and in 1D can take only the values 0 and π (*modulo* 2π). Thus, it turns out that γ_c/π and γ_s/π are topological quantum numbers which are related to changes in the total polarization and the difference between polarizations for spin up and down respectively [40].

Defining a vector $\gamma = (\gamma_c, \gamma_s)$, it is easy to see [40] that for a CDW (SDW) with maximum order parameter one has $\gamma = (0, 0)$ ($\gamma = (\pi, \pi)$), and these values are consistent with the change in up and down polarizations when the electrons of spin down of one phase are moved to the other sublattice to form the other phase. Since γ jumps in π only at the phase transitions, the values $\gamma(\text{CDW}) = (0, 0)$ and $\gamma(\text{SDW}) = (\pi, \pi)$ are valid for any non-zero magnitude of the corresponding order parameters. These values are also consistent with the canonical transformation.

$$c'_{j,\uparrow} = c_{j,\uparrow}, c'_{j,\downarrow} = (-1)^j c_{j,\downarrow}^\dagger \quad (9)$$

under which the CDW and SDW are interchanged and the Berry phases modulo π transform as:

$$\gamma' = \gamma + \pi. \quad (10)$$

Since the ground state for $U = V = 0$ is invariant under equation (9), equation (10) implies that for the third phase present in the diagram $\gamma_c(TS) = \gamma_s(TS) + \pi$ (numerically it turns out that $\gamma(TS) = (0, \pi)$), and thus, at least one of the topological numbers γ_c/π , γ_s/π jumps at each boundary. Thus, this method combined with finite-size scaling is able to determine accurately the phase diagram (see Fig. 2).

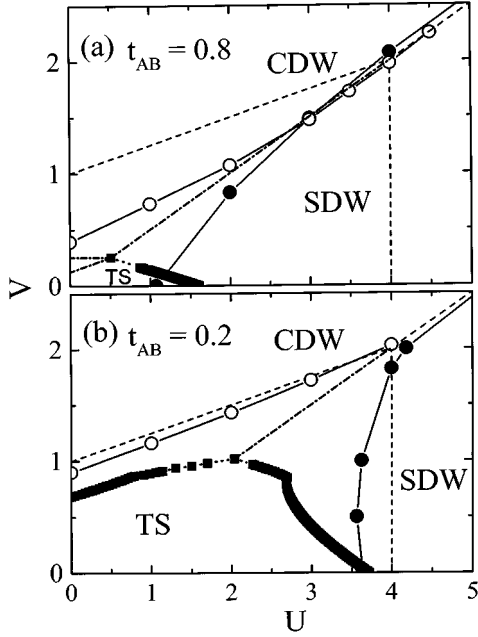


Fig. 2. Phase diagram of the model (3) in 1D for one particle per site, $t_{AA} = t_{BB} = 1$ and two different values of t_{AB} . Solid (open) circles are determined from the jump of γ_c (γ_s). Solid squares, dotted and dot-dashed lines are HF BCS results. The dashed lines are exact results in the limit $t_{AB} \rightarrow 0$ [36]. Full lines are guides to the eye. The small difference between the results from both Berry phases at the CDW-SDW boundary is due to finite-size effects.

The best previous numerical methods to determine phase diagrams of this type were based on the size dependence of SDW and CDW order parameters, and their probability densities in a Monte-Carlo sampling [38, 52, 54]. However, these quantities as well as different correlation functions vary smoothly at the transition and it is very difficult to obtain accurate boundaries [52–55]. Instead, the use of topological numbers as order parameters necessarily leads to sharp transitions.

In Figure 2 we show the phase diagram of the model (3) in 1D obtained with the above mentioned method, for two values of t_{AB} , and compare it with the corresponding HF BCS results and with the exact result for $t_{AB} \rightarrow 0$ [36]. Although, as mentioned in the previous section, the HF BCS results are not expected to have quantitative validity in 1D for large values of the interaction, for small t_{AB} the resulting phase diagram is in reasonable agreement with that obtained with the above explained more reliable numerical method. The results of the latter tend to the exact phase diagram as $t_{AB} \rightarrow 0$. The comparison also shows that the TS phase in 1D extends beyond the expectations of the HF BCS results. This is particularly clear for $t_{AB} \sim t_{AA} = t_{BB}$ and $U \sim 2V$, and is probably related to the fact that, in the continuum limit theory, the backscattering and Umklapp terms coming from the U and V terms of the Hamiltonian (ultimately responsible of the insulating behaviour), nearly cancel each other on the line $U = 2V$ [54, 56].

We should note that the method of the topological transitions alone, is not able to identify the nature of the TS phase, since different phases can have the same topological numbers. For example, we find $\gamma = (0, 0)$ not only for the CDW, but also in the negative- U Hubbard model with small negative V , for which s -wave singlet pairing occurs [56, 57]. We also find it for our model (Eq. (3)) with $t_3 = V = 0$ and small U , for which also singlet superconducting correlations dominate at large distances, as explained in Section 2.

In the following we summarize the evidence in favour of the triplet superconducting phase in 1D.

a) Superconductivity

- Since each time the Berry phase is evaluated, the ground state energy as a function of the flux $E(\phi)$ is computed at the same time, we have checked that there is a tendency to AFQ (*i.e.* $E(\phi) \simeq E(\phi + \pi)$) inside almost all the TS phase.
- Our previous calculations of the correlation exponent K_ρ for $V = 0$ show the dominance of superconducting correlations at large distances ($K_\rho > 1$) for $U < U_c$, and an opening of a charge gap for $U > U_c$ [39, 42]. The value of U_c has been estimated as $U_c \sim 3.5$ for $t_{AB} = 0.2$ and $t_{AA} = t_{BB} = 1$ [42] in good agreement with the result shown in Figure 2. For $t_{AB} = 0.6$, from K_ρ one obtains $U_c = 2.05 \pm 0.05$ [39], while from the topological transition we obtain $U_c = 2.11$ [40].
- For a “metallic” gapless phase with $K_\rho \leq 1$ (as in the non-interacting case), one expects undetermined Berry phases [40, 66] instead of the result $\gamma = (0, \pi)$ for the TS phase.

b) Triplet character

- The HF BCS decoupling in any dimension leads to unstable singlet and stable triplet superconductivity.
- For known cases of singlet superconductivity (mentioned above) we obtain $\gamma = (0, 0)$ in contrast to the result $\gamma(TS) = (0, \pi)$.
- We find that in rings of 10 sites the nearest-neighbour triplet-triplet correlations are larger than the singlet-singlet ones at the largest distance in the ring (5 sites).
- Numerically, we obtain a non-degenerate ground state inside the TS phase which should transform into itself under the symmetry transformation (9) for $U = V = 0$, since the Hamiltonian is invariant at that point. An ordinary BCS singlet solution transforms into a SDW under this transformation, leading necessarily to a degenerate ground state for $U = V = 0$. Instead, using $c_{k,\downarrow}^\dagger = c_{-k+Q,\downarrow}$, $|0\rangle = \prod_k c_{k,\downarrow}^\dagger$ and $\cos(k_\alpha + Q_\alpha) = -\cos(k_\alpha)$, it can be easily checked that our p -wave triplet BCS solution in the x -direction (see Sect. 3 after Eq. (8)):

$$|p_x\rangle = \prod_{k\sigma, k_x > 0} (u_k + v_k c_{k,\sigma}^\dagger c_{-k,\sigma}^\dagger) |0\rangle \quad (11)$$

is invariant under equation (9).

- Finite-size scaling is consistent with the absence of a spin gap inside the TS phase. Continuum-limit theory predicts that triplet superconducting correlations dominate at large distances (due to logarithmic corrections) when $K_\rho > 1$ and a spin gap is absent [67].

5 Summary and discussion

We have studied the occurrence of superconductivity in the generalized Hubbard model (3). This model contains the most important physical ingredients expected to describe transition metals in general [26] or cuprate superconductors [21–24]. In 1D, most of the parameters of the model appropriate for systems like trans-polyacetylene have been estimated [25,48] and are consistent with several regions of parameters for which we find superconductivity.

When the three-body term $t_3 = 2t_{AB} - t_{AA} - t_{BB}$ vanishes, singlet s -wave superconductivity is expected for electron densities per site $n \neq 1$ or very small values of U . For n not too near one and $V = 0$, equation (4) describes qualitatively the values of U below which superconducting correlations dominate at large distances in 1D. However, numerical results suggest that equation (4) underestimates these values by a factor ~ 1.4 . For $n = 1$, the region of superconducting behaviour is very small.

Instead, for $n = 1$ and $t_{AB} < t_{AA} = t_{BB} = 1$, we find evidence of a p -wave triplet superconducting phase (TS) for small values of U and V . The Hartree-Fock BCS approximation gives a stable TS for sufficiently small U and V in any dimension. In 1D, the numerical method of the Berry phases, described in the previous section, predicts a stable TS even for small $1 - t_{AB}$ and large values of $U \sim 3$ near the line $U = 2V$.

While a definite proof of the triplet character of this phase does not exist so far, there are several arguments in favour of it enumerated at the end of the previous section. In contrast to the previous case of s -wave superconductivity ($2t_{AB} = t_{AA} + t_{BB}$) mentioned above, for $t_{AB} < t_{AA} = t_{BB}$, the effect of doping seems to weaken the TS in favour of the SDW at $V = 0$ [42].

Experimentally, evidence of a triplet odd-parity superconducting order parameter exists in some quasi-1D organic conductors [68]. In 1D, our solution is compatible with a nodeless superconducting gap, as evidenced by thermal conductivity measurements in (TMTSF)₂ClO₄ [68].

The effect of phonons, particularly in 1D, can stabilize insulating CDW states, or favour s -wave superconducting states. However, based on the general study performed in 1D using bosonization [67], we believe that our results remain qualitatively valid in presence of a small or moderate electron-phonon coupling. In addition, if phonons are treated in the adiabatic approximation, the model (3) retains its form [21b].

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