Superconductivity and Topological Numbers in the Hubbard Chain with Bond-Charge Interaction

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We determine the quantum phase diagram of the Hubbard chain with electron-hole symmetric correlated hopping at 1/2- and 1/4-filling using geometric concepts and continuum limit field theory. The long distance behavior of various correlation functions show a very rich phase diagram with several insulating, metallic, and superconducting phases, which might be relevant to \((\text{TMTSF})_2X\) compounds. The closing of charge and spin gaps are accurately resolved as topological transitions (jumps in \(\pi\) of Berry phases). The metallic or insulating character of each thermodynamic phase is obtained from the ground-state expectation value of a displacement operator in reciprocal space.

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Superconductivity studies in the Bechgaard salts with the generic formula \((\text{TMTSF})_2X\) have enriched our knowledge of low-dimensional conductors with the new physics discovered. Although at very low temperatures, the transverse hopping should play a role, the extremely large anisotropy suggests that a one-dimensional (1D) model should be a good starting point for understanding these compounds. Tight-binding calculations suggest that only one band crosses the Fermi level. Therefore, one can construct an effective 1D one-band model, retaining only the ground state (GS) of each unit cell for zero, one, and two holes and can map these states into the corresponding ones of a Hubbard model. This is a formidable task, in contrast to cuprate superconductors and has not been done yet. However, it is evident that the effective hopping should depend upon the occupation of the sites involved, and one expects an important on-site interaction \(U\). These
physical considerations lead to the following effective Hamiltonian

$$H = \sum_{\langle i,j \rangle} \sigma (c_i^\dagger c_j + h.c.) + t_{AA}(1-n_i)(1-n_j) + t_{BB} n_i n_j + t_{AB} [n_i (1-n_j) + n_j (1-n_i)] + U \sum_i \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right)$$

in standard notation, with one hole per unit cell (1/2-filling, \( n = 1 \)). We restrict the present study to the electron-hole symmetric case \( t_{AA} = t_{BB} = 1 \).

Another possible starting point is to retain the states of lowest energy of only one organic molecule TMTSF (instead of the unit cell). The resulting Hamiltonian is similar to (1), but now the operators \( c_i^\dagger \sigma, c_i \sigma \) act on low-energy states of one molecule (labeled by \( i \)), the parameters are different, and the appropriate filling is one hole each two sites (1/4-filling, \( n = 1/2 \)).

In this work we determine the quantum phase diagram of \( H \), both for 1/2- and 1/4-filling, using recent developments based on geometrical concepts, Lanczos diagonalization, and density-matrix renormalization group (DMRG) methods. We also extend away from 1/2-filling previous studies using continuum limit field theory (CLFT), valid for small values of the interactions. Varying the parameters of the model, we obtain several thermodynamic phases with noticeable correspondence to the observed ones.

The basic tool for determining accurate phase boundaries are the charge (\( \gamma_c \)) and spin (\( \gamma_s \)) Berry phases. \( \gamma_c (\gamma_s) \) is the phase captured by the GS of a system of length \( L \), when twisted boundary conditions \( c_{i+L} = e^{i\Phi} c_i^\dagger \sigma \) are varied in the cycle \( 0 \leq \Phi \leq 2\pi \), keeping \( \Phi = \Phi_{\uparrow} = \Phi_{\downarrow} (\Phi = -\Phi_{\uparrow} = \Phi_{\downarrow}) \).

For systems with inversion symmetry, \( \gamma_c \) and \( \gamma_s \) can only be either 0 or \( \pi \) (mod \( 2\pi \)). Then, there are only four possible values of the topological vector \( \vec{\gamma} = (\gamma_c, \gamma_s) \). In this model, for \( n = 1 \), these values correspond to the four thermodynamic phases which can be obtained by varying the parameters. A jump by \( \pi \) in \( \gamma_c \) (\( \gamma_s \)) signals the opening of a charge \( \Delta_c \) (spin \( \Delta_s \)) gap and a change by \( e/2 \) in the polarization (difference between up and down polarizations) of the system. For the present \( H \) and any filling \( \gamma_s = \pi \) if and only if \( \Delta_s = 0 \), and for \( n = 1, \gamma_c = 0 \) if and only if \( \Delta_c = 0 \).

For a system of arbitrary length \( L \), in contrast to any other observable, \( \vec{\gamma} \) jumps at the transitions, and the location of this jump in parameter space has a very small size dependence. Close to \( n = 1 \), the \( L \to \infty \) phase boundaries (extrapolated from \( L = 6, 8, 10, \) and 12), are displayed in Fig. (a). We estimate the error in the critical value of \( U \) to be less than 1%.

Dotted lines correspond to results obtained using the CLFT. Agreement with the topological transitions is excellent for small \( t_{AB} - 1 \) and \( U \), in particular, for \( 0.6 \leq t_{AB} \leq 1.2 \). For large negative \( U \) and \( n = 1 \), the dominant correlation functions (CF) at large distances are those for the singlet
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Fig. 1. (a) Quantum phase diagram for $n \rightarrow 1$. The vector Berry phase $\vec{\gamma} = (\gamma_c, \gamma_s)$ of each thermodynamic phase is indicated. Dotted lines are the phase boundaries according to the CLFT. (b) Localization parameter $|z_L|$ for $t_{AB} = 0.6$ as a function of $U$. Solid circles are results for $L = 12$, and the solid line is a polynomial extrapolation in $1/L$ using $L = 4, 6, 8, 10$ and 12.

superconductor (SS) and a charge density wave (CDW), as in the negative-$U$ Hubbard model. For $n \neq 1$, SS CF prevail. For $0 < U < 4$, $n = 1$, and lowering $t_{AB}$, the nature of the different thermodynamic phases is the following: a dimerized spin (and pseudospin) Peierls (SP) phase, one with dominating spin density wave (SDW) CF, and one with identical triplet superconducting (TS) and bond SDW (BSDW) CF. We have established the dominant CF of this phase using DMRG, since, by symmetry, the correlation exponent $K_\rho = 1$ and all CF decay with the same leading power law factor. Slightly away from $n = 1$, where Umklapp processes in the CLFT become irrelevant, $K_\rho > 1$ and then, the TS CF are larger than all others at large distances. Therefore, in materials with weakly coupled chains and $n = 1$, fluctuations in the density of each chain should also favor the TS CF.

Increasing $U$, there is a Mott transition TS$\rightarrow$SDW which can be studied using the quantity $z_L = \langle g_L | \hat{O} | g_L \rangle$, where $\hat{O} = \exp(i \frac{2\pi}{L} \sum_j j \sigma j \tilde{n}_j \sigma)$ and $|g_L\rangle$ is the GS of the system ($\langle g_L | g_L \rangle = 1$) with $L$ sites and $L$ particles. Note that $\hat{O}$ shifts the wave vector of each particle in $2\pi/L$. Then, if $|g_L\rangle$ describes a Fermi or Luttinger liquid with a well-defined Fermi surface in the thermodynamic limit, $\lim_{L \rightarrow \infty} z_L = 0$. Instead, for an insulator, $|z_L| - 1$ goes to zero in the same way as the Drude weight $D_c$. Furthermore, from a cumulant expansion of $z_L$, it can be shown that $\ln |z_L|$ is a measure of the fluctuations of the polarization (specifically $2(\frac{2\pi}{L})^2 \ln |z_L| = \langle \sum j \sigma j \tilde{n}_j \sigma \rangle^2 - \langle (\sum j \sigma j \tilde{n}_j \sigma)^2 \rangle$), which are qualitatively different in an insulator and in a metal. The above discussion shows that except for some pathological cases, $\lim_{L \rightarrow \infty} |z_L| = 0$.
in a metal, while \( \lim_{L \to \infty} |z_L| = 1 \) in an insulator. In Fig. 1(b) we show \( |z_L| \) as a function of \( U \) for a case in which the topological transition is at \( U_c = 2.051 \). For \( U < U_c \), \( |z_L| \) decreases with \( L \), while above \( U_c \) (\( U \sim 3.5 - 4 \)), the extrapolated values saturate near 1.

We studied the evolution of the phase diagram with doping, using numerical calculations and the extension of the CLFT approach away from \( n = 1 \). For \( n = 2/3, 1/2 \), the topological transitions do not completely determine the phase diagram, and the calculation of the appropriate generalization of \( \gamma_c \) presents some technical problems. The jump in \( \gamma_s \) still very accurately determines the opening of \( \Delta_s \). For \( n = 1/2 \), the transition to dominating superconducting CF at large distances (\( K_\rho > 1 \)) is determined using numerical data for 8, 12 and 16 sites and finite-size scaling. While at \( n = 1 \) the computation of \( K_\rho \) has large finite-size effects, for \( n = 1/2 \) we compared \( K_\rho \) with available Bethe-ansatz results for \( t_{AB} = 1 \) with \( U = -2 \) and \( U = -4 \) and found the difference to be less than 1%.

As the system is doped away from 1/2-filling, the SDW advances gradually over the TS, and a strong increase in the SS region at the expense of the former SP takes place. The numerical phase diagram for \( n = 1/2 \) is shown in Fig. 2(a). Within the CLFT we obtained simple analytical expressions \( U_s = 2\sqrt{2}(t_{AB} - 1) \) for the transition at \( K_\rho = 1 \), and \( U_g = \sqrt{2}(8/\pi + 2)(t_{AB} - 1) \) for the value of \( U \) at which \( \Delta_s \) closes. As shown in Fig. 2(a), these expressions are again in excellent agreement with the numerical results, for small \( U \) and \( t_{AB} - 1 \). However, at intermediate values of the interactions, the deviations are much stronger than at 1/2-filling, and
The regions in which superconducting CF dominate are larger than those predicted by the CLFT. The extension of the SS region for $t_{AB} > 1$ and repulsive $U$ is particularly noticeable.

The nature of each thermodynamic phase, particularly the TS one, was confirmed by direct calculation of CF using DMRG. An example is shown in Fig. 2(b). The CF are defined as in Ref. [4]. The slower decay of the TS CF for $t_{AB} = 0.6$, and $U = -1$ is consistent with the fact that this point lies inside the TS phase in Fig. 2(a).

In summary, we determined the phase diagram of a model, expected to describe the low-energy physics of some organic superconductors, using recently developed geometrical concepts, and other numerical and analytical techniques. The phase diagram is very rich. At 1/2-filling ($n = 1$), there are all possible combinations of open or closed charge and spin gaps, and two different Mott transitions take place as a function of the Coulomb on-site interaction $U$. There is a wide region in which triplet superconducting CF dominate. This region includes positive values of $U$ if $0.57 < n < 1.43$.

The relevance of the model to (TMTSF)$_2$X compounds cannot be demonstrated until the low-energy reduction is performed. However, it is remarkable that for $n \sim 1$ and positive $U$, the sequence of phases predicted by the model with decreasing $t_{AB}$ is the same as that observed with increasing applied pressure. We expect that $n \sim 1$ might be more appropriate than $n \sim 1/2$ if the observed dimerization is physically important.

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