Phase Diagrams from Topological Transitions: The Hubbard Chain with Correlated Hopping

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The quantum phase diagram of the Hubbard chain with correlated hopping is accurately determined through jumps in \(\pi\) in the charge and spin Berry phases. The nature of each thermodynamic phase, and the existence of charge and spin gaps, is confirmed by calculating correlation functions and other fundamental quantities using numerical methods, and symmetry arguments. Remarkably we find striking similarities between the stable phases for moderate on-site Coulomb repulsion: spin Peierls, spin-density-wave and triplet superconductor, and those measured in (TMTSF)\(_2\)X.

The search for electronic mechanisms of superconductivity and the study of superconduction and Mott phase transitions are among the most interesting subjects of the physics of strongly correlated systems. In few cases, exact results have helped to elucidate the nature of these transitions \[4\]. In general one has to rely on numerical calculations of finite systems for which quantities like the Drude weight \(D_c\) (which should vanish for an insulator in the thermodynamic limit \[3\]), or any other correlation function, vary smoothly at the transition. Consequently, for instance, the boundaries between a charge-density-wave (CDW) or spin-density-wave (SDW) insulators and metallic phases in half-filled generalized Hubbard models were difficult to establish \[8\].

The Berry phase is a general geometrical concept which finds realizations in various physical problems \[4\]. It is the anholonomy associated to the parallel transport of a vector state in a certain parameter space. In condensed matter, the charge Berry phase \(\gamma_c\) is a measure of the macroscopic electric polarization in band or Mott insulators \[3\] while the spin Berry phase \(\gamma_s\) represents its spin polarization \[2\]. In systems with inversion symmetry \(\gamma_c\) and \(\gamma_s\) can attain only two values: 0 or \(\pi\) (mod \(2\pi\)). Thus, if two thermodynamic phases differ in the topological vector \(\vec{\gamma} = (\gamma_c, \gamma_s)\) this sharp difference allows us to unambiguously identify the transition point even in finite systems. This “order parameter” was recently used to detect metallic, insulator and metal-insulator transitions in one-dimensional lattice fermion models \[9\].

In this Letter we determine the quantum phase diagram of the Hubbard chain with correlated hopping at half-filling using topological transitions. The phase diagram is very rich showing two metallic and two insulating thermodynamic phases each characterized by one of the four possible values of the topological vector \(\vec{\gamma}\). One of the metallic phases corresponds to a Tomonaga-Luttinger liquid with dominant triplet superconducting correlations at large distances (TS). This is interesting since there is experimental evidence indicating that the Bechgaard salts (TMTSF)\(_2\)ClO\(_4\) and (TMTSF)PF\(_6\) under pressure are TS \[1\] \[3\]. Furthermore, the insulating SDW and spin gapped spin-Peierls phase observed in (TMTSF)PF\(_6\) as the pressure is lowered \[4\] are also present in the model phase diagram.

The effective model Hamiltonian is:

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

(1)

\(H\) contains the most general form of hopping term describing the low energy physics of a broad class of system Hamiltonians in which four states per effective site \(\gamma\) are retained. In particular, the Hamiltonian \(H\) in Eq. (1) has been derived and studied for transition metals, organic molecules and compounds \[2\], intermediate valence systems, cuprates and other superconductors \[12\]. In the continuum limit, the only relevant interactions at half-filling are \(U\) and \(t_{AA} + t_{BB} - 2t_{AB}\). Therefore, we restrict the present study to the electron-hole symmetric case \(t_{AA} = t_{BB} = 1\) which has spin and pseudospin SU(2) symmetries, the latter with generators \(\eta^+ = \sum_i (-1)^i c_i^{\dagger \uparrow} c_i^{\uparrow}\), \(\eta^- = (\eta^+)^\dagger\), and \(\eta^z = \frac{1}{4} \sum_i (\sum_{\bar{\sigma}} n_i^{\bar{\sigma}} - 1)\). The canonical transformation (CT) \(c_i^{\dagger \uparrow} \rightarrow c_i^{\dagger \uparrow}\), \(c_i^{\dagger \downarrow} \rightarrow (-1)^i c_i^{\dagger \downarrow}\) changes the sign of \(U\) in \(H\) and interchanges the total spin and pseudospin operators \((\eta^\alpha \leftrightarrow S^\alpha)\). These symmetry properties become crucial in this work. For \(t_{AB} = 0\), the model has been solved exactly \[3\] with the result that the ground state (GS) is highly degenerate. For \(t_{AB} \neq 0\) the physics of the model is still unclear and constitutes our main concern.

For the present case \(\gamma_{c,s}\) are defined as \[1\]

\[\gamma_{c,s} = i\int_0^{2\pi} \ d\phi \ \langle g_K(\phi, \pm \phi) \partial_\phi g_K(\phi, \pm \phi) \rangle,
\]

(2)

where \(\langle g_K(\phi_i, \phi_\downarrow) \rangle\) is the GS in the subspace with total wave vector \(K\) and other quantum numbers kept fixed, with fluxes \(\phi_\sigma\) for spin \(\sigma\). Changes in macroscopic polarization with spin \(\sigma\), \(P_\sigma\), are related to the corresponding
changes in the Berry phase by: $\Delta P = \Delta P' = e\Delta\gamma_{c,s}/2\pi \pmod{e}$ [8-10]. Thus, a phase transition will be detected by a jump in $\gamma_c (\gamma_s)$ if and only if both thermodynamic phases differ in $P_\uparrow + P_\downarrow$ ($P_\uparrow - P_\downarrow$) by $e/2 \pmod{e}$. For example, if one of the phases is a CDW with maximum order parameter (CDWM) and the other a Néel state (N), one is transformed into the other transforming half of the charges (those with a given spin) one lattice parameter. In addition, as explained below, in the present model topological transitions in $\gamma_c$ and $\gamma_s$ indicate the opening of the charge and spin gap $\Delta_c$, $\Delta_s$.

We find that the minimum of the GS energy as a function of fluxes, $E_g(\phi_\uparrow, \phi_\downarrow)$, corresponds to the so-called closed shell conditions (CSC): if the number of sites (assumed even) is $L = 2 \pmod{4}$, then $K = \phi_\sigma = 0$, while for $L$ multiple of four $K = \phi_\sigma = \pi$ (which is equivalent to taking antiperiodic boundary conditions and $K = 0$ in a system without fluxes).

For any finite system and fixed $t_{AB}$, varying $U$, two topological transitions occur in the model, corresponding to a jump in either $\gamma_c$ or $\gamma_s$. We have determined those transitions in rings of length $L = 6, 8, 10, 12$ using the Lanczos method. The results extrapolated with a cubic polynomial in $1/L$ are represented in Fig. 1. In contrast to other physical quantities which show large finite-size effects, particularly near $t_{AB} = 0$, the topological transitions converge rapidly to the thermodynamic limit (for example, for $t_{AB} = 0.05$, $\gamma_c$ jumps at $U = 3.451$, 3.681, 3.788, and 3.846 for $L = 6 - 12$, and the extrapolated value is $U = 3.932$). The numerical convergence becomes problematic for smaller $t_{AB}$ values. At $t_{AB} = 0$ the transition points are determined from the exact solution [8] as those values of $U$ where $\Delta_c$ and $\Delta_s$ open. Those critical values are $U_{c,s} = \pm 4$ and match smoothly with the rest of the curves in Fig. 1. It is easy to see that under CT the geometrical phases transform as $\gamma_c \leftrightarrow \gamma_s + \pi$ [8]. Thus, as seen in Fig. 1, a jump in $\gamma_c$ at $U_c$ (full line) implies a jump in $\gamma_s$ at $-U_c$ (dashed line), and vice versa.

In the case where all particles are localized one can easily determine the value of $\gamma_c$ as $\gamma_c = \Im \ln z_{c,s}^\gamma$, where $z_{c,s}^\gamma = (g|e^{i\sum_{j} \gamma(n_j, \pm n_j)}|g)$, (3) was recently used to study quantum localization [7,8].

In the thermodynamic limit $z_{c,s}^\gamma$ vanishes for a conductor while $|z_{c,s}^\gamma| \to 1$ for an insulator. Clearly, $\gamma_c(\text{CDWM}) = (0, 0)$, while $\gamma_s(\text{N}) = (\pi, \pi)$, and by continuity $\gamma_c(\text{CDW}) = (0, 0)$, $\gamma_s(\text{SDW}) = (\pi, \pi)$. On the other hand, it is not easy to predict the values of $\gamma_c$ in conducting phases. However, for $U = 0$, the model is invariant under CT. Therefore $\gamma_c = (\pi, 0)$, or $\gamma_s = (0, \pi)$, indicating a topological difference with the above mentioned CDW and SDW states.

![FIG. 1. Quantum phase diagram of the correlated hopping Hubbard chain. The vector Berry phase $\vec{\gamma} = (\gamma_c, \gamma_s)$ and the nature of each stable phase is indicated: Luther-Emery liquid with equally decaying singlet superconductor and CDW correlations (SS-CDW), Tomonaga-Luttinger liquid with triplet superconducting and bond SDW correlations dominating at large distances (TS-BS-DW), SDW insulator (SDW), and spin and pseudospin dimerization (S,PS).](image1)

![FIG. 2. Spin gap $\Delta_s$ as a function of $U$ for $t_{AB} = 0.6$, obtained with DMRG.](image2)

$\Delta_c$ ($\Delta_s$) vanishes at the left (right) of the full (dashed) line in Fig. 1, and is different from zero at the right (left). It has been shown, that in spin SU(2) symmetric systems the opening of $\Delta_s$ can be detected as a level crossing of triplet and singlet states for boundary conditions opposite to the CSC ones (periodic if the number of particles with a given spin $N_\sigma$ is even, and antiperiodic if $N_\sigma$ is odd) [9]. It is precisely this crossing which causes the jump in $\gamma_s$ [9]. A direct evaluation of $\Delta_s$ has large finite-size effects, and an accurate calculation requires use of the Density Matrix Renormalization Group (DMRG) method [12]. Fig. 2 displays $\Delta_s$ for $t_{AB} = 0.6$ extrapolated from calculations of open chains with length $L \leq 40$. For $-2 < U < -1$, $\Delta_s$ vanishes within numerical accuracy ($\sim 0.01$) while for smaller values of $U$ it increases rapidly. These results are consistent with $\Delta_s$ opening near $U_s \approx -2.1$ with a singular growth (exponentially small as in the $t - J$ model [13]). The result derived from the topological transition is $U_s = -2.051$. 


The system forms an exact solution for interchanged as of lowest energy are pseudospin ones [3]. In addition, usual in finite systems pseudospin counterparts of $\Delta$ are always decreases (increases) with $U$ in a system of more than 16 sites.

The solid lines are polynomial extrapolations in $1/U$ values (isolated values suggest a tendency to reach the insulating phase $L \to \infty$ as in the quarter-filled infinite Hubbard model as a function of the nearest-neighbor repulsion $U$) [21], i.e. on-site singlet superconducting and charge CF have the same distance dependence. This, in turn, implies $K_{\rho} = 1$ in the conducting phases [22], meaning that the large distance behavior is dominated by logarithmic corrections. Also, using CT and spin rotations one obtains $\chi_{c}(d, U) = \chi_{sz}(d, -U)$ and $\chi_{s}(d, U) = \chi_{c}(d, -U) = (-1)^d \chi_{bsdwd}(d, U)$.

We restrict our study to odd values of $d$ for which the oscillatory factors of the CF in the continuum limit are maximum [22]. In addition we took $L = 2d$, motivated by results on the Heisenberg model [23], showing that $\lim_{L \to \infty} \chi_{sz}(d, L) = C\chi_{sz}(d, 2d)$, where $C$ is a constant independent of $d$. This also true, if $d$ is odd, for all CF of our model in the non-interacting case, with $C = (\pi/2)^2$.

The above mentioned symmetry relations and analytical results in the non-interacting limit allowed us to check the accuracy of the DMRG results. A summary for each non-equivalent topological region is described below:

a) $\tilde{\gamma} = (\pi, 0)$, $\Delta_{c} \neq 0$, $\Delta_{s} \neq 0$. All CF decay exponentially. To understand the nature of this insulating phase we use symmetry arguments and the following correlation functions (CF) (see Fig. 4):

$$\chi_{t(s)}(d) = \frac{1}{2} \langle (c_{0\uparrow}^{\dagger}c_{d\downarrow} + c_{d\uparrow}c_{0\downarrow}) (c_{d+1\uparrow}c_{0\downarrow} + c_{d+1\downarrow}c_{0\uparrow}) \rangle$$

$$\chi_{os}(d) = \langle c_{0\uparrow}^{\dagger}c_{d\uparrow}c_{d\downarrow} \rangle$$

$$\chi_{c}(d) = -\frac{1}{2} \langle (n_{0\uparrow} + n_{0\downarrow} - 1)(n_{d\uparrow} + n_{d\downarrow} - 1) \rangle$$

$$\chi_{bsdwd}(d) = \frac{1}{2} \langle (c_{0\uparrow}^{\dagger}c_{1\downarrow} + c_{1\uparrow}^{\dagger}c_{0\downarrow})(c_{d\downarrow}^{\dagger}c_{d+1\uparrow} + c_{d+1\downarrow}^{\dagger}c_{d\uparrow}) \rangle$$

$$\chi_{sz}(d) = -2\langle S_{0}^{x}S_{d}^{z} \rangle, \quad (4)$$

computed with DMRG and CSC [21]. The CF are defined such that, in the non-interacting case, $\lim_{L \to \infty} \chi(d, L) = 1/(\pi d)^2$, with $d$ an odd number. $\chi_{bsdwd}(d)$ corresponds to correlations between spins located in bonds [6].

The GS for CSC is always a spin and pseudospin singlet. Invariance under pseudospin rotations implies that $\chi_{c}(d) = (-1)^{d+1}\chi_{c}(d)$, i.e. on-site singlet superconducting and charge CF have the same distance dependence. This, in turn, implies $K_{\rho} = 1$ in the conducting phases [22], meaning that the large distance behavior is dominated by logarithmic corrections. Also, using CT and spin rotations one obtains $\chi_{c}(d, U) = \chi_{sz}(d, -U)$ and $\chi_{s}(d, U) = \chi_{c}(d, -U) = (-1)^d \chi_{bsdwd}(d, U)$.

Fig. 3. Drude weight $D_{c}$ and $z_{L}^{\rho}$ for $t_{AB} = 1.4$ as a function of $U$ for $L = 12$ (open circles) and $L = 24$ (solid triangles). The solid lines are polynomial extrapolations in $1/L$.

The symmetry transformation CT implies that if $\Delta_{s}$ opens at $U_{s}$, a pseudospin gap $\Delta_{\rho}$ opens at $-U_{s}$. Pseudospin excitations form a subset of all charge excitations.

In our case the charge velocity $v_{s}$ and $\Delta_{c}$ (computed as usual in finite systems $L \leq 12$ [19]) coincide with their pseudospin counterparts $v_{\rho}$ and $\Delta_{\rho}$ for opposite $U$) [22]. This is consistent with the exact solution for $t_{AB} = 0$ where the charge excitations of lowest energy are pseudospin ones [3]. In addition, the charge-charge and spin-spin correlation functions are interchanged as $U$ changes sign (see below). The opening of $\Delta_{c}$ where $\gamma_{c}$ jumps from 0 to $\pi$ is also consistent with calculations of $z_{L}^{\rho}$, $D_{c}$, superconducting correlation functions, $K_{\rho}$ and central charge $c$.

For $t_{AB} > 1$, $\Delta_{c}$ opens more slowly and the detection of the transition becomes more difficult. However, as shown in Fig. 3 $D_{c}$ and $z_{L}^{\rho}$ display a similar behavior near the jump in $\gamma_{c}$ ($U_{c} = -1.702$) as in the quarter-filled infinite $U$ extended Hubbard model as a function of the nearest-neighbor repulsion $V$ [18] where a metal-insulator transition takes place at $V = 2t$. At large $|U|$ the only relevant energy scale is $4t_{AB}^{2}/|U|$ and therefore, $D_{c}$ increases with $U$ for large negative $U$. Near $U_{c}$ there is a drastic change of behavior of $D_{c}$ and $z_{L}$ vs $U$, and for $U > U_{c}$, the extrapolated values suggest a tendency to reach the insulating values ($D_{c} = 0$, $z_{L} = 1$), in the thermodynamic limit. $z_{L}^{\rho}$ always decreases (increases) with $L$ at the left (right) of $U_{c}$. This is the first accurate (DMRG) calculation of $z_{L}^{\rho}$ in a system of more than 16 sites.

In order to further characterize each thermodynamic phase we use symmetry arguments and the following correlation functions (CF) (see Fig. 4):

$$\chi_{t(s)}(d) = \frac{1}{2} \langle (c_{0\uparrow}^{\dagger}c_{d\downarrow} + c_{d\uparrow}c_{0\downarrow}) (c_{d+1\uparrow}c_{0\downarrow} + c_{d+1\downarrow}c_{0\uparrow}) \rangle$$

$$\chi_{os}(d) = \langle c_{0\uparrow}^{\dagger}c_{d\uparrow}c_{d\downarrow} \rangle$$

$$\chi_{c}(d) = -\frac{1}{2} \langle (n_{0\uparrow} + n_{0\downarrow} - 1)(n_{d\uparrow} + n_{d\downarrow} - 1) \rangle$$

$$\chi_{bsdwd}(d) = \frac{1}{2} \langle (c_{0\uparrow}^{\dagger}c_{1\downarrow} + c_{1\uparrow}^{\dagger}c_{0\downarrow})(c_{d\downarrow}^{\dagger}c_{d+1\uparrow} + c_{d+1\downarrow}^{\dagger}c_{d\uparrow}) \rangle$$

$$\chi_{sz}(d) = -2\langle S_{0}^{x}S_{d}^{z} \rangle, \quad (4)$$

computed with DMRG and CSC [21]. The CF are defined such that, in the non-interacting case, $\lim_{L \to \infty} \chi(d, L) = 1/(\pi d)^2$, with $d$ an odd number. $\chi_{bsdwd}(d)$ corresponds to correlations between spins located in bonds [6].
metry arguments, for \( U = 0 \), all CF except \( \chi_s \) show the same \( 1/d^2 \) decay (apparently without logarithmic corrections). Renormalization group arguments show that when \( \Delta_c = 0 \), \( \chi_s \) should decay more slowly than \( \chi_s \), and therefore dominate for small \( |U| \). As \( U \) increases, \( \chi_s \) decays more rapidly, while the opposite happens with \( \chi_{sz} \). Near the opening of \( \Delta_c \) (at \( U_c \approx 2.05 \) for \( t_{AB} = 0.6 \)), both CF seem to decay in a similar fashion. For \( U > 0 \), as \( t_{AB} \) is decreased a similar sequence of quantum phase transitions takes place as pressure is applied \([4]\). This general approach can be extended to spatial dimensions higher than one \([5]\), and applied to more general models which do not necessarily have SU(2) pseudospin symmetry \([6]\).

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![Graph](image_url)

**Fig. 4.** Correlation functions (CF) times the square of the distance \( d \) as a function of \( d \) for \( t_{AB} = 0.6 \): nearest-neighbor triplet \( |\chi(d)| = |\chi_{badw}(d)| \) (squares) and singlet \( \chi_s(d) \) (circles) pair CF, on-site pair and charge CF \( |\chi_{sz}(d)| = |\chi_c(d)| \) (downward triangles), and spin CF \( \chi_{sz}(d) \) (upward triangles). See Eq. (4).

In conclusion, we have constructed the quantum phase diagram of Eq. (1) from topological considerations. Each thermodynamic phase is associated to a topological vector, and changes in that quantity signal the transition point. A key finding is the identification of a triplet superconducting phase degenerate with a bond-located SDW for \( t_{AB} < 1 \) and small \( |U| \). Taking into account the slight dimerization in (TMTSF)_2X compounds, an effective Hamiltonian similar to Eq. (1) can be realized, where only four low-energy states per unit cell are kept. Assuming that additional interactions stabilize the TS with respect to the BSDW it is remarkable that, for

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