Phase Diagram of a Model of Correlated Hopping of Electrons in a Lattice of Berry Molecules

Giuseppe Santoro,1,2 Nicola Manini,1,2 Alberto Parola,1,3 and Erio Tosatti1,2,4
1 Istituto Nazionale di Fisica della Materia (INFM)
2 International School for Advanced Studies (SISSA), Via Beirut 4, I-34013 Trieste, Italy
3 Istituto di Fisica, Via Lucini 3, Como, Italy
4 International Centre for Theoretical Physics (ICTP), P.O. Box 586, I-34014 Trieste, Italy

The 1D phase diagram of a model for correlated hopping of electrons in a lattice of Berry phase molecules is presented. Electrons hop in presence of an extra orbital degree of freedom at each site. This is mimicked as a spin-1 variable whose allowed states depend on the electron occupancy so as to take into account the orbital degeneracies of different molecular occupancies. In the 1D case we find that at low electron densities \( n << 1 \) there is a region with dominant superconducting correlations surviving an additional repulsive on-site interaction \( U \) as strong as the bandwidth, \( W = 4t \). The critical value \( U_c \) of \( U \) below which superconductivity is found to be dominant decreases with increasing density \( n \). For \( n = 1/2 \) we find \( U_c/t \approx 1 \), whereas at \( n = 1 \) (half-filling) our (less accurate) results are compatible with \( U_c/t \approx 0 \). For \( U > U_c(n) \) and away from half-filling \( (n \neq 1) \) the system is metallic with dominant 2\( k_F \) charge density wave (CDW) correlations. At half-filling a charge gap opens for \( U > U_c \) and the system becomes an insulator. A spin-gap characterizes the phase-diagram for all densities and for all values of \( U \), even in the metallic regime \( U > U_c \).
I. INTRODUCTION

In the normal theory of metals not much attention is usually devoted to orbital phenomena. The atomic orbital angular momentum is first of all largely quenched by crystal fields, which split part of the orbital degeneracy. Subsequently, the electron kinetic energy, usually large, completes the job by eliminating residual degeneracies except at special points in the Brillouin zone.

The scope of this paper is to explore and describe in some detail a possible scenario emerging in the opposite limit. This is realized considering “molecular” sites with a well-defined orbital degeneracy, unquenched by crystal fields, and with a coherent, but extremely weak, electron hopping energy \( t \) between the sites. The specific extra ingredients which we consider are: (a) the orbital degeneracy depends on electron occupancy; (b) inter-site electron hopping forces a switch of orbital degeneracy for both the initial and final site.

This kind of model is closely inspired by our previous studies [1,2] of the physics of C\(_{60}\) ions, present in molecular fullerides. An isolated C\(_{60}\) ion undergoes a dynamical Jahn-Teller (JT) effect, which, as we found, is affected by an electronic Berry phase when \( n \) is odd, but not when it is even. As a result, the molecular ground state has \( L = 1 \) in the former case and \( L = 0 \) in the latter as in point (a) above.

A realistic model for the superconducting compounds A\(_2\)C\(_{60}\) (A=K,Rb) should take into account the electronic and molecular degrees of freedom of C\(_{60}\); the three degenerate \( t_{1g} \) electronic orbitals (LUMO) at each molecule and the eight \( H_g \) 5-dimensional phonon multiplets which are allowed to couple, by symmetry, with the electronic orbitals. The energies of these phonons range from 30 to 200 meV, i.e., comparable to the typical electronic bandwidth \( W \approx 0.4 \) eV in the solid. In such a situation, a standard Eliashberg approach, heavily based on Migdal’s theorem (neglect of electron-phonon vertex corrections) and on the smallness of \( \hbar \omega_{\text{Debye}}/W \), is hard to justify from first principles, even if empirically successful.

We explore here a different route, based on the opposite limit in which the hopping matrix element \( t \) is the smallest energy scale in the problem. The basic ingredients of the model we will study are the different degeneracies associated to molecular states with different electronic occupation, as suggested by a careful treatment of the JT effect of each molecule. While well aware of the limitations of such an approach – the real situations being in the intermediate regime \( t \approx \hbar \omega \) – we still believe it illustrates the potentially interesting role played by orbital degeneracies in molecular crystals.

The basic ideas can be illustrated in a model which is much simpler than that of C\(_{60}\), i.e., a system of “\( e \otimes E \)” molecules [3] with two electronic orbitals per site \( c_{\pm,\sigma} \), coupled to a two-dimensional JT active phonon multiplet \( b_{\pm} \) of energy \( \hbar \omega \):

\[
H = -t \sum_{\pm} \sum_{<r,r'>} \sum_\sigma [c_{\pm,\sigma}^\dagger (r') c_{\pm,\sigma} (r) + H.c.] + \hbar \omega \sum_{\pm} \sum_r [b_{\pm}^\dagger (r) b_{\pm} (r) + \frac{1}{2}]
\]

\[
H_{e-\text{ph}} = \frac{g \hbar \omega}{2} \sum_r \sum_\sigma \left\{ c_{+,\sigma}^\dagger (r) c_{-,\sigma} (r) [b_+^\dagger (r) + b_+ (r)] + H.c. \right\}.
\]

Such a simplified model has been considered in Ref. [3] and studied using a strong coupling \( (g \rightarrow \infty) \) approach to the electron-phonon molecular Hamiltonian. Consider first the case in which there is no hopping \( (t = 0) \). The molecular Hamiltonian commutes with an angular momentum-like operator

\[
j(r) = [b_+^\dagger (r) b_+ (r) - b_-^\dagger (r) b_- (r)] + \frac{1}{2} \sum_\sigma [c_{+,\sigma}^\dagger (r) c_{+,\sigma} (r) - c_{-,\sigma}^\dagger (r) c_{-,\sigma} (r)].
\]

One finds that molecules with an odd number of electrons \( n \) \((n = 1,3)\) have an associated electronic Berry phase of \( \pi \) and a four-fold degenerate ground state \( (j = \pm 1/2, \sigma = \pm 1/2) \). On the contrary, molecules with an even number of electrons \( (n = 0,2) \) have no Berry phase and a non-degenerate singlet ground state \( (j = 0, S = 0) \). For \( g > 1 \), excited molecular states are separated from the ground state by terms of order \( h \Omega = \hbar \omega/g^2 \).

However, the validity of this analysis is not restricted to a strong coupling regime. For \( g << 1 \), conventional 2\(^{nd}\)-order perturbation theory in \( H_{e-\text{ph}} \), neglecting retardation effects, gives an effective phonon-mediated electron-electron interaction of the type [3]

\[
H_{e-e} = -\frac{g^2 \hbar \omega}{4} \sum_r \sum_{\sigma,\sigma'} \left\{ c_{+,\sigma}^\dagger (r) c_{-,\sigma} (r) c_{+,\sigma'}^\dagger (r) c_{-,\sigma'} (r) + H.c. \right\}.
\]
It is simple to verify that the four degenerate $n = 1$ states $c^\dagger_{\cdot\cdot,\sigma}|0\rangle$ have an energy $E_{n=1} \approx -g^2\hbar\omega/4$, whereas the lowest $n = 2$ state is the inter-orbital singlet $(c^\dagger_{\cdot\cdot,\uparrow} - c^\dagger_{\cdot\cdot,\downarrow})|0\rangle$ with energy $E_{n=2} \approx -g^2\hbar\omega$. Once again, $(j = \pm1/2, \sigma = \pm1/2)$ for the $n = 1$ states, whereas $(j = 0, S = 0)$ for the lowest $n = 2$ state.

Equation 3 shows that the inclusion of the JT effect proves already important in providing a sizable pairing energy which acts as a kind of effective negative Hubbard-$U$ term, therefore reducing the effect of the local Hubbard repulsion between electrons. It is therefore not surprising that, in absence of strong repulsive e-e interactions, the phonon-mediated local attraction leads to superconductivity. Manini, Tosatti and Doniach have found that this pairing attraction is important at least as long as $t < \hbar\Omega$. Shelton and Tsvelik have studied, using bosonization in 1D, the purely electronic model consisting of the hopping term $T$ and the effective non-retarded electron-electron interaction $H_{e-e}$ in Eq. 3. They too find a strong tendency to superconductivity. However, these negative Hubbard $U$’s can in practice be easily canceled with Coulomb repulsive Hubbard $U$’s.

We will show here that there are effects, induced by orbital degeneracy, which can lead to superconductivity even when repulsive interactions overwin the polaronic attraction. These effects will be found to be more pronounced at low carried density.

As argued above, singly occupied states have an extra degeneracy of orbital origin $(j = \pm1/2)$ while the lowest doubly occupied state is non-degenerate $(j = 0)$. If the hopping $t$ is much smaller than the lowest local excitation energy, we can effectively restrict the Hilbert space at each site by keeping only the ground state for each electronic occupation. We are thus led to considering a Hubbard-type model in which each site of the lattice carries an extra pseudospin-1 degree of freedom, with the following constraint: a singly-occupied site has, in addition to the usual spin occupation. Manini, Tosatti and Doniach have introduced and studied this EP model in one-dimension and at half-filling. In this paper we present the results we have obtained for the full phase diagram of the model in 1D, whereas a doubly occupied (or empty) site must have $S^z = 0$ and is therefore non-degenerate,

\[
\begin{align*}
    n_r &= 1 \quad \implies \quad S_r^z = \pm 1, \\
    n_r &= 0, 2 \quad \implies \quad S_r^z = 0.
\end{align*}
\]

The electron-pseudospin (EP) working Hamiltonian $H$ is written as follows:

\[
H = -\frac{t}{2} \sum_{<rr'>} \sum_{\sigma} (c^\dagger_{r,\sigma} c_{r',\sigma} + H.c.) (S^+_{r} S^-_{r'} + H.c.) + U \sum_r n_{r\uparrow} n_{r\downarrow},
\]

where the $S^z$'s are spin-1 ladder operators at each site, and the remaining notation is completely standard. It is worth stressing that while $H$, and in particular the hopping term, conserves the constraint in Eq. 4, the model is still highly non-trivial even for $U = 0$.

Manini, Tosatti and Doniach have introduced and studied this EP model in one-dimension and at half-filling. By small ring exact diagonalizations and a BCS-like mean field calculation they show that the effect of the correlated hopping, even in the absence of any negative-$U$ term, is to induce pairing between electrons of opposite spin. In this paper we present the results we have obtained for the full phase diagram of the model in 1D, which is illustrated in Fig. 1. We find that at low densities $n << 1$ there is a region with dominant superconducting correlations surviving repulsive interactions as strong as the bandwidth, $W = 4t$. The critical value $U_c$ of $U$ below which superconductivity is found to be dominant decreases with increasing density $n$. For $n = 1/2$ we find $U_c/t \approx 1$, whereas at half-filling our results (not very accurate, due to marginal umklapp terms) are compatible with $U_c/t \approx 0$. For $U > U_c(n)$ and out of half-filling ($n \neq 1$) the system is metallic with dominant $2k_F$ charge density wave (CDW) correlations. At half-filling a charge gap opens up for $U > U_c$ and the system becomes an insulator. A spin-gap characterizes the phase-diagram for all densities and for all values of $U$, even in the metallic regime $U > U_c$.

II. SOME DEFINITIONS AND A FEW EXACT RESULTS, MAINLY IN 1D

As we will discuss more in detail in Section 3, only charge degrees of freedom remain gapless in our model. As a consequence, the large-distance physics distances is characterized by a quantity $K_\rho$ – determining the behavior of the correlation functions decaying as power-laws – and by the velocity $v_\rho$ of the sound-like collective excitations. As we will see in Section III, the relevant correlation functions are density-density ($N(x)$) and singlet superconductive ($S(x)$), behaving as

\[
\begin{align*}
    N(x) &= -\frac{K_\rho}{2\pi^2} \frac{1}{x^2} + A_2 \frac{\cos(2k_F x)}{x K_\rho} + A_4 \frac{\cos(4k_F x)}{x^4 K_\rho} + \cdots \\
    S(x) &= \frac{B_2}{x^{1/K_\rho}} + \cdots.
\end{align*}
\]
For general values of $U$ and of the density $n$, results for $K\rho$ can be obtained in a standard way \[4\] from a knowledge of the charge velocity $u_\rho$,

$$u_\rho = \lim_{L \to \infty} \frac{L}{2\pi} [E_L(S = 0, k = 2\pi/L) - E_L] ,$$

of the inverse compressibility $\kappa^{-1}$

$$\frac{1}{\kappa n^2} = \lim_{L \to \infty} \frac{L}{2} \frac{\partial^2 E_L}{\partial N^2} = \frac{\pi}{2} \frac{u_\rho}{K\rho} ,$$

and of the Drude peak strength $D_c \[12,13\]

$$D_c = \lim_{L \to \infty} \frac{L}{2} \frac{d^2 E_L(\Phi)}{d\Phi^2} \bigg|_{\Phi = 0} = \frac{1}{\pi} u_\rho K\rho .$$

Here $E_L(S = 0, k = 2\pi/L)$ is the energy of the lowest excited singlet state with total momentum $k = 2\pi/L$ with respect to the ground state of energy $E_L$ in a ring of size $L$, and $E_L(\Phi)$ is the ground state energy in presence of a magnetic flux $\Phi$.

In general, we resort to exact diagonalizations of the model on small rings of size $L$ (with $L$ up to 16), and use Eq. \[5\] to estimate $u_\rho$ and Eq. \[8\] or \[9\] to extract $K\rho$ \[14\]. Three regions of the phase diagram are, however, well under control using different approaches: the low density limit $n \to 0$, \[15\] and the limit of large repulsion or attraction $U \to \pm \infty$. \[16,17\] We summarize here, for the reader’s convenience, the most important results concerning these three regions.

### A. The low-density limit: solution for two electrons

Consider the two-electron problem first. A state in the two-particle Hilbert space with total $\z$-component of the spin $M_\z = 0$ (for both the electrons and the spin-1 states) can be written as

$$|\Psi\rangle = \sum_{r,r'} \left[ \left| \psi_{+-}(r, r') S^z_+ S^-_r + \psi_{-+}(r, r') S^-_r S^+_r \right| c^\dagger_{r\uparrow} c^\dagger_{r\downarrow} |0\rangle \right] ,$$

where the vacuum $|0\rangle$ is the state without fermions and with $S^z = 0$ at each site. In writing $|\Psi\rangle$ one takes into account the two possibilities of associating a $S^z = 1$ spin state to the up and down electrons: $\psi_{+-}$ is the amplitude for having $S^z = +1$ associated to the $\uparrow$-electron (and $S^z = -1$ to the $\downarrow$-electron), while $\psi_{-+}$ is the amplitude for other possible choice. The Schrödinger equation for $\psi_{+-}(r, r')$ is

$$E\psi_{+-}(r, r') = -t \sum_a \left[ \psi_{+-}(r + a, r') + \psi_{+-}(r, r' + a) \right] + U \delta_{r,r'} \psi_{+-}(r, r')$$

$$-t \left( \sum_a \delta_{r+a, r'} \left[ \psi_{++}(r, r) + \psi_{--}(r', r') \right] \right) ,$$

where $a$ denotes a nearest neighbor vector ($a = \pm 1$ in 1D). A similar equation is obtained for $\psi_{-+}(r, r')$ by just exchanging $\psi_{+-}$ and $\psi_{-+}$ everywhere. The last term in Eq. \[14\] is the crucial outcome of the extra (orbital) degeneracy of singly occupied states, and deserves a few comments. When the two electrons are far enough in the otherwise empty lattice, the EP Hamiltonian $H$ simply allows the hopping to a nearest neighbor site of the “composite” object (see Fig. 2a) formed by an electron and the associated spin-1 state (first term in Eq. \[15\]). In other words, each electron retains its orbital index during the hopping process. Things are more subtle when two electrons come to the same site $r$. In such a case (see Fig. 2b), from a doubly occupied site with $S^z = 0$ one can reach, upon hopping, two possible final states: either each electron keeps its own spin-1 label or the spin-1 labels associated to the two electrons are exchanged. It is precisely this second possibility of exchanging spin-1 states that is responsible for the presence of $\psi_{+-}$ in the equation for $\psi_{+-}$ and vice-versa (last term in Eq. \[15\]).

The Schrödinger equation is easily solved (on a square lattice in any D), in momentum space, where it reads:

$$[E - 2\epsilon_k] \psi_{+-}(k) = \frac{U}{L^D} \sum_p \psi_{+-}(p) + \frac{2\epsilon_k}{L^D} \sum_p \psi_{-+}(p) .$$

\[12\]
Here the case of total momentum $P = 0$ has been considered, for simplicity, and $\epsilon_{k}$ is the tight-binding dispersion of the free-electron problem ($\epsilon_{k} = -2t \sum_{\alpha} \cos k_{\alpha}$). Introducing the quantity $J_{+}- = L^{-D} \sum_{p} \frac{1}{E - 2\epsilon_{k}} + J_{-} = \frac{1}{L^{D}} \sum_{k} \frac{2\epsilon_{k}}{E - 2\epsilon_{k}}$. (The equation for $J_{-}$ is obtained by exchanging $J_{+}$ with $J_{-}$ everywhere.) The set of solutions among which the ground state is found have $J_{+} = J_{-}$ and their eigenvalues $E$ satisfy the equation

$$\frac{1}{L^{D}} \sum_{k} \frac{1}{E - 2\epsilon_{k}} = \frac{2}{E + U}. \quad (14)$$

It is worth mentioning that in the ordinary Hubbard case, the right-hand side of Eq. (14) would simply read $1/U$. A graphical analysis of Eq. (14) readily shows that a bound state solution is present even for $U > 0$ up to $U_{c} = 4Dt$ in $D \leq 2$. In $D \geq 3$ a finite attractive $U$ is needed to produce a bound state.

The bound state solution has been worked out analytically in the $1D$ case. The bound state wavefunction naturally provides a picture of bound pairs approximately localized on adjacent lattice sites. Remarkably, the rather strong attraction responsible for this binding is generated by the kinetic term alone via the presence of the additional degrees of freedom. The critical value of the Hubbard repulsion $[U_{c} = 4t$ in $1D]$ is considerably larger than the ground state binding energy at $U = 0$ $[E_{b}/t = (8/\sqrt{3} - 4) \sim 0.618$ in $1D]$ showing that this kind of pairing mechanism is rather insensitive to the presence of on-site Coulomb repulsion. The same feature is also present in two dimensions where $U_{c} = 8t$: The enhancement is due to the the larger coordination of the 2D lattice which provides an even more efficient delocalization of the electron pair.

This interpretation of the two-particle ground state, plus the additional finding that there is no phase separation, leads to a simple picture, at least for $U < U_{c}$, of the low density limit of model both in one and two dimensions: the system behaves as a weakly interacting, dilute gas of bosons with an extended core. A superfluid ground state must be expected at zero temperature. In one dimension, of course, off-diagonal long range order cannot occur and only a long range power-law decay of the density matrix is possible, while in two dimensions a genuine $T = 0$ Bose condensate will form. In terms of the original electrons this implies a standard strong coupling BCS superconducting ground state with localized Cooper pairs. A similar scenario has also been proposed in the framework of the one dimensional $t - J$ model where bound pairs are formed at low density and $2 < J/t < 2.95$. In that case, however, the model is unstable to phase separation, which in fact occurs massively at larger values of $J/t$, whereas the present model shows no such tendency at least in $1D$.

From a low-density expansion of the ground-state energy and of the charge velocity an analytic determination of the exponent $K_{p}$ in the limit $n \rightarrow 0$ has been given in Ref. [13]. It is found that $K_{p} = 2$ for $U < U_{c}(n = 0) = 4t$, whereas $K_{p} = 1/2$ for $U > 4t$.

B. $U \rightarrow +\infty$ limit

The strong coupling expansion of the EP model has been worked out in Ref. [16]. The resulting Hamiltonian, to $O(t^{2}/U)$, is defined in the subspace of empty or singly occupied sites where electrons are characterized by two internal spin-1/2 degrees of freedom: The usual spin ($\sigma$) and a pseudospin ($\tau$). The latter takes into account the two possible states of the original spin-1 rotators allowed by the constraint (4). The resulting Hamiltonian, exactly like in the $t - J$ model, contains a kinetic term (with coupling constant $-t$) and a spin (and pseudospin) dependent contribution which scales as $t^{2}/U$. In $1D$, analogously to the Hubbard model case, the total wavefunction factorizes, at $U \rightarrow \infty$, for all densities: The position of the electrons is determined by a (free) spinless fermion wavefunction while the spin (and pseudospin) ordering on the squeezed chain is governed by the effective spin Hamiltonian

$$H_{\sigma \tau} = -J_{\text{eff}} \sum_{\langle i, j \rangle} \left[ 2\bar{\sigma}_{i} \cdot \bar{\sigma}_{j} - \frac{1}{2} \left( 2\bar{\tau}_{i} \cdot \bar{\tau}_{j} - \frac{1}{2} \right) \right] \quad (15)$$

where the effective coupling constant depends on the electron density $n$ as $J_{\text{eff}} = \frac{\Delta^{2}}{n}[1 - \sin(2\pi n)/(2\pi n)]$. It turns out that, in contrast with the Heisenberg case, the Hamiltonian in Eq. (15) has a (doubly degenerate) valence bond ground state and is characterized by a spin gap of order $J_{\text{eff}}$. Therefore, we conclude that our model (Eq. (5)), at arbitrary (finite) density has a spin gap for $U \rightarrow \infty$. The charge degrees of freedom are, on the contrary, gapless and tend to approach the spinless fermion case as $U \rightarrow \infty$. 

5
Quantities such as the charge velocity and Drude peak can be obtained analytically for any lattice size $L$ by this large-$U$ mapping of the charge degrees of freedom to free spinless fermions. The expression for the charge velocity $u_\rho$ reads:

$$u_\rho(U = +\infty) = 2t \frac{L}{\pi} \sin(\pi/L) \sin(\pi n) \xrightarrow{L \to \infty} 2t \sin(\pi n),$$

whereas the Drude peak strength $D_c$ is given by

$$D_c(U = +\infty) = t \frac{\sin(\pi n)}{L \sin(\pi/L)} \xrightarrow{L \to \infty} t \frac{\pi}{\pi} \sin(\pi n).$$

As a result, $K_\rho = 1/2$ for all densities $n \neq 1$ on the boundary line $U = +\infty$. \[11\]

C. $U \to -\infty$ limit

The third, rather trivial, region where the physics is under control is that of large on-site attraction. Indeed, in the limit $U \to -\infty$, only doubly occupied and empty sites are allowed. The extra degeneracy of singly occupied sites plays therefore no special role, and the model behaves as the corresponding negative $U$ Hubbard model. \[21\] In analyzing our data in this limit we will use, for comparison, the numerical results for the Hubbard case obtained from Bethe Ansatz. \[12\] At half-filling, the mapping of the $U \to -\infty$ limit into the antiferromagnetic Heisenberg chain (with $J = \frac{8t^2}{|U|}$ in the present case \[21\]) provides analytic $L = \infty$ results for the Drude peak $D_c$ and the charge velocity $u_\rho$. \[17,13\] We get \[22\]

$$u_\rho = \frac{\pi}{2} J + \cdots = \frac{\pi}{2} \frac{8t^2}{|U|} + \cdots$$

$$D_c = 4 \frac{J}{8} + \cdots = \frac{1}{2} \frac{8t^2}{|U|} + \cdots .$$

(The dots indicate higher order corrections in $t/U$.) The corresponding value of $K_\rho$ at half-filling for large negative $U$ is therefore given by $K_\rho = 1$. \[11\]

III. THE PHASE DIAGRAM (1D)

In order to study the model using standard 1D Fermi gas techniques, we have to represent the extra spin–1 degeneracy and the associated constraint in a suitable way. A possible procedure is to first represent the Hamiltonian in Eq. \[5\] in terms of additional hard-core boson operators $d_{r\sigma}$ as follows:

$$H = -t \sum_{<rr'>} \sum_{\sigma,\sigma'} \{ c_{r\sigma}' c_{r'\sigma} d_{r\sigma}' d_{r'\sigma'} + H.c. \} + \frac{U}{2} \sum_r [n_{r\uparrow} n_{r\downarrow} + n_{r\uparrow}^d n_{r\downarrow}^d] ;$$

the constraint now being that, at each site,

$$n_{r\uparrow}^d = n_{r\downarrow}^c.$$  \[20\]

Eqs. \[19\] and \[20\] give a faithful representation of all the matrix elements of the original model. The idea behind this representation is that the extra label $S^z = +1$ (or $-1$) at each singly-occupied site $r$ is represented by a hard-core boson $d_{r\uparrow}$ (or $d_{r\downarrow}$). Empty sites have no bosons, whereas the $S^z = 0$ state of a doubly occupied site is represented by two bosons $d_{r\uparrow}^d d_{r\downarrow}^d$.

In 1D, we can transform the hard-core bosons $d_{r\sigma}$ into spinful fermions, by a Wigner-Jordan transformation. \[13\] We are then led to consider a problem of correlated hopping of two species of fermions in 1D with a conserved constraint (Eq. \[20\]). A possible way of treating this problem is to enlarge the Hilbert space by removing the constraint in Eq. \[20\] and to introduce a term $V \sum_r (n_{r\uparrow}^c - n_{r\uparrow}^d)^2$ with $V \to \infty$ in the Hamiltonian. The correlated hopping term can then be regarded as a second-order process obtained from a standard free hopping of the $c$ and $d$ particles as follows:
\[ H_V = -\tilde{t} \sum_{\langle rr' \rangle} \sum_{\sigma} \left\{ c_{r\sigma}^\dagger c_{r'\sigma} + d_{r\sigma}^\dagger d_{r'\sigma} + H.c. \right\} + \frac{U}{2} \sum_r \left[ n_{r\uparrow} n_{r\downarrow}^c + n_{r\downarrow} n_{r\uparrow}^d \right] + V \sum_r (n_{r\uparrow}^c - n_{r\uparrow}^d)^2 + \Delta H_V \]

\[ \Delta H_V = \frac{\tilde{t}^2}{V} \sum_{\langle rr' \rangle, \sigma, \sigma'} \left\{ c_{r\sigma}^\dagger c_{r\sigma'} c_{r'\sigma} c_{r'\sigma'} + d_{r\sigma}^\dagger d_{r\sigma'} d_{r'\sigma} d_{r'\sigma'} \right\}, \] (21)

where \( \tilde{t}^2/V = t \), and \( V \) is understood to be large. The extra term \( \Delta H_V \) is included in order to cancel unwanted terms generated by second-order perturbation theory in the hopping \( t \). We have thus obtained a reasonably standard form of two-chain problem, which we treat in weak-coupling in \( U \) and \( V \) (assuming continuity with the large \( V \) regime), by linearizing the band around the two Fermi points at \( \pm k_F \) and introducing right (\( p = L = + \)) and left (\( p = L = - \)) fermion fields \( \psi_{\alpha \sigma}(x) \) for every species of fermions (\( \alpha = c, d \), and \( \sigma = \uparrow, \downarrow \)). Luckily, the “g-ology” of this two-chain problem turns out to be a particular case of the two-chains in presence of transverse hopping treated by Fabrizio et al. [24]. We can therefore directly use the RG equations of Ref. [24] calculated up to third order in the couplings (two-loops). Away from half-filling (i.e., when umklapp terms are irrelevant) the result is that the model scales to a strong-coupling fixed point and gaps open in all sectors with the exception of the totally symmetric one, which remains gapless. Correlation functions can be calculated by bosonizing the strong coupling fixed point. [24] We introduce a bosonic representation of the fermion fields

\[ \psi_{\alpha \sigma}(x) = \frac{e^{ipk_F x}}{(2\pi \alpha)^{1/2}} e^{i\sqrt{\pi}(\Phi_{\alpha \sigma}(x) + p\Phi_{\alpha \sigma}(x))}, \] (22)

where \( \Phi_{\alpha \sigma}(x) \) and \( \Theta_{\alpha \sigma}(x) \) are boson fields such that \( \Pi_{\alpha \sigma}(x) = -\nabla \Theta_{\alpha \sigma}(x) \) is the momentum conjugate to \( \Phi_{\alpha \sigma}(x) \), and \( \alpha \) is a short-distance cut-off. In terms of charge/spin and symmetric/antisymmetric combinations of the fields

\[ \Phi_{\alpha \sigma}(x) = \frac{1}{\sqrt{2}} \{ \Phi_{\alpha \uparrow} \pm \Phi_{\alpha \downarrow} \}, \]

\[ \Phi_{\alpha \sigma}(x) = \frac{1}{\sqrt{2}} \{ \Phi_{c\alpha \sigma} \pm \Phi_{d\alpha \sigma} \}, \] (23)

the bosonized Hamiltonian for the gapless field \( \Phi_{\alpha \sigma}^\pm \) reads

\[ \mathcal{H} = \frac{1}{2} \int_0^L dx \left[ u_{\rho} K_{\rho}^+ (\Pi_{\rho}^+)^2 + \frac{u_{\rho}}{K_{\rho}^+} (\nabla \Phi_{\rho}^+)^2 \right] + \frac{\pi}{8L} \frac{u_{\rho}}{K_{\rho}^+} (\hat{N} - N_0)^2 + u_{\rho} K_{\rho}^+ J^2, \] (24)

whereas the other fields are effectively locked to their strong-coupling values \( \Phi_{\rho}^- = \Phi_{\rho}^\pm = 0 \). Here \( \hat{N} \) is the operator counting the total number of particles of both species (\( N_0 \) is its ground state value), and \( J \) is the associated current operator. [10] We do not calculate \( u_{\rho} \) and \( K_{\rho}^+ \) perturbatively, since we are interested in the physical limit \( V \to \infty \).

We will therefore extract the correct \( u_{\rho} \) and \( K_{\rho}^+ \) numerically from finite size exact diagonalizations (see below).

From Eq. [24] the compressibility relation can be immediately derived. [10][13] It reads:

\[ L \frac{\partial^2 E_L}{\partial N^2} = \frac{\pi}{4} \frac{u_{\rho}}{K_{\rho}^+}, \] (25)

where \( N = 2N_c \) is the total number of particles of both species. Similarly, the Drude peak is found to be given by

\[ D_c = \frac{1}{2\pi} u_{\rho} K_{\rho}^+. \] (26)

It is simple to verify that the correlation functions which decay as a power-law at large distances are the density-density correlations \( N(x) = \langle n_{\sigma}^c n_{\sigma}^d \rangle \) and the singlet superconductive correlations \( S(x) = \langle P_{\uparrow}^1 P_{\uparrow} \rangle \) with \( P_x = \psi_{\sigma \uparrow}(x) \psi_{\sigma \uparrow}(x) \psi_{\sigma \downarrow}(x) \psi_{\sigma \downarrow}(x) \). Expressing the fermionic fields in terms of the bosonic ones, and using the Hamiltonian in Eq. [24], we readily find that:

\[ N(x) = -\frac{K_{\rho}^+}{4\pi^2} \frac{1}{x^2} + A_2 \cos \left( \frac{2k_F x}{x K_{\rho}^+/2} \right) + A_4 \cos \left( \frac{4k_F x}{x K_{\rho}^+/2} \right) + \cdots \]

\[ S(x) = \frac{B_2}{x^{2/K_{\rho}^+}} + \cdots . \] (27)
We emphasize that all the relations obtained so far, from the compressibility to the correlation functions, have exactly the same form they would take in the negative-\(U\) Hubbard case if we define \(K_\rho = K^+_\rho /2\). The corresponding forms of the correlation functions, compressibility, and Drude peak are then given by Eqs.\(\{13\}\). (In the compressibility relation, a factor 4 is absorbed by the fact that \(N = 2N_c\), \(N_c\) being the number of electrons.)

To facilitate the comparison with the Hubbard case we will use in the following the notation \(K_\rho = K^+_\rho /2\), so that the latter will be directly comparable to the Hubbard model’s \(K_\rho\).\(\{23\}\)

From Eq.\(\{22\}\) we observe that regions with \(K_\rho (= K^+_\rho /2) > 1\) and \(K_\rho < 1\) are characterized by dominant correlations (i.e., correlations with the slowest decay) of the superconductive and \(2k_F\)–CDW type, respectively. We recall that, in the low-density limit \(n \to 0\), \(K_\rho = 4/\pi\) for \(U > U_c = 4t\) and \(K_\rho = 2/\pi\) for \(U < U_c\).

This defines the left \((n = 0)\) border of the phase diagram in Fig. 1. For \(U < U_c\), the dominant correlations are superconductive, decaying as \(1/\sqrt{x}\), exactly as in a dilute \((n \to 0)\) hard core boson gas. For \(U > U_c\), the correlation function with the slowest decay is the \(2k_F\) density-density response, with an inverse square root behavior \(1/\sqrt{x}\), implying a divergence in the \(2k_F\)–CDW susceptibility, except at \(U = \infty\) where the \(2k_F\) response function has vanishing amplitude, like in the Hubbard model, and the corresponding singularity is therefore absent.

### A. Numerical results

We are now ready to discuss the results of the finite-size exact diagonalization data of the EP Hamiltonian.\(\{3\}\). First we will show that a spin gap – which is expected all over the phase diagram, and not just in the superconducting region – is indeed found for all the values of \(U\) studied, at \(n = 1/2\) and \(n = 1\).

Figs.\(\{3\}\) and \(\{4\}\) show the finite-size gaps between the ground state and the lowest triplet state, \(\Delta E_L (S = 1)\), as a function of the inverse lattice size \(1/L\) for both the quarter-filled (Fig.\(\{3\}\)) and the half-filled case (Fig.\(\{4\}\)) and for several values of \(U\). As expected, \(\Delta E_L (S = 1)\) always extrapolate to a finite non-zero value in the infinite volume limit for all the values of \(U\) studied.

The extrapolated values of the spin gap \(\Delta E_\infty (S = 1)\) (see Fig.\(\{2\}\) inset for the \(n = 1\) case) decrease with increasing \(U\) in agreement with the result that, as \(U \to +\infty\), the spin gap should be proportional to \(J_{\text{eff}} = 2\mu_B [n - \sin(2\pi n)/(2\pi)]\).

Next we turn to the exponent \(K_\rho\) for finite values of the density \(n\). The exact eigenvalues of \(L\)-site rings provide determinations of the three quantities \(u_\rho\) (Eq.\(\{1\}\)), \(D_c\) (Eq.\(\{3\}\)), and \(\partial^2 E_L / \partial N_c^2\) (Eq.\(\{3\}\)). In particular, the magnetic flux \(\Phi\) through the ring in the evaluation of the Drude peak \(\{4\}\) is implemented simply by changing the hopping matrix element \(t \to te^{i\Phi/L}\) (a procedure equivalent to twisting the boundary conditions) and calculating the second derivative with respect to \(\Phi\) numerically. Moreover, as usual, the second derivative of the energy with respect to the number of electrons \(N_c\), appearing in the compressibility \(\{8\}\), is approximated by the finite difference expression \(L[E_L(N_c + 2) + E_L(N_c - 2) - 2E_L(N_c)]/4\).

Figs.\(\{3\}\) and \(\{4\}\) show the finite-size values of the Drude peak \(D_c\) and of the charge velocity \(u_\rho\) (inset) for the quarter-filled \((n = 1/2)\) and half-filled \((n = 1)\) case, for several values of \(U\). The \(U = +\infty\) values of \(D_c\) and \(u_\rho\) for \(n = 1/2\) (see Eqs.\(\{17\}\) and \(\{18\}\)) are shown in Fig.\(\{3\}\) by solid lines. In the quarter-filling case – representative of the \(0 < n < 1\) region of the phase diagram – a finite non-zero Drude peak, signal of a metallic ground state, is obtained for any \(U\).

Correspondingly, the charge velocity \(u_\rho\) scales to a finite value for any \(U\). On the contrary, at half filling and for positive enough \(U\) \((n=1, \text{ Fig.}\{4\}\) the Drude peak vanishes in the thermodynamic limit, indicating insulating behavior.

This is due to the opening of a gap in the charge sector above some critical value of \(U\) close to 0. In Fig.\(\{4\}\) the finite-size charge gap at half-filling

\[
\Delta_c = \frac{1}{2}[E(N_c = L + 2) - E(N_c = L) - U]
\]

is plotted: \(\Delta_c\) scales nicely to 0 as \(L \to \infty\) for negative \(U\), whereas it extrapolates towards finite nonzero values (roughly proportional to \(U\) for large \(U\)) for positive enough \(U\). The extrapolated values of the charge gap for several values of \(U\) are shown in the inset of Fig.\(\{4\}\), together with the positive \(U\) Hubbard model values, for comparison.

Finally, Figs.\(\{3\}\) and \(\{4\}\) show the finite-size estimates of the exponent \(K_\rho\) \(\{14\}\) for \(n = 1/2\) and \(n = 1\), respectively, and for several values of \(U\). For the quarter-filling case (Fig.\(\{3\}\)) it is instructive to compare \(K_\rho\) with the corresponding Hubbard model result, obtained from a numerical solution of the Bethe Ansatz equations.\(\{12\}\) The arrows in panel \((a)\) of Fig.\(\{3\}\) indicate the values of \(K_\rho\) for the Hubbard model at the corresponding value of \(U\).

The most important information, however, is contained in the \(U = 0\) data of Fig.\(\{4\}\). the exponent \(K_\rho\) at \(U = 0\) scales to a value somewhat larger than the critical value 1, which is also the value of \(K_\rho\) for the non-interacting Hubbard model. This indicates (see Eq.\(\{27\}\) with \(K_\rho = K^+_\rho /2\)) that our model has dominant superconducting correlations even in absence of attractive interactions. Panel \((b)\) of Fig.\(\{4\}\) shows that the superconducting state survives, for \(n = 1/2\),
up to a positive $U/t$ of order 1. Fig. 3 shows the values of $K_p$ at half-filling, together with the Hubbard model results (solid squares). At half-filling, umklapp processes are marginal even in the gapless regime, introducing logarithmic corrections to the size scaling. The data for the Hubbard model show clearly the consequence of such a non-trivial size scaling: an extrapolation based on the data at small sizes gives sizable errors (of the order of 10%). In view of this non-trivial size scaling, it is hard to make definite statements on the critical value of $U$ above which a charge gap opens and the system starts to be an insulator. Nevertheless, the $U = 0$ data for $K_p$ (panel (b) of Fig. 3) seem to be definitely below the value of 1, where umklapp processes should become relevant. We are therefore inclined to believe that a charge gap should be present even at $U = 0$ (see also the comparison with the Hubbard results of Fig. 7), although the $U = 0$ Drude peak results of Fig. 3 might suggest a conducting behavior.

The phase diagram in Fig. 4 summarizes our results on the model in Eq. (5) in $D = 1$. The most remarkable feature is in the low density region $n < 1$, where superconducting correlations are found to be dominant up to positive values of the on-site coulomb repulsion $U$ comparable to the electronic bandwidth. We believe that the physics at small densities is robust. The bound states discussed in Section II.A should lead to Bose condensation of strongly localizes Cooper pairs in 2D. In 3D no bound state is found but a superconducting instability should still occur in the presence of a Fermi surface. On the other hand, other features of the model, like the presence of a spin gap over all the phase diagram – including the positive $U$ metallic regime – are probably confined to the low dimensionality 1D case.

IV. CONCLUSIONS

We have studied the 1D phase diagram of a model of electrons which hop weakly between molecular sites. Due to the Berry phase mechanism, each molecular site possesses an unquenched orbital degeneracy, only when its electron occupancy is odd. Upon electron hopping, the orbital degeneracies must correspondingly switch, as the occupancies of the initial and final states change. By adding adjustable on-site Hubbard $U$ term, we can effectively remove from the problem all polaronic effects, and we can thus study the effect of orbital degeneracy, and of its hopping-induced switch, in isolation. The working model (5) is therefore Hubbard-like, but embodies the orbital degeneracy part in the form of a pseudospin-1 on-site variable. We have studied its zero-temperature phase diagram as a function of electron filling and of Hubbard $U$.

Through a series of mappings – all of which are exact for what concerns the asymptotic behavior of correlations in 1D – we find that the problem is equivalent to a particular variant of two coupled 1D chains, whose behavior is generally well studied [24]. This mapping predicts that there will generally be no charge gap (except at half filling for $U > U_c$) while there will always be a spin gap, for all $n > 0$ and all $U$. The zero charge gap is related to either sliding CDW conductivity or superconductivity, and we have distinguished these two different regions in the phase diagram. A quantitative study of the phase diagram, conducted by exact diagonalization and finite size scaling, has led to the overall picture of Fig. 4.

The most interesting fact in the phase diagram is the dominance of superconducting behavior extending even into the (moderately) repulsive-$U$ region. Pairing is associated with new orbital correlations – as foreshadowed by an exact 2-electron solution – which permit a lowering of kinetic energy through an enhanced nearest neighbor pair scattering. This feature represents an important novelty brought about by orbital degeneracy, and should reasonably carry over to more complex and realistic situations in higher dimensions. This pairing mechanism is not easily destroyed by a repulsive $U$, it is more effective at low carrier density, and is apparently immune from the polaron self-trapping, which depresses $T_c$ in strongly coupled electron-phonon systems.

Another new feature found in this model in 1D is the presence of an overall spin gap, including the nonsuperconductive region of the phase diagram, where sliding CDW $2k_F$ correlations dominate. It is at this stage not clear in what way this behavior (which appears rather specific of 1D) will change in higher dimensions.

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[1] A. Auerbach, N. Manini, and E. Tosatti, Phys. Rev. B 49, 12998 (1994); N. Manini, E. Tosatti, and A. Auerbach, ibid. 49, 13008 (1994). See also Ref. [1].
[2] E. Tosatti, and N. Manini, Chem. Phys. Lett. 223, 61 (1994).
[3] L. Pietronero, S. Strassler, and C. Grimaldi, Physica B 204, 222 (1995).
[4] O. Gunnarsson et al., Phys. Rev. Lett. 74, 1875 (1995); O. Gunnarsson, Phys. Rev. B 51, 3493 (1995).
Higher $n = 2$ states are either intra-orbital singlets $c_{\uparrow,1}^\dagger c_{\downarrow,1}^\dagger |0\rangle$, with $E_0 \approx -g^2 \hbar \omega / 2$, or triplet states ($E_T = 0$).

[10] F. D. M. Haldane, J. Phys. C 14, 2585 (1981).

The extrapolations are obtained through weighted quadratic polynomial fit to finite size data. The large-$U$ behavior is apparent at the right side of the plot.

[11] The notation adopted here differs from that of Ref. [15] where $K_p$ is used to indicate what we call here $K_p^\dagger$. In this paper we use $K_p$ to indicate the quantity $K_p^\dagger / 2$, which is directly comparable to the Hubbard model’s $K_p$.

[12] H. Schulz, Phys. Rev. Lett. 64, 2831 (1990).

For $U \to -\infty$, in particular, the model maps into a Heisenberg problem with $J = 8t^2 / |U|$ instead of simply $4t^2 / |U|$ as in the Hubbard case. This is due to the additional degeneracy of the singly occupied states which appear as intermediate states in second order perturbation theory.

[13] B. S. Shastry, Mod. Phys. Lett. B. 6 1427 (1992). B. S. Shastry and B. Sutherland, Phys. Rev. Lett. 65, 243 (1990).

For the positive-$U$ Hubbard case, due to the absence of a spin gap, the density-density and superconductive correlation functions are not given by Eq. [4] in terms of $K_p$. The relationships determining $K_P$ (Eqs. [5]), on the contrary, hold for the positive-$U$ Hubbard as well.

[14] Introducing the finite-size values of the three quantities $L \partial^2 E_L / \partial N_c^2$, $u_p$ and $D_c$ in relations [3] and [4] we get, in general, two independent estimates of the exponent $K_p$.

[15] G. Santoro, M. Airoldi, N. Manini, E. Tosatti, and A. Parola, Phys. Rev. Lett. 74, 4039 (1995).

[16] A. Parola, G. Santoro, and E. Tosatti (unpublished).

[17] F. D. M. Haldane, Phys. Rev. Lett. 45, 1358 (1980).

[18] A. Parola et al. in “Proc. Nato Advanced Research Workshop on Dynamics of Magnetic Fluctuations in High Temperature Superconductors”, ed G. Reiter, P. Horsch and G. Psaltakis (N.Y. Plenum 1990).

[19] M. Ogata, M. U. Luchini, S. Sorella, and F. F. Assaad, Phys. Rev. Lett. 66, 2388 (1991).

[20] M. Ogata, H. Shiba, Phys. Rev. B 41, 2326 (1990).

[21] For $U \to -\infty$, in particular, the model maps into a Heisenberg problem with $J = 8t^2 / |U|$ instead of simply $4t^2 / |U|$ as in the Hubbard case. This is due to the additional degeneracy of the singly occupied states which appear as intermediate states in second order perturbation theory.

[22] The extra-factor 4 in the expression for $D$, relative to the Heisenberg case, is due to the fact that if a flux $\Phi$ is included in the hopping, $t \to t e^{i \Phi / L}$, the $J$-coupling is modified as $J \to J e^{i \Phi / L}$ so that $E_{U \to -\infty}(\Phi) = E_{\text{Heisenberg}}(2\Phi)$, generating a factor 4 in the Drude peak, related to the second derivative of the energy.

[23] J. Sólyom, Adv. Phys. 28, 201 (1979).

[24] M. Fabrizio, Phys. Rev. B 48, 15838 (1993); M. Fabrizio, A. Parola, and E. Tosatti, Phys. Rev. B 46, 3159 (1992).

[25] For the positive-$U$ Hubbard case, due to the absence of a spin gap, the density-density and superconductive correlation functions are not given by Eq. [4] in terms of $K_p$. The relationships determining $K_p$ (Eqs. [5]), on the contrary, hold for the positive-$U$ Hubbard as well.

[26] J. L. Cardy, J. Phys. A 19, L1093 (1986). See also F. D. M. Haldane and Y. Tu, UCSD-preprint (1990).

FIG. 1. The 1D phase diagram for the EP model (Eq. [2]) discussed in the present paper. For details see Sect. [7].

FIG. 2. The hopping mechanism of an up-electron starting from a singly (a) or doubly (b) occupied site.

FIG. 3. The spin-gap, defined as the difference in energy between the lowest triplet state and the ground state (singlet), for $n = 1/2$ and $U = 0, 2t$ and $4t$, as a function of the inverse lattice size $1/L$.

FIG. 4. The spin-gap for $n = 1$ and $U/t = 0, 1, 4, 10$ and 100. Inset: the extrapolated values of the spin-gap in the thermodynamic limit. The extrapolations are obtained through weighted quadratic polynomial fit to finite size data. The asymptotic $1/U$ behavior is apparent at the right side of the plot.

FIG. 5. The Drude peak $D_c$ and the charge velocity $u_p$ (inset) for $n = 1/2$ (quarter-filling). The lines for the Drude peak are fit to the finite-size data. The large-$U$ behavior (solid line) is discussed in Sect. [9].

FIG. 6. The Drude peak $D_c$ and the charge velocity $u_p$ (inset) at half-filling ($n = 1$). The data for $U = 2t$ and $10t$ show clear indication of $D_c$ vanishing in the thermodynamic limit, while for negative $U$, $D_c$ remains finite. The data for $U = 0$ seem also to converge to a nonzero value, but there are evidences (see Sect. [9]) in favour of insulating behavior ($D_c = 0$).
FIG. 7. The charge gap at half filling, obtained as the difference in energy between the lowest $N_c = L + 2$ state and the $N_c = L$ ground state (Eq. 28). The inset reports the extrapolations obtained through weighted quadratic polynomial fit to finite-size data, together with the Hubbard model values, for comparison. The charge gap seems to vanish at some point close to $U = 0$.

FIG. 8. The exponent $K_\rho$ for the EP model at quarter filling obtained (Eq. 8) as $K_\rho = \pi D_c / u_\rho$. Panel (a): $U/t = -100, -4$ and 0; arrows mark the asymptotic values of $K_\rho$ for the Hubbard model obtained by Bethe Ansatz. Panel (b): $U = t$ and $4t$; squares mark the scaling of $K_\rho$ for the Hubbard model at the corresponding values of $U$, for comparison.

FIG. 9. The exponent $K_\rho$ for the EP model at half filling obtained (Eqs. 8 and 9) as $K_\rho = \pi \left( D_c / 2L \frac{\partial^2 E_G}{\partial N_c^2} \right)^{1/2}$. Square dots represent the scaling of the same quantity for the Hubbard model at the corresponding values of $U$. Notice the non-trivial size scaling, due to marginal umklapp terms. Panel (a): $U = -20t$ and $-2t$. Panel (b): $U = 0$ and $t$. 
Spin gap

Extrapolated

Spin gap

$n=1$

$U=0$

$U=t$

$U=4t$

$U=10t$

$U=100t$

$1/L$
Drude peak $D_c$

$1/L$

$n=1/2$

$U=\infty$

$U=0$

$U=4t$

$U=100t$

$U=\infty$
\[ U = -2t \]

\[ \frac{1}{U} = 2t \]

\[ U = 0 \]

\[ U = -10t \]

\[ n = 1 \]

Drude peak \( D_c \) vs. \( 1/L \)
Extrapolated Charge gap

Charge gap

$U/t$

$U=3t$

$U=2t$

$U=0$

$U=-10t$

Hubbard

EP

$n=1$
$K_\rho(n=1)\begin{cases} U=-20t \\ U=-2t \\ U=0 \\ U=t \end{cases}$