Strongly Enhanced Superconductivity in Coupled t-J Segments

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The t-J Hamiltonian is one of the cornerstones in the theoretical study of strongly correlated copper-oxide based materials. Using the density-matrix renormalization group method we obtain the phase diagram of the one-dimensional t-J chain in the presence of a periodic hopping modulation, as a prototype of coupled-segment models. While in the uniform 1D t-J model the near half-filling superconducting state dominates only at unphysically large values of the exchange coupling constant $J/t > 3$; we show that a small hopping and exchange modulation very strongly reduces the critical coupling to be as low as $J/t \sim 1/3$—well within the physical regime. The phase diagram as a function of the electron filling also exhibits metallic, insulating line phases and regions of phase separation. We suggest that a superconducting state is easily stabilized if t-J segments creating local spin-singlet pairing are coupled to each other—another example is the ladder system.

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Introduction.—Since its introduction at the end of the 1980s, the t-J model Hamiltonian [1] has formed one of the cornerstones in the theoretical study of high temperature superconductors (HTSs). It is a minimal low-energy model for the electronic and magnetic structures of the copper-oxide planes in HTSs and can be derived from the Hubbard model in the strong coupling limit [2]. Although the initial interest in the t-J model focused on its two-dimensional (2D) realization, its one-dimensional (1D) version, which is of direct relevance to, for instance, doped spin-chain materials, provides a number of interesting phases that are also observed in the 2D context, such as a spin-gap phase and the occurrence of phase separation [3,4]. The 1D t-J model actually also displays a superconducting instability, even if all this is in a parameter range where the ratio of the exchange J and hopping t, near half filling is $J/t \sim 3$, which is not of relevance to real materials—the HTSs are rather in the regime where $J/t \sim 1/3$. In the latter regime, quasi-1D systems, e.g., t-J *ladders* can support superconductivity [5–9] which is related to the substantial binding energy for two holes in even-leg ladders, giving rise to the presence of preformed Cooper pairs on the rungs. However, in a 1D system this binding energy vanishes for physically relevant values of J/t [10].

In this Letter, we consider the 1D t-J model in the presence of a periodic local modulation of t and J; within segments of length S_l the hopping and exchange are constant, but the coupling *between* these segments is somewhat weaker, see Fig. 1. In a solid, such a local modulation might, for instance, result from a periodic structural modification or from electronic self-organization. Using the density-matrix renormalization group (DMRG) method we establish that for hole-doped systems close to half filling in the presence of a weak modulation not only the spin gap forms but also the holes pair up already for small values of J/t. A calculation of the Luttinger parameter suggests the stabilization of a superconducting (SC) state in a wide region of the phase diagram, also in the physically relevant low-doping regime with $J/t \sim 1/3$. The stability of the SC state weakly depends on the segment length and apart from superconductivity also metallic, insulating, and phase separated regions are present.

Model and method.—To investigate the effect of the modulation, we consider the model Hamiltonian $H = H_0 + H_\delta$, where H_0 is the uniform 1D t-J part $H_0 = -t\sum_{i\sigma}(c^\dagger_{i,\sigma}c_{i+1,\sigma} + \text{H.c.}) + J\sum_i(\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \frac{1}{4}n_i n_{i+1})$, and H_δ describes the local modulation

$$H_\delta = \delta t\sum_{j\sigma}(c^\dagger_{jS_l,\sigma}c_{jS_l+1,\sigma} + \text{H.c.}) - \delta J\sum_j\left(\mathbf{S}_{jS_l} \cdot \mathbf{S}_{jS_l+1} - \frac{n_{jS_l}n_{jS_l+1}}{4}\right). \quad (1)$$

Here, the sum is over all integers i (j) labeling the sites (segments), $c^\dagger_{i\sigma}$ is the electron creation operator at site i with spin σ, $\mathbf{S}_i$ is the spin-$\frac{1}{2}$ operator, and n_i the electron number operator. Equation (1) represents the reduction in hopping integral δt and exchange interaction δJ on the bonds connecting edge sites of segments with length S_l. The

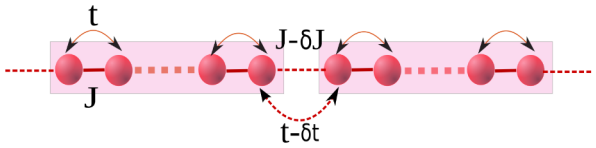

FIG. 1. Schematic picture of the model for coupled t-J segments.

modulated bond consists of the rightmost site of jth segment and the next site to it, which are indexed by jS_l and (jS_l+1), respectively, see Fig. 1. To stay within the perturbative framework in which the t-J model is derived from the Hubbard Hamiltonian, we retain the direct relation between δt and δJ from second-order perturbation theory. As $J = 4t^2/U$, where U is the on-site Coulomb repulsion, we have

$$\frac{J-\delta J}{J} = \left(\frac{t-\delta t}{t}\right)^2. \tag{2}$$

In units of t, we are thus left with only two energy scales: $\delta t/t$ and J/t. The parameter $\delta J/J$ is fixed by the relation in Eq. (2). Clearly, for $\delta t = 0$ the model reduces to the usual 1D t-J Hamiltonian. The electron density is denoted by n. This model also gives a fascinating playground from the points of view of the SC state as a doped spin liquid [11] and of the SC state laying near charge ordering [12].

The quantities of interest, e.g., Luttinger parameter, spin gap, and binding energy, were calculated by the DMRG method [13,14] on a lattice with up to $L = 288$ sites and finite-size extrapolations were performed to obtain them in the thermodynamic limit [15]. We have studied the systems with segment lengths $S_l = 2$, 4, 6, 8, 12. The electron filling is defined as $n = N/L$, where N is the total number of electrons. We kept up to 2000 density-matrix basis states and the typical discarded weight is $\sim 10^{-8}t$.

Spin gap and pair binding.—We start our discussion with spin gap Δ_s. The uniform t-J model (i.e., $\delta t = 0$) in 1D gives the spin-gap phase only at low *electron* density and at large exchange $J/t > 2$ [3,4,16,17]—a parameter regime that is barely relevant to real materials. We show below that the spin-gap phase can appear at small J/t and for weak hole doping (i.e., $n \approx 1$) when a nonzero δt is introduced.

The singlet-triplet excitation energy is given by the energy difference $\Delta_s = E(N, S_z^T = 1) - E(N, S_z^T = 0)$. Here, $E(N, S_z^T)$ is the ground state energy with N electrons and total z component of spins S_z^T. At half filling, $n = 1$, the uniform t-J model corresponds to a Mott insulator with zero spin gap. But if δt is switched on, the spin gap opens and increases monotonically, see Fig. 2(a). The gap reaches its maximum in the limit of decoupled Heisenberg segments, i.e., $\delta t/t = 1$. However, the situation changes drastically when the system is doped with holes, see Figs. 2(b) and 2(c). The overall spin gap is much reduced but kept to be finite. The gap reaches its maximum for *small* $\delta t/t$ and gradually vanishes for larger values of $\delta t/t$. Figure 2(b) shows the spin gap at $J/t = 0.8$ for $S_l = 2$, 4, and 6 as a function of $\delta t/t$ in the limiting density $n \to 1$, which corresponds to putting only two holes in different-length systems and extrapolating Δ_s to the thermodynamic limit [15].

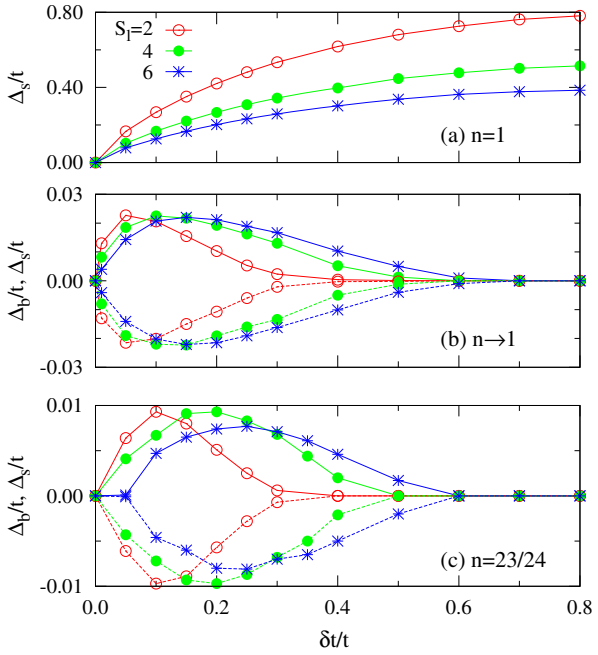

FIG. 2. Spin gap and binding energy at $J/t = 0.8$ for (a) $n = 1$, (b) $n \to 1$, and (c) $n = 23/24$. The red empty circles, green filled circles, and blue star points connected with solid (dotted) lines represent the spin gap (binding energy) for segment size $S_l = 2$, 4, and 6, respectively.

Surprisingly, a very small $\delta t = 0.01$ is already enough to produce a sizable spin gap. The spin gap increases first as in the half-filled case, but then decreases to zero for larger $\delta t/t$. It is interesting that the maximum of the spin gap is not really sensitive to S_l. We notice that the occurrence of the maximum of Δ_s shifts to higher δt if we increase S_l. It is related to a slower reduction of (electron or hole) bandwidth by δt for larger S_l. We also calculated the pair binding energy, which measures the stability of pairing and is defined as $\Delta_b = E(N \pm 2, S_z^T = 0) + E(N, S_z^T = 0) - 2E(N \pm 1, S_z^T = \pm 1/2)$. The plot of Δ_b is shown in Fig. 2(b) for $S_l = 2$, 4, and 6 with the same symbols and colors as Δ_s but connected by dotted lines. The negative values of Δ_b indicate the stability of pairing and a relation $\Delta_s = |\Delta_b|$ in a metallic (M) regime suggests an occurrence of the spin-singlet SC state. The spin gap and pair binding energy at a finite hole density of $n = 23/24$ are shown in Fig. 2(c). Compared to the limit of half filling $n \to 1$, their magnitudes are smaller but the overall behaviors are almost unchanged.

Superconductivity and phase diagram.—The DMRG calculations allow us to map out the phase diagram for the modulated 1D t-J model including the potential SC state. It should be noted that the uniform 1D t-J model shows a transition from M to the SC state at $J/t \geq 2$ in the dilute electron regime. An even higher J/t is necessary to get the SC phase with increasing n [4]. In order to examine the possibility of superconductivity, we estimate the M-SC

transition point by calculating the Luttinger parameter K_ρ: In the conformal field theory the SC and density-density correlations are known to decay in power law as $\sim 1/x^{1/2K_\rho}$ and $\sim 1/x^{2K_\rho}$ at large distances x, respectively. Therefore, we can find the dominant correlations, namely, a paramagnetic metal for $K_\rho < 1$ and a superconductor for $K_\rho > 1$ [18,19]. The Luttinger parameter is extracted from the slope of the charge structure factor $C(q)$ at the wave vector $q \to 0$ limit [20–22]:

$$K_\rho = \pi \lim_{q \to 0^+} \frac{C(q)}{q}, \tag{3}$$

where $q = 2\pi S_l/L$ for finite systems and $C(q)$ is the Fourier transform of density-density correlation $C(q) = (1/L)\sum_{l=1}^{L}(\langle N_i N_{i+l}\rangle - \langle N_i\rangle\langle N_{i+l}\rangle)$, where $N_i = \sum_{j\in S_l} n_j$ is the total density of the ith segment. Equation (3) is still valid for a modulated system [23]. More details are discussed in the Supplemental Material [15].

For fixed n, S_l, and δt, we determined the M-SC transition point J^c/t (the value of J/t at which $K_\rho = 1$). At large J/t, the system separates into electron- and hole-rich regions and the onset of phase separation (PS) has been estimated by inverse compressibility or as a divergent point of K_ρ [15]. The resulting n-J/t phase diagrams containing PS, M, and SC phases are shown in Figs. 3(a)–3(c) for $\delta t/t = 0.2$ and $S_l = 2$, 4, and 6, respectively. The blue star symbol represents J^c/t in the $n \to 1$ limit. It is remarkable that close to half filling (even for a system with only two holes, i.e., $n \to 1$) J^c/t is significantly reduced for all the cases of S_l as shown in Fig. 3. Apparently, the critical value can be as small as $J^c/t \sim 0.35$ for a relatively weak modulation $\delta t/t = 0.2$. It has been also confirmed by comparing the decay ratios of the density-density and SC correlation functions with the distance [15]. This significant reduction of K_ρ would be related to a wide region of the SC phase near half filling in the t-J ladder model [9].

This observation motivates us to study how J^c/t changes as a function of $\delta t/t$. Since a large reduction of J^c/t can be acquired near half filling, we fix the filling at $n = 23/24$ and plot J^c/t in Fig. 4 for $S_l = 2$, 4, 6, 8, 12. For each S_l even a weak modulation $\delta t/t$ causes a large drop in J^c/t from ~ 3.2 for the uniform case $\delta t = 0$. Depending on S_l the lowest J^c/t is reached for $\delta t/t$ between ~ 0.1 and ~ 0.3. This implies that an increase of δt helps electrons in each segment to form singlet pairs which can move easily unless $\delta t/t$ becomes too large, which then tends to localize electrons on individual segments for large $\delta t/t$. This explains the steep minimum and then slow rise in J^c/t. At small $\delta t/t$, J^c/t increases with S_l because the pair formation gets weakened as the segment becomes larger. Ultimately, at very large S_l, the system approaches to the uniform t-J model. On the other hand, at large $\delta t/t$ the pair formation is most effective but the movement of pairs is restricted due to the narrowing of bandwidth and a high J^c/t is given accordingly. An intriguing thing is that even for $S_l = 12$ the strong reduction of J^c/t is obtained despite $J^c/t \sim 3.2$ for any $\delta t/t$ in the $S_l \to \infty$ limit. It means that a system with $S_l = 12$ is still far from the uniform t-J model. We also notice that as we increase $S_l = 2$ to 12 J^c/t at large $\delta t/t$ decreases rapidly for smaller $S_l(\lesssim 4)$ and then almost saturates for larger $S_l(\gtrsim 6)$. To explain this behavior, we plot the spin gap of decoupled segments (i.e., $\delta t/t = 1$) as a function of S_l in the inset of Fig. 4. As expected, we see a sharp (slow) decrease of the spin gap at small (large) S_l.

Insulating line phases.—Unlike the uniform t-J model, we notice some insulating regions (vertical lines in Fig. 3) appearing at various commensurate fillings. This type of insulating region is well known in ladder systems [24]. Because of the restriction in hopping as we introduce δt, the electrons may form a superstructure in each segment which leads to the insulating behavior of the system. The insulating to M transition of the $S_l = 2$ system at $n = 1/2$, which is shown in Fig. 3(a), has been discussed in terms of the melting of Mott insulating states [25]. We briefly recap its intuitive understanding which will guide us to understand the insulating regions at other fillings and $S_l = 4$, 6 systems.

Let us first consider the $S_l = 2$ system with no exchange interaction, i.e., $J \to 0$. Then the tight binding model with $\delta t > 0$ at $n = 1/2$ forms bonding and antibonding states

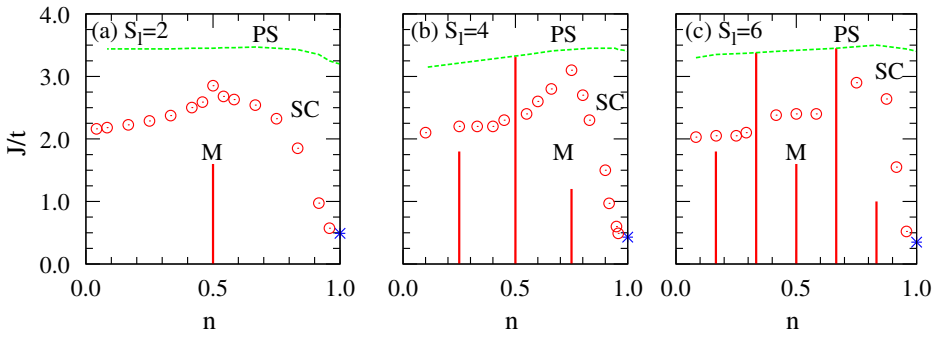

FIG. 3. (a)–(c) Phase diagrams on n-J/t plane at $\delta t/t = 0.2$ for $S_l = 2$, 4, and 6 systems, respectively, containing superconducting (SC), metallic (M), and phase separated (PS) phases. The empty circles represent the M to SC transition and the blue star indicates the M-SC critical point in the $n \to 1$ limit. The vertical lines at commensurate fillings represent insulating line phases.

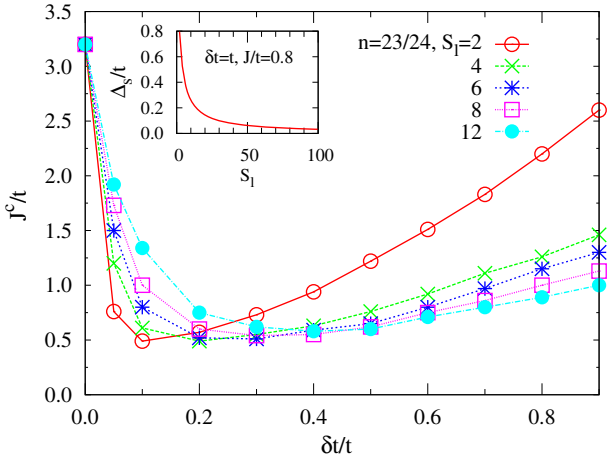

FIG. 4. Critical point between metallic and superconducting phases at $n = 23/24$ for systems with $S_l = 2, 4, 6, 8, 12$. Inset: Δ_s for decoupled segments with different sizes S_l at $J/t = 0.8$.

with spin σ, i.e., t-dimer states: $|t\text{-dim}\rangle_\sigma = (|\sigma 0\rangle \pm |0\sigma\rangle)/\sqrt{2}$ separated by a dimerization gap $\Delta_d = 2\delta t$ at each segment. Thus, due to the t dimerization one electron is trapped in the bonding state of a segment and the system becomes a Mott insulator. Then, if we increase J, a tendency to make singlet pairs is introduced at each segment due to J dimerization, which leads to a transition to the M state. If we further increase J, the system goes into SC and finally reaches to PS. Such a melting of insulating states happens also in the $S_l = 4$ system at $n = 1/4$, $3/4$ and the $S_l = 6$ system at $n = 1/6$, $3/6$, $5/6$ as shown in Figs. 3(b) and 3(c), respectively. No effective pairing with an odd number of electrons in a segment at these fillings causes the melting of insulating states with increasing J. However, an even number of electrons on a segment as in the $S_l = 4$ system at $n = 1/2$ and the $S_l = 6$ system at $n = 2/6$, $4/6$ prevents melting by making an effective pairing between themselves even with increasing J. As a result, the insulating states continue to exist until the PS boundary as shown in Figs. 3(b) and 3(c). These insulating line phases and metal-insulator transitions were captured by calculating charge gap $\Delta_c = [E(N+2,0) + E(N-2,0) - 2E(N,0)]/2$.

Conclusions.—Using the DMRG method we confirmed that a metal to superconducting transition can occur in a physically relevant regime of exchange and hopping parameters (i.e., $J/t \sim 1/3$) in the 1D system with coupled t-J segments. As compared to the uniform 1D t-J model, only a moderate modulation of the hopping integral causes an order of magnitude reduction of critical exchange coupling to the superconducting state near half filling. We presented n-J phase diagrams at $\delta t/t = 0.2$ with different segment sizes containing, besides phase separation, metallic and superconducting phases also insulating line phases at commensurate fillings. These results may be of relevance to certain quasi-1D materials, including cuprates in which typical exchange coupling is $J/t \sim 1/3$ [26]. An example is the spin-Peierls system $CuGeO_3$ [27] which consists of linear spin-$\frac{1}{2}$ CuO_2 chains with alternating exchange and hopping, corresponding to a $S_l = 2$. Our results may suggest that doping with a few holes may turn the system to be superconducting. Such values of exchange and hopping parameters can in principle also be achieved in 1D ultracold fermionic quantum gases [28] and with polar molecules [29] on optical lattices. It will be most interesting to establish whether in such quantum simulator experiments a superconducting state can be stabilized by a relatively benign modulation of the 1D t-J Hamiltonian as we propose here. In this Letter, the segments are an open chain coupled linearly as a simplest 1D case. However, any shape of segment can be allowed if it creates a locally finite spin excitation gap. The network between the segments would also be flexible. We think that this simple condition possibly will be a great help for superconducting material design. For example, the ladder t-J system is a special case of the coupled-segment systems.

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