Spin Gap and Superconductivity in the One-Dimensional $t$-$J$ Model with Coulomb Repulsion

M. Troyer$^{(a,b,c)}$, H. Tsunetsugu$^{(a,b)}$, T.M.Rice$^{(b)}$
J. Riera$^{(d)}$ and E. Dagotto$^{(d)}$

$^{(a)}$Interdisziplinäres Projektzentrum für Supercomputing, Eidgenössische Technische Hochschule, CH-8092 Zürich, Switzerland
$^{(b)}$Theoretische Physik, Eidgenössische Technische Hochschule, CH-8093 Zürich, Switzerland
$^{(c)}$Centro Svizzero di Calcolo Scientifico, CH-6924 Manno, Switzerland
$^{(d)}$Department of Physics, Center for Materials Research and Technology, and Supercomputer Computations Research Institute, Florida State University, Tallahassee, FL 32306, USA.

(Received )

The one-dimensional $t$-$J$ model with density-density repulsive interactions is investigated using exact diagonalization and quantum Monte Carlo methods. A short-range repulsion pushes phase separation to larger values of $J/t$, and leads to a widened precursor region in which a spin gap and strengthened superconducting correlations appear. The correlation exponent is calculated. On the contrary, a long-range repulsion of $1/r$-form suppresses superconductivity in the precursor region.
I. INTRODUCTION

The $t$-$J$ model is one of the most actively studied model Hamiltonians for the cuprate superconductors [1,2]. Two essential features of these materials are correctly implemented in this model, namely the strong on-site Coulomb repulsion at Cu sites and strong antiferromagnetic (AF) spin fluctuations in the ground state. Although much effort has been devoted to the search for superconductivity in this model, the parameter values where superconductivity may appear and the symmetry of the superconducting order parameter remain to be definitively established. Two arguments have been given that suggest the presence of superconducting correlations in this model. One proposal is based on the strong AF fluctuations that occur in the region of small hole doping away from the AF-ordered state at half-filling [3]. The second is based on the occurrence of phase separation at larger values of $J/t$ [4]. In particular, in several papers it has been argued that superconductivity may appear in the precursor region to phase separation. Only recently, numerical studies have been carried out in this region. Dagotto and Riera [5] examined the $t$-$J$ model at quarter-filling in one (1D) and two (2D) dimensions. In particular, they found that adding a short-range density-density repulsion pushes phase separation to larger values of $J/t$ and leads to strengthened signs of superconducting correlations. Those authors provided an intuitive physical picture of the origin of this effect, based on the effect of the nearest-neighbor repulsion to form pairs of electrons in the ground state [6]. The analysis in 2D is similar to what occurs in 1D. In particular, Dagotto and Riera have recently shown that a superconducting state with $d_{x^2-y^2}$ symmetry may exist in the more realistic case of the 2D $t$-$J$ model near phase separation [7]. A recent study of a 1D two band model also shows that superconducting correlations are enhanced near the phase separation boundary [8].

Although the parameter region where superconductivity was observed is not obviously directly relevant for the high-$T_c$ cuprates, it is not excluded that both regions are analytically connected. Thus, it is important to continue the study of this phenomenon. This is the purpose of the present paper. Our calculations are restricted to 1D for simplicity.
In this case a reliable finite-size scaling analysis can be implemented, and exact diagonalization results can be extrapolated to infinite size. Another advantage of the 1D problem is that quantum Monte Carlo (QMC) methods can be used on large samples down to low temperatures without encountering the sign problem. Finally, the correlation exponents can be conveniently calculated using conformal field theory (CFT). Previous studies \cite{5} have convincingly shown that there are strong analogies between 1D and 2D systems, and thus our results may be valid also in higher dimensions.

The 1D $t$-$J$ model without repulsive density-density interactions has been investigated in detail by Ogata et al. \cite{9} using finite size diagonalization, and by Assaad and Würtz \cite{10} using QMC methods. This 1D $t$-$J$ model shows three different ground state behaviors in the plane defined by the electron density, $\rho$, and the ratio of spin exchange interaction to hopping amplitude, $J/t$. First, a Tomonaga-Luttinger liquid (TLL) exists at all $\rho \neq 1$ for not so large exchange coupling $J/t$. This phase is characterized by gapless charge and spin excitations, and by power-law correlation functions in space and time \cite{11}. Second, there is a phase-separated region for large $J/t$ at all densities $\rho$. In this region, the charge fluctuations are completely suppressed except for the center-of-mass motion of the electron condensed part, while the spin excitations are gapless. Third, there is a spin gap phase \cite{9}, which exists between the previous two regimes but at small $\rho$-values (at $\rho = 1/3$ or larger the spin gap is no longer observed). It has gapless charge excitations, but exponentially decaying spin correlation functions. In the regions with gapless charge excitations, power-law behaviors of correlation functions are determined by a single parameter $K_\rho$ \cite{11,12}. Superconductivity is the most dominant correlation in the regime where $K_\rho > 1$, for both the TLL and the spin gap phases. This region is found close to the phase separation boundary \cite{9} and is caused by an attractive interaction via spin exchange. In the large $J/t$ region, phase separation overcomes the competition with superconductivity. Therefore, at least naively we may expect a wider superconducting region if we can suppress phase separation by including other terms in the Hamiltonian. This can be easily achieved. Phase separation can be suppressed
by the long-range part of the Coulomb repulsion between electrons. This long-range term is neglected in the Hubbard and \( t-J \) models. However, this term plays a crucial role in and near the phase separated region. In this paper we will study the problem of whether the long-range Coulomb repulsion can enhance the superconductivity by suppressing phase separation and causing a large precursor region.

Another central issue of this paper is to analyze if this precursor region is characterized by a gap in the spin excitation spectrum. As proposed first by Anderson [1] and by Kivelson et al. [13] afterwards, a possible mechanism of the high-\( T_c \) superconductivity is that upon doping of holes local spin-singlet electron pairs, which would constitute a spin liquid state in the undoped insulator, start to move coherently, resulting in an off-diagonal long-range order (ODLRO). If the hole motion does not destroy the local character of singlet pairs completely, the lowest spin excitation is given by a singlet-to-triplet excitation of a local pair, and thus it will have a finite gap, even though its absolute value may be reduced by virtual pair-breaking effects due to charge fluctuations. Therefore, a finite spin gap is indicative of the short-range resonating valence bond (RVB) mechanism of superconductivity. Following this scenario, the effect of hole doping has been examined for several models which have an insulating ground state with a spin gap at half filling [14,15], and strong superconducting correlations are found upon doping. In this paper, we will study the models where a spin gap is caused by doping holes into an antiferromagnetic insulator with gapless spin excitations. This is consistent with experiments on several high-\( T_c \) materials, particularly in underdoped materials [16,17]. However, the question of how these local spin-singlet pairs are stabilized when holes are mobile is not well understood. The existence of a spin gap also has a strong relation with the internal symmetry of superconductivity. In the TLL phase (i.e., no spin gap), the nearest-neighbor singlet and triplet pairing have the same exponent in the superconducting correlation functions [1]. Once the spin gap becomes finite by changing coupling constants in the Hamiltonian or electron concentration, the system is scaled to another universality class, the Luther-Emery fixed point in the \( g \)-ology [11,18]. Thus, the line where the gap
opens corresponds to the phase boundary between two different universality classes, the TLL phase and the spin gap (Luther-Emery) phase, and physical properties change their long-range behaviors drastically on this line [11]. In the spin gap phase, the triplet and singlet superconductivity are no longer degenerate and the triplet superconductivity is suppressed relative to the singlet one, since making a triplet pair costs a finite energy.

In this paper, we will study the effects of long-range Coulomb repulsion on superconducting correlations and the spin gap, using three modifications of the $t$-$J$ model with different interaction ranges. The first one is the $t$-$J$ model plus nearest-neighbor repulsions [5,6,19],

$$H_{t-J-V} = -t \sum_{i,\sigma} \left( \mathcal{P} c_{i,\sigma}^\dagger c_{i+1,\sigma} \mathcal{P} + h.c. \right) + J \sum_i \left( \mathbf{S}_i \cdot \mathbf{S}_{i+1} - \frac{1}{4} n_i n_{i+1} \right) + V \sum_i n_i n_{i+1},$$

where $c_{i,\sigma}^\dagger$ creates an electron at site $i$ with $z$-component of spin $\sigma = \uparrow, \downarrow$, $n_i = \sum_\sigma c_{i,\sigma}^\dagger c_{i,\sigma}$, and $\mathbf{S}_i$ are electron spin operators. The projector $\mathcal{P} = \Pi_i \left( 1 - n_{i,\uparrow} n_{i,\downarrow} \right)$ projects out states with doubly occupied sites. By taking the $V \to 0$ limit, one recovers the original $t$-$J$ model. Secondly, we will study a model which includes next-nearest-neighbor repulsions:

$$H_{t-J-V-V' } = H_{t-J-V} + V' \sum_i n_i n_{i+2}.$$  

The last modification is a model with a bare Coulomb repulsion and a spatial decay proportional to $1/r$ [20]. For a finite lattice, we will use the following Hamiltonian,

$$H_{V/r} = -t \sum_{i,\sigma} \left( \mathcal{P} c_{i,\sigma}^\dagger c_{i+1,\sigma} \mathcal{P} + h.c. \right) + J \sum_i \left( \mathbf{S}_i \cdot \mathbf{S}_{i+1} - \frac{1}{4} n_i n_{i+1} \right) + \frac{V_L}{2} \sum_{i,j} \frac{(n_i n_j - \rho^2)}{d_{ij}},$$

where $\rho \equiv (\sum_i n_i)/L$ is the electron concentration, and the “distance” $d_{ij}$ between the sites $i$ and $j$ is defined as

$$d_{ij} = \frac{L}{2\pi} \sin \left( \frac{2\pi}{L} |i - j| \right),$$

on our finite lattice of $L$ sites. In the $L \to \infty$ limit, $d_{ij} \to |i - j|$. The last term in the Hamiltonian is a constant and gives the contribution of a uniform positive-charge background, which keeps the ground state energy per site finite in the limit $L \to \infty$. 
II. NUMERICAL METHODS

We use both exact diagonalization and QMC methods to investigate the ground state properties of the models described in the previous section. Exact diagonalization gives results with high accuracy for small lattices. It also allows the calculation of dynamical properties in real time. QMC can be used to investigate static properties of larger lattices. For the exact diagonalization method, the Lanczos algorithm [21] is used to obtain the energy eigenvalues and the eigenvectors for the ground state as well as for the first few excited states. The relative error of the eigenvalues, and the residue of the eigenvector are both less than $10^{-9}$ for lattices of up to 20 sites. In order to carry out a systematic finite size analysis, the boundary conditions must be chosen carefully. One choice is to select boundary conditions which keep all one particle orbitals either fully occupied or empty in the noninteracting case. We will call this choice closed shell boundary conditions (CSBC). In practice, we use periodic boundary conditions (PBC) for systems with $N = 4n + 2$ particles ($n$ is an integer) and antiperiodic boundary conditions (APBC) for $N = 4n$ particles. The opposite choice of antiperiodic boundary conditions for systems with $N = 4n + 2$ particles and periodic boundary conditions for $N = 4n$ particles will be called open shell boundary conditions (OSBC). The ground state of the 1D $t$-$J$ model is always a spin singlet with CSBC, but it changes the spin quantum number depending on the parameters for OSBC. In most cases we use CSBC. In cases where a more careful analysis is necessary to study finite size effects, we use both CSBC and OSBC.

By QMC methods considerably larger systems can be studied at low temperatures. Here, we use the world line algorithm [22] with a four-site cluster decomposition [23]. Since there is no negative sign problem for the 1D $t$-$J$ model [10], simulations could be performed on lattices with up to $L = 96$ sites at inverse temperatures up to $\beta t = 64$. The systematic error of order $O(\Delta \tau^2)$ due to the finite Trotter time step $\Delta \tau$ is controlled by extrapolating the results obtained at $\Delta \tau t = 0.25$ and $\Delta \tau t = 0.5$. The usual zero winding number boundary conditions were used. For more details on the algorithm we refer to Refs. [10,22,23].
To study the properties of the $t$-$J$-$V$ model we first calculate the spin gap by exact diagonalization and QMC. Next we calculate the charge and spin structure factors by both methods. Furthermore we measure pairing correlations by exact diagonalization. The charge and spin structure factors are defined as the Fourier transform of the correlation functions in real space:

$$S_{\text{charge}}(q) = \frac{1}{L} \sum_{j,m} e^{i q (j-m)} \langle (n_{j,\uparrow} + n_{j,\downarrow})(n_{m,\uparrow} + n_{m,\downarrow}) \rangle,$$

$$S_{\text{spin}}(q) = \frac{1}{L} \sum_{j,m} e^{i q (j-m)} \langle (n_{j,\uparrow} - n_{j,\downarrow})(n_{m,\uparrow} - n_{m,\downarrow}) \rangle = 4 \frac{1}{L} \sum_{j,m} e^{i q (j-m)} \langle S^z_j S^z_m \rangle. \tag{6}$$

The singlet pairing correlations are defined as $\langle P^\dagger(r) P(0) \rangle$, where

$$P^\dagger(r) = \frac{1}{\sqrt{2}} \left( c^\dagger_{r,\uparrow} c^\dagger_{r+1,\downarrow} - c^\dagger_{r,\downarrow} c^\dagger_{r+1,\uparrow} \right) \tag{7}$$

is the creation operator of a nearest-neighbor electron singlet pair. The superconducting structure factor is defined as its Fourier transform, i.e.

$$S_{\text{pair}}(q) = \frac{1}{L} \sum_{j,m} e^{i q (j-m)} \langle P^\dagger(j) P(m) \rangle. \tag{8}$$

III. PHASE SEPARATION

In the $t$-$J$ model it is well known that phase separation occurs for large values of $J/t$. At low hole doping this effect arises in order to minimize the number of broken antiferromagnetic bonds in the system. For low electron doping, the $J$-term is an explicitly attractive term for electrons. For large values of $J$ this attraction overcomes the repulsion due to the kinetic term and the system is separated into a particle-rich phase and a sea of holes. Close to the phase separation boundary the system is still homogeneous but the attraction already produces bound states of holes or electrons, depending on the doping. Precisely this effect led to recent studies of that region in both 1D and 2D to search for indications of...
superconductivity in this type of models. Superconductivity will be investigated in detail in Sec. V.

In this section, we will determine the boundary of the phase separation region by exact diagonalization techniques. This boundary is defined by those points in parameter space where the inverse compressibility $\kappa^{-1}$ vanishes. On a lattice with $N$ particles and $L$ sites, $\kappa^{-1}$ can be calculated as

$$\kappa^{-1} = \frac{N^2}{L} \left( \frac{E(N + 2; L) + E(N - 2; L) - 2E(N; L)}{4} \right),$$  \hspace{1cm} (9)$$

where $E(N; L)$ is the ground state energy of the finite system with $N$ particles on $L$ sites. Equation (9) is simply a discrete version of the second derivative of the energy with respect to the number of particles. The phase separation boundary can also be estimated using QMC methods. Here, phase separation is characterized by a divergence of the long-wavelength charge fluctuations $S_{\text{charge}}(q = 2\pi/L)$ when the system size $L$ is increased (for details we refer the reader to Ref. [10]). The results obtained by both methods agree very well. Comparing results for different system sizes $L$, we estimate the error on this boundary to be of the order of $\Delta J \sim 0.1t$.

Figure 1 shows the inverse compressibility for the $t$-$J$, $t$-$J$-$V$, and $t$-$J$-$V$-$V'$ models at quarter band-filling. It can clearly be seen that, as expected, the repulsive $V$-term pushes the phase separation boundary to larger couplings $J/t$. In the phase diagrams (Figs. 2 and 3), this behavior is clearly seen in the $J$-dependence of the phase separation line (thick line in the figures). The next-nearest-neighbor repulsion $V'$ shifts phase separation into even larger values of $J$.

The case of a long-range repulsion of $1/r$-form is different. On a finite size lattice, a large enough $J > J_c$ will result in phase separation but the critical value $J_c$ diverges with the system size. Thus, in an infinite lattice no phase separation will occur. This is easily understood since the contribution of the long-range repulsion to the energy diverges in the phase separated state. When $J$ is increased the system does not phase separate but rather forms a charge density wave (CDW) consisting of larger and larger clusters of...
antiferromagnetically aligned spins.

IV. SPIN GAP

Several well-studied models of interacting electrons present a nonzero spin gap. For example, the extended Hubbard model for $V > U/2$ has a gap in the spin excitation spectrum $[1]$. The attractive-$U$ Hubbard model in 2D has both a superconducting and a spin-gap at all fillings $[24]$. The Luther-Emery model is an example of an exactly solvable model with a spin gap $[18]$. Also spin models with ground states made only of local spin singlet pairs, e.g. the AF Heisenberg chain with a frustrating next-nearest-neighbor interaction $[25]$, have a nonzero spin gap. Doping holes into such a chain leads to the $t$-$J$-$J'$ model with charge carriers which also exhibits a spin gap near half filling $[15]$. However, studies of the $t$-$J$ model in 1D at quarter band-filling $[9]$ did not show indications of such a gap. This has to be contrasted against the recent analysis of the $t$-$J$-$V$ model by Dagotto and Riera where at large and intermediate values of $V/t$, a nonzero spin gap was observed. In this section, we clarify this situation by an analysis of the spin gap in the $t$-$J$-$V$ model at all values of the coupling $V/t$ using Lanczos and QMC methods.

First, let us consider the classical limit $t = 0$. In this case the ground state can be obtained exactly following, for example, the procedure of Ref. $[3]$. Both the $t$-$J$-$V$ and $t$-$J$-$V$-$V'$ models have a spin gap for $V - 2V' < J < (V + 2V')/(2 \log 2 - 1)$ at quarter band-filling. In this parameter region the ground state consists of nearest-neighbor singlet pairs separated by two holes ($2k_F$ CDW). Other configurations are also possible in this regime since a pair of electrons in the previous state can be moved one lattice spacing to the right or the left without additional cost in energy. A similar analysis can be carried out in higher dimensions leading also to the presence of a spin gap $[3,4]$. Therefore the spin excitations have a gap $\sim J$. The problem is whether this spin gap will survive for finite $t$. To study this issue we calculated the spin gap using exact diagonalization methods on lattices with up to $L = 20$ sites at quarter band-filling ($\rho = 1/2$). The spin gap on a finite lattice, $\Delta(L)$, is
evaluated directly as the difference between the energies of the lowest lying spin singlet and triplet states. The spin gap $\Delta$ in infinite systems is then obtained by extrapolating $\Delta(L)$ to the bulk. As a scaling function we have used the following form (for fixed fillings $\rho = N/L$):

$$\Delta^{BC}(L) = E^{BC}_0(L) - E^{BC}_1(L) = \Delta + \frac{a^{BC}_1}{L} + \frac{a^{BC}_2}{L^2},$$

where $E^{BC}_0(L)$ and $E^{BC}_1(L)$ are the lowest eigenenergies in the spin singlet and triplet subspaces, respectively. The superscript $BC$ denotes the boundary conditions. Both CSBC and OSBC were used. We have observed that including a $1/L^3$ term changes $\Delta$ by only a few percent, and thus our results seem stable. We have tested this extrapolation using the $t$-$J$ model, where no spin gap was reported at quarter band-filling. In the case of a finite spin gap we expect that asymptotically for large $L$ the spin gap follows an exponential scaling. The results of QMC for systems with $L = 48$ and $L = 96$ sites indicate such a behavior, but for the small system sizes that can be investigated using exact diagonalization we are not yet in this exponential regime and the fitting function Eq.(10) is the best. In the QMC simulations the spin gap is calculated as the difference between the energies of the $M_z = 0$ and $M_z = 1$ subspace. ($M_z$ is the $z$-component of the total magnetization). As shown in Figure 4, the scaling function Eq.(10) somewhat underestimates $\Delta$, as expected from the correct asymptotic exponential behavior. Therefore, the spin gap $\Delta$ calculated following our procedure should be considered as a lower bound for the actual value of the gap.

In Figure 5 the spin gap for the quarter-filled $t$-$J$-$V$ model is shown. The parameters are chosen along the line $J = 3t + 2V$, which is inside the superconducting region close to phase separation. The spin gap $\Delta$ increases with $J$ and $V$. In the phase diagram shown in Fig. 2 we plot the contour lines for several values of constant gap $\Delta$. A prominent feature is that the spin gap region expands with increasing $V$, which is consistent with the result in the classical limit $t = 0$. As mentioned above, the effect of the $V'$ term on the spin gap is also estimated qualitatively by considering the limit $t \to 0$. The $V'$ term expands the spin gap region in the strong coupling regime.

Figure 5 shows that the spin gap is nonzero in the bulk limit for all the values of $V/t$...
that we have analyzed, starting at $V/t = 0.5$. Then, it may occur that for a certain range of $J/t$-values $V/t = 0$ is a singular point and that a small perturbation away from it, opens a gap immediately. Such a behavior was recently suggested [5], but by no means proved, based on a mapping of the large $V/t$ results into the attractive Hubbard model. We know that the last model opens a spin gap as soon as the interactions are turned on. Of course, we cannot exclude the possibility that for all values of $J/t$ there is a “critical” value of $V/t$ larger than 0, where the gap opens. We expect that the spin gap is sensitive to the value of $J/t$. The investigation of this behavior certainly deserves more work.

V. SUPERCONDUCTIVITY

In this section we will study superconducting correlations, and discuss their relation to the phase separation and spin gap regions. As discussed in Sec. I, our main concern is whether intermediate and long-ranged Coulomb interactions can enhance superconductivity by suppressing phase separation, which destroys superconductivity otherwise. For this purpose, we have calculated several quantities to investigate superconducting correlations in the ground state. First, we have measured the absolute value of the superconducting structure factor $S_{\text{pair}}(q = 0)$. Then, we study the real-space pairing correlations $\langle P^\dagger(r)P(0) \rangle$ as a function of distance. Finally, we will investigate the width of the superconducting region by analyzing the correlation exponents in Sec. VII.

In the $t$-$J$-$V$ model, it was shown by Dagotto and Riera [5] that increasing the value of $V/t$ from zero, the nearest-neighbor density-density repulsion enhances both the peak value of $S_{\text{pair}}(q = 0)$, and the pairing correlations at large distances compared to the $t$-$J$ model. Furthermore, a similar qualitative behavior was observed in the more realistic 2D case [5,7]. For larger values of $V/t$, the pairing correlations are eventually suppressed and they decay to zero when $V/t \to \infty$, due to the lack of mobility of the pairs [5]. In these previous studies, it was observed that the inclusion of the repulsive term shifts not only the phase separation boundary to larger values of $J/t$, but the superconducting region is shifted as well, always...
existing as a narrow strip close to phase separation.

Since the nearest-neighbor term enhances superconductivity \[^{[5]}\], let us consider the effect of a next-nearest-neighbor repulsion term \(V'\) (Hamiltonian Eq.\(^{[2]}\)), which further suppresses phase separation. Figures \(^{[4]}\) and \(^{[5]}\) show the uniform component of the superconducting structure factor \(S_{\text{pair}}(q = 0)\) for \(V/t = 1\) at quarter band-filling \((\rho = 1/2)\) and for \(\rho = 2/3\), respectively. A small repulsion \((V'/V = 0.25\) and \(V'/V = 0.5\)) enhances the peak value of the superconducting structure factor for both dopings. The maximum is around \(V'/V = 0.5\). At large values of \(V' > V/2\) superconductivity is reduced, and actually at \(V'/t = 2\) it is strongly suppressed. For larger values of \(V/t\), the effect of \(V'/t\) is less important. Actually, for \(V/t \sim 3\) or larger, we observed that the \(V'\)-term suppresses superconductivity as soon as it is turned on. However, these values may be unphysically large in the real materials. As in the \(t-J\) model the superconducting structure factor is largest in a region near the phase separation boundary. The suppression of superconductivity with large \(V'\) is due to a competition with CDW correlations, as will be shown in the next section.

As emphasized in a recent paper \[^{[5]}\], the \(q = 0\) component of the superconducting structure factor, \(S_{\text{pair}}(q = 0)\), contains both the short and long distance correlations. Thus, it is very important to study the pairing correlations in real space to observe its asymptotic behavior. For the \(t-J-V\) model \((V' = 0)\), and the \(t-J-V'-V'\) model at \(V' = V/2 = t/2\), we have calculated \(\langle P^t(r)P(0)\rangle\) for quarterband-filling on lattices of \(L = 12, 16\) and \(20\) sites, and, additionally, for a filling of \(\rho = 2/3\) on lattices of \(L = 12, 15, 18\). In Fig.\(^{[8]}\) several typical results are plotted for values of \(J/t\) at the maximum of the superconducting structure factor. They show an increase in the long-range pairing correlations with \(V'\), as suggested by Fig.7. The features become more prominent with an increase of the system size. From this evidence we conclude that our results are valid for the infinite system and the next-nearest-neighbor interaction indeed further increases the long-range pairing correlations. The behavior observed in the susceptibility is thus indicative of long distance properties of the ground state.
As mentioned above, the system with a $1/r$ long-range repulsion does not undergo phase separation in the thermodynamic limit. However, the long-range repulsion also suppresses the superconducting pairing correlations (see Figs. 7 and 8) at large distances. For this particular example, note that the study of the large distance behavior of the correlations is crucial. From Fig. 4 it would have been concluded that $1/r$ interactions also enhanced superconductivity. However, this is a short distance effect. Actually, in Fig. 8 for distances smaller than three lattice spacings, correlations for different models are all similar, while only at large distances it can be observed that the correlations for the $1/r$ interaction are strongly suppressed.

To summarize the results of this section, we have observed that a short-range Coulomb repulsion suppresses phase separation, and enhances both the superconducting structure factor and the long-distance pairing correlations. For the particular case of $V' = 0$ this is in agreement with previous results [3]. On the other hand, the long-range $1/r$ repulsion does not enhance pairing correlations in the ground state, in spite of the fact that it suppresses phase separation. The reason is that two effects are in competition against superconductivity: one is phase separation, and the other is CDW order. In other words, in a region of electron pairs, as that found in the $t = 0$ limit, we can have superconducting or CDW correlations in the ground state once the hopping $t$ becomes nonzero. This can be clearly seen in the attractive Hubbard model where at half-filling, both types of orders are exactly degenerate. Away from that special point we expect the degeneracy to be lifted. While phase separation is pushed further away by the long-range repulsion both CDW and superconducting correlations are enhanced, but the CDW correlation are dominant.

VI. CHARGE AND SPIN STRUCTURES

In this section we will examine the competition between phase separation, superconductivity, CDW and spin density wave (SDW) order in the ground state of the several models under consideration. We have calculated the correlation functions and structure factors of
the $t$-$J$-$V$ model Eq. (1) on large systems with up to $L = 96$ by using QMC techniques at $\rho = 1/2$ and $V/t = 1$. For the long-range $1/r$ model Eq. (3), we have carried out exact diagonalization calculations for systems of up to $L = 20$ sites, since the world line algorithm of the QMC method requires the interactions to be local.

At small values of $J/t$ the $t$-$J$-$V$ model shows similar qualitative behavior of the charge and spin structures as the $t$-$J$ model. The system is characterized by $4k_F$ CDW correlations showing a power law decay like in the $t$-$J$ and Hubbard models. The spin degeneracy of the case $J = 0$ is lifted by an infinitesimal $J$, leading to dominating $2k_F$ SDW fluctuations. Consequently the charge and spin structure factors present a cusp at $q = 4k_F$ and $q = 2k_F$, respectively ($J/t = 0.5$ in Fig. 9a and b).

Let us now increase $J/t$, while keeping $V/t$ fixed. At larger values of $J/t$ the particles form nearest-neighbor singlet pairs, as was discussed in previous sections and Refs. [5,6]. This effect suppresses the $4k_F$ charge and $2k_F$ spin fluctuations, while enhancing $2k_F$ charge fluctuations. In the structure factors this effect can be seen by a decrease in the $2k_F$ spin singularity and the development of a $2k_F$ charge structure ($J/t = 4$ in Figs. 9a and b). While the Coulomb repulsion enhances the formation of nearest-neighbor singlet pairs, the CDW correlations still dominate the pairing correlations. The real-space spin correlations show a strong AF nearest-neighbor correlation. The amplitude of the longer-range correlations is, on the other hand, very small. This makes it hard to distinguish the TLL region, where the spin correlations show a power-law decay, from the spin gap region where they show an exponential decay. Therefore it is necessary to combine the CFT and numerical calculations to obtain the correlation exponents as will be done in the next section.

At even larger values of $J/t$, the system is dominated by the superconducting correlations. As a typical example, charge and spin correlation functions are shown for $J/t = 4.75$ in Fig. 9a and b. There the particles tend to form nearest-neighbor singlet pairs and the spin excitations have a gap. This is reflected by the spin structure factor which is similar to that of a gas of nearest-neighbor singlet pairs.
Finally, at $J/t > 5$ phase separation occurs. The inverse compressibility becomes zero and the $q = 2\pi / L$ component of the charge structure factors increases strongly and diverges with increasing system size.

If the long-range interactions of $1/r$ form are used, the CDW correlations are dominant for the whole-range of couplings $J/t$ as can be seen from the charge structure factor (Figs. 10a and b). At small $J/t$, we can again see a $4k_F$ cusp in the charge structure factor, and a cusp at $2k_F$ in the spin structure factor ($J/t = 2$ in Fig. 10a and c). Increasing $J/t$, a $2k_F$ peak in $S_{\text{charge}}(q)$ develops, while the spin structure has a maximum at $q = \pi$ and looks similar to that of a gas of nearest-neighbor singlet pairs ($J/t = 5$ in Fig. 10a,c). At larger $J/t$ there is no phase separation but, as discussed before, the particles form larger and larger clusters of AF spin chains. This can be seen in the charge structure factor as the shift of the peak towards smaller $q$. The spin structure factor resembles that of an AF Heisenberg chain with a peak at $q = \pi$. In the long-range model the CDW correlations always dominate the superconducting correlations.

VII. CORRELATION EXPONENTS

In this section we will calculate the correlation exponents of the $t$-$J$-$V$ model. The correlation exponents can be used to decide which correlations dominate the long-range behavior. It is in general hard to determine the correlation exponents directly from the numerical calculations of the correlation functions. However, in many 1D Fermion systems, by combining conformal field theory (CFT) with numerical simulations, one can determine the correlation exponents from thermodynamic quantities which can be calculated more easily and accurately than the long-range correlations [11,12].

Depending on the coupling constants two main regimes can be distinguished. In the TLL regime both the charge and spin excitations are gapless and the correlation functions show a power-law decay. The exponents can be described by a single dimensionless exponent $K_\rho$.
\[ \langle n(r)n(0) \rangle \sim A_0 r^{-2} + A_1 \cos(2k_F r) r^{-(1+K_\rho)} + A_2 \cos(4k_F r) r^{-4K_\rho}, \]

\[ \langle S_z(r)S_z(0) \rangle \sim B_0 r^{-2} + B_1 \cos(2k_F r) r^{-(1+K_\rho)}, \quad (11) \]

\[ \langle P^\dagger(r)P(0) \rangle \sim C_0 r^{-\left(1+\frac{1}{K_\rho}\right)} + C_1 \cos(2k_F r) r^{-\left(K_\rho+\frac{1}{K_\rho}\right)}. \]

Logarithmic corrections have been omitted in these formulas. Models belonging to the TL regime include the \(t\)-\(J\) model before phase separation and the repulsive Hubbard model, as well as many generalizations of these models without a spin gap. The other regime is the spin gap phase, typically represented by the Luther-Emery model. This phase has a finite gap in the spin excitation spectrum but gapless charge excitations. Here the spin correlations have an exponential decay, and the other correlations again present a power law decay:

\[ \langle n(r)n(0) \rangle \sim A_0 r^{-2} + A_1 \cos(2k_F r) r^{-K_\rho} + A_2 \cos(4k_F r) r^{-4K_\rho}, \]

\[ \langle P^\dagger(r)P(0) \rangle \sim C_0 r^{-\frac{1}{K_\rho}}. \quad (12) \]

The extended Hubbard model includes both the TLL and spin gap phases. It is apparent that the superconducting pairing correlations are dominant for \(K_\rho > 1\) in both phases.

Because the \(t\)-\(J\)-\(V\) model shows qualitatively similar behavior in the correlation functions as the \(t\)-\(J\) model, we expect it to belong to the same universality class. This is further confirmed by calculation of their central charges. The CFT predicts the following finite size corrections of the ground state energy for a TLL [12]:

\[ E(L)/L = \epsilon - \frac{\pi}{6}(v_c + v_s) \frac{c}{L^2}, \quad (13) \]

with the central charge \(c = 1\). Here, \(E(L)\) is the ground state energy of the finite system with \(L\) sites and \(\epsilon\) is the energy per site in the infinite system. The parameters, \(v_c\) and \(v_s\), are the charge and spin velocities, respectively. They can be calculated as the derivative of the charge and spin excitation energies with respect to total momentum. We calculated them by using

\[ v_c = \left[ E_0(q = 2\pi/L) - E_0(q = 0) \right]/\frac{2\pi}{L}, \quad (14) \]

\[ v_s = \left[ E_1(q = 2\pi/L) - E_0(q = 0) \right]/\frac{2\pi}{L}, \quad (15) \]
where $E_0(q)$ and $E_1(q)$ are the lowest energy eigenvalues in the spin singlet, respectively triplet, subspace of total momentum $q$. The central charge was then obtained by fitting the ground state energies according to Eq. (13). Our calculations give $c \sim 1.04$, which is in agreement with $c = 1$ within the finite size errors in the velocities of the order of a few percent. This value of $c$ is nearly $J$ and $V$ independent. The deviations from unity are always smaller than the estimated error in the velocities which are about 10%.

The correlation exponent $K_\rho$ can now be calculated from the relation \[ K_\rho = \pi v_c \rho^2 \kappa / 2, \] with $\rho$ being the particle density, and $\kappa$ the compressibility. In Fig. 2 we show contour lines of constant $K_\rho$ in the $J$-$V$ plane at quarter band-filling. In addition, Fig. 3 shows the phase diagram of the $t$-$J$-$V$ model at $V/t = 1$ for all fillings.

Several regions can be distinguished in the phase diagram. For large values of $J$ the system is phase separated. As a precursor to phase separation there is a region of width $\Delta J \sim t$ where the correlation exponent $K_\rho > 1$, and thus the superconducting correlations correspondingly dominate the long-range behavior. At smaller values of $J/t$, $K_\rho < 1$ and, therefore, the CDW correlations are dominant. Another important line is the boundary of the spin gap region (the line $\Delta = 0$ in the phase diagram). Although the lines of constant $K_\rho$ seem to be continuous at that boundary, a large change in the long-range correlations occurs there. A direct consequence is, of course, that the spin correlation functions change their space-time dependence from a power law in the TLL phase to an exponential form in the spin gap phase. A more noticeable effect is the jump in the exponents of charge and superconducting correlations. The charge exponent jumps from $1 + K_\rho$ to $K_\rho$, while the superconducting exponent $1 + 1/K_\rho \to 1/K_\rho$ (compare Eqs. (11) and (12)). As a consequence, the exponent of the most dominant correlations is always greater than or at least equal to unity in the spin gap phase. This means that the corresponding structure factor is divergent. On the other hand, in the TLL phase, even the most dominant exponent is less than unity, leading to a cusp in the structure factors instead of a divergent peak.
This implies a strong increase in the superconducting correlations in the spin gap region due to the repulsive interactions.

**VIII. CONCLUSIONS**

We have examined in detail the precursor region to phase separation for the 1D $t$-$J$ model including repulsive density-density interactions. These repulsive interactions, as expected, move the phase separation boundary to larger value of $J/t$ but at the same time open up a wider precursor region where strengthened superconducting correlations appear. Our numerical calculations confirm earlier reports of superconductivity in the precursor region and show clear evidence for the existence of a spin gap and an enhanced range of superconducting correlations for short-range repulsions. However, we find that the form of the repulsive interaction strongly influences the precursor region, and in certain cases, such as a long-range $1/r$-interaction, it favors a CDW state over a superconducting state.

What is the relevance of these results to the high-$T_c$ superconductors? At first sight, it might seem that our results have no relation with the cuprates since they have been obtained in 1D, at large $J/t$ and mainly at dopings $\rho = 1/2$ and $2/3$. However, note two important issues: first, recent work has shown that regarding superconductivity there is no drastic qualitative difference between 1D and 2D. Although there is no possibility of real long-range order in 1D, both in 1D and 2D superconducting correlations seem dominant in the same region, namely close to phase separation. Second, it has been observed that numerically the signals of superconductivity are maximized near quarter filling in both cases.

Then, it is possible to make some speculations about 2D models based on the results of the 1D systems. For example, note that in Fig. 3 the region where superconductivity dominates exists at dopings as close to half-filling as $\rho \sim 0.875$. However, the numerically calculated amplitude of the superconducting correlation decreases when $\rho$ changes from $1/2$ to $2/3$, as shown in Figs. 7 and 8. This result implies that superconductivity may exist near half-filling but is difficult to observe numerically through pairing-pairing correlation.
functions, mainly because the number of pairs contributing to superconductivity decreases to zero when \( \rho \to 1 \). Certainly, it could be that we have a similar situation in 2D, i.e. that the strip of superconductivity \( (K_\rho > 1) \) at quarter-filling reaches the neighborhood of half-filling, with a small order parameter hard to detect numerically. In the 2D \( t-J \) model phase separation near half-filling starts at a coupling close to \( J/t \sim 1 \), and thus the region of superconductivity may exist in the realistic region of \( J/t \sim 0.3 - 0.4 \) and low doping. We believe that it is very important to test these speculations.

**ACKNOWLEDGMENTS**

The quantum Monte Carlo calculations were done on the Cray Y/MP-464 of ETH Zürich. The exact diagonalization studies were performed on the NEC SX-3/22 of the Centro Svizzero di Calcolo Scientifico CSCS Manno, and also at the CRAY-2 of the National Center for Supercomputing Applications, Urbana, IL, USA. The work was supported by the Swiss National Science Foundation under grant number SNF 21-27894.89 and by an internal grant of ETH Zürich. We wish to thank F.F. Assaad, M. Imada, M. Luchini, A. Moreo, M. Ogata, and D. Würtz for helpful discussions.
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FIGURES

FIG. 1. Inverse compressibility for the \( t-J \) model, the \( t-J-V \) model (at \( V/t = 1 \)) and the \( t-J-V-V' \) model (at \( V/t = 1, V'/t = 0.5 \)) at quarter band filling on a chain with \( L = 16 \). The phase separation boundary \( (\kappa^{-1} = 0) \) is shifted towards larger \( J/t \) with inclusion of Coulomb repulsions.

FIG. 2. Phase diagram of the 1D \( t-J-V \) model at quarter filling. The thick line denotes the phase separation boundary. Contour lines of constant \( K_{\rho} \) (solid lines) and constant spin gap \( \Delta \) (dashed lines) are shown. The error of \( \Delta = 0 \) line is estimated about \( \Delta J \sim 0.5t \), while it is about \( \Delta J \sim 0.1t \) for the other \( \Delta \) and \( K_{\rho} \) lines. These contour lines were obtained from interpolating results on a grid with a spacing of 0.25\( t \) in the \( J \) and \( V \) direction.

FIG. 3. Phase diagram of the 1D \( t-J-V \) model in the \( \rho-J \) plane for \( V/t = 1 \). \( L = 16 \). The solid line is the phase separation boundary, and the others are contour lines of constant \( K_{\rho} \). These contour lines were obtained from interpolating results on a grid with a spacing of 0.25\( t \) in the \( J \) direction for systems with an even number of particles and CSBC. The errors on the \( K_{\rho} \)-lines are estimated to be smaller than \( \Delta J \sim 0.1t \)

FIG. 4. Finite size scaling of the spin gap in the \( t-J-V \) model for \( J/t = 9 \) and \( V/t = 3 \) at \( \rho = 1/2 \). Data for up to \( L = 20 \) are calculated by exact diagonalization with CSBC and OSBC. Data for \( L = 16, 24, 48 \) and 96 are calculated by QMC at an inverse temperature of \( \beta t = 24 \). Included are the extrapolations to the \( L \rightarrow \infty \) limit using polynomials of second, respectively third, order in \( 1/L \).

FIG. 5. The extrapolated spin gap along the line \( J = 3t + 2V \) in the \( t-J-V \) model at \( \rho = 1/2 \).

FIG. 6. Superconducting structure factor for the \( t-J-V-V' \) model for \( V/t = 1 \) and various values of \( V' \) at quarter band-filling. \( L=16 \) with CSBC.
FIG. 7. Superconducting structure factors of the \( t-J-V \), \( t-J-V' \), and the long-range repulsion models. (a) 10 particles on 20 sites \( (\rho = 1/2) \); (b) 12 particles on 18 sites \( (\rho = 2/3) \). Both CSBC and OSBC are used. The small peak around \( J/t = 8 \) for the long-range model is due to finite size effects and vanishes with increasing the system size. The jump seen for OSBC at \( J/t \sim 4 \) is due to a level crossing of the ground state. At small values of \( J/t \), the ground state is spin triplet for OSBC. With the opening of the spin gap, the singlet spin state becomes the ground state.

FIG. 8. (a), (b) Pairing correlations for the same models as in Fig. 7. at the \( J \)-values where the superconducting structure factor has its maximum for that model. Note that in the finite system this peak, while being close to the phase separation boundary, is actually at \( J \) values where the infinite system is phase separated. In the infinite system the peak is located exactly at the phase boundary. (c) Pairing correlations for \( L = 20 \) and \( \rho = 1/2 \) with CSBC for three different \( J \)-values: \( J/t = 3 \), where CDW correlations are dominant; \( J/t = 5 \) where superconductivity is dominant; and at \( J/t = 7 \), which is in the phase separated region. The increase of the pairing correlation for \( J/t = 7 \) at \( r = 10 \) is a finite size effect which vanishes when larger lattices are considered.

FIG. 9. Monte Carlo results of (a) charge and (b) spin structure factors in the \( t-J-V \) model at \( V/t = 1 \) for different values of \( J/t \). The lattice size was \( L = 96 \) sites with \( N = 48 \) particles, the inverse temperature \( \beta t = 24 \) or \( \beta t = 64 \). The imaginary time step \( \Delta t = 0.25 \) was chosen small enough to see the properties of the ground state.

FIG. 10. Charge and spin structure factors for the long-range model obtained by exact diagonalization. \( L = 20 \) and \( N = 10 \) with CSBC. (a) Charge structure factors for small values of \( J/t \). (b) Charge structure factors for large values of \( J/t \). (c) Spin structure factors for the entire coupling range.