Pairing fluctuations in a one-dimensional copper oxide model

E. B. Stechel
Sandia National Laboratories, MS-0345, Albuquerque, New Mexico 87185

A. Sudbø
Institutt for Fysikk, Norges Tekniske Høgskole, 7034 Trondheim-NTH, Norway

T. Giamarchi
Laboratoire de Physique des Solides, Universiteé Paris-Sud, 91405 Orsay, France

C. M. Varma
AT&T Bell Laboratories, Murray Hill, New Jersey 07974
(Received 16 May 1994)

The exact ground-state energy $E_0(\Phi)$ is calculated for a one-dimensional copper-oxide model defined on a ring of finite length L, threaded by an external flux Φ. It includes on-site and nearest-neighbor intersite Coulomb repulsion V, as well as a nonzero bare "oxide" gap Δ_0 between the orbitals in the unit cell. The correlation exponent K_ρ of the corresponding low-energy Hamiltonian shows that singlet (extended s-wave) superconductivity has the most rapidly diverging susceptibility as $T\to 0$ ($K_\rho > 1$). This superconducting phase is located close to a phase-separation instability of the model, indicated by $K_\rho \to \infty$. Longer range of the Coulomb interaction tends to frustrate phase separation, enhances the range of V for which $K_\rho > 1$, and slightly broadens the regime of V where $1 < K_\rho < \infty$.

I. INTRODUCTION

The discovery of high-T_c superconductivity in copper-oxide-based materials, has focused much attention on the physics of low-dimensional strongly correlated fermion systems with repulsive interactions. Since obtaining a correct description of the low-energy excitations in the normal state of these materials remains a theoretical challenge, obtaining an understanding of the mechanism by which superconductivity occurs also remains elusive.

Shortly after this discovery three distinct electronic models were proposed to describe the essential physics of the two-dimensional (2D) CuO sheets in the cuprates. Extensive investigation of these models have followed. Anderson suggested that the cuprates can be described by a 2D model with strong on-site Coulomb interactions between the electrons in the partially filled band of Cu $3d$ levels.[1] This is the well-known single-band Hubbard model, for which Lieb and Wu[2] provided an exact solution in 1D. A related model is the t-J model which can be derived from the Hubbard model in the limit $U/t \to \infty$, i.e., $J = 4t^2/U \ll 1$. The t-J model can be considered independent of the Hubbard model as a generic model for studying the interplay between charge and spin degrees of freedom. An exact solution is known in 1D at $J/t = 2$, where the ground state of the system is a dimerized spin liquid with no diverging superconducting pairing fluctuations.[3,4] (At $J/t = 2$ it is no longer obvious what connection, if any, the t-J model has to the Hubbard model.) Varma, Schmitt-Rink, and Abrahams (VSA) presented a 2D model consisting of three orbitals per unit cell,[5] namely the Cu $3d_{x^2-y^2}$, and oxygen $2p_x, 2p_y$. The model contains hopping between Cu and oxygen (t_{pd}) and a repulsive interaction at the Cu and oxygen sites (U_d and U_p, respectively.) In addition, it contains a nearest-neighbor copper-oxygen interaction V. Independently, Emery presented a closely related three-band model,[6] in which the parameter V was assumed to play no role. No rigorous results exist for the VSA or Emery models for general values of the parameters. Furthermore, the nature of their ground states is not known as yet in the entire parameter space or range of possible fillings (number of electrons per unit cell).

An important question is, which minimal microscopic Hamiltonian is necessary to correctly describe the various states of these materials? If one believes that an electronic mechanism is responsible for the observed superconductivity it is necessary to understand how repulsive Coulomb interactions can provide an effective attraction between the relevant electronic excitations. That this cannot happen for the 1D repulsive Hubbard model is well known.[2] We emphasize that this does not preclude the possibility of a superconducting ground state in the 2D one-band repulsive Hubbard model. However, if it is superconducting, the physics of the Hubbard model must be quite different in 2D than it is in 1D. The t-J model at large values of J/t can have diverging superconducting fluctuations, but large values of J/t essentially correspond to putting in an attractive interaction by hand, and the physics is thus *a priori* qualitatively different from that of the repulsive 1D Hubbard model. This is also obvious from the Bethe-ansatz solutions to both models in 1D: The t-J model at $J/t = 2$ exhibits complex pseudomomenta (which are the quantum numbers of the charge degrees of freedom, i.e, "holons") in the ground-state manifold. This is characteristic of bound or anti-

bound states, whereas the repulsive Hubbard model always exhibits real pseudomomenta for the holons, characteristic of scattering states.

Reference 5 argued that the three-band model with V included (hereafter denoted as the VSA model) is the minimum model necessary to describe the unconventional low-energy physics of the metallic ground states of the copper oxides. It was also argued that such fluctuations promote a superconducting instability. More recently, it was argued the repulsive interaction may also lead to the anomalous normal metallic-state properties of the high-T_c cuprates[7] which at half-filling (defined to be one hole per unit cell) are charge-transfer insulators.

Although the common structural element of the cuprate superconductors is the two-dimensional CuO_2 planes, for which the above models were developed, much work has been done on one-dimensional systems. The reasons are (i) 1D systems are easier to work with, and there is hope that intuition may be gained that could be relevant to higher-dimensional systems. For instance, if dominant superconducting fluctuations are found in a 1D system they will very likely also be found in 2D. (ii) A lowering of the dimensionality is expected to present an increasingly hostile environment for promoting superconducting pairing. For numerical purposes 1D systems are more convenient, since one can consider systems with larger linear dimensions.

In this paper, a brief version of which has been presented elsewhere,[8] we consider a 1D version of the VSA model of Eq. (1); in 1D it is a two-band model. The central question which we are interested in investigating is the role of the parameter V in inducing paring in 1D. This repulsive interaction will turn out to be crucial in inducing an effective attraction on O sites and will moreover be more effective in this respect in 2D than in 1D, as could be seen from a simple electrostatic argument. On a lattice, coherent single-particle hopping contributes a pair-breaking effect for real-space superconductive pairing (and other paired, but nonsuperconducting states), and this may be an increasingly efficient competing effect as the dimensionality is increased.[9] It is thus *a priori* not clear what the net effect on superconductivity an increase of dimensionality will have, although one expects that it in general is beneficial.

This paper is organized as follows. Section II defines the model we consider. Section III discusses the effects of twisted boundary conditions on ground-state energies and some transport coefficients. Pairing in nonsuperconducting states and phase separation is discussed in Sec. IV. Sections V and VI consider pairing correlators in general and in the 1D Cu-O model, respectively.

II. THE MODEL

The 1D version of the copper-oxide model is defined by

$$H_{\mathrm{CuO}}=T(\Phi)+\Delta\sum_i[n_{p,i}-n_{d,i}]+U_d\sum_i n_{d,i,\uparrow}n_{d,i,\downarrow}+U_p\sum_i n_{p,i,\uparrow}n_{p,i,\downarrow}+V\sum_i n_{d,i}[n_{[p,i-1}+n_{p,i}]\ . \tag{1}$$

In Eq. (1), we have

$$n_{\alpha,i}=\sum_\sigma n_{\alpha,i,\sigma}=\sum_\sigma c^\dagger_{\alpha,i,\sigma}c_{\alpha,i,\sigma}\ , \tag{2}$$

where α denotes an orbital index [$\alpha\in(d,p)$], and σ a spin index [$\sigma\in(\uparrow,\downarrow)$]. Throughout, $\sum_i$ is taken to run over unit cells, chosen such that the oxygen is to the right of copper. We have introduced the parameter $\Delta\equiv(E_p-E_d)/2$, with $E_p>E_d$ in a hole notation, where E_p and E_d are site energies on the oxygen and copper sites, respectively, and the zero of energy has been chosen at $(E_p+E_d)/2$. The quantity $T(\Phi)$ is the kinetic energy operator of the system in the presence of an external flux Φ, and will be specified below. The model defined by Eq. (1) contains the Emery-model and the one-band Hubbard model, as well as the extended Hubbard model as special cases: The Emery model has $V=0$. The one-band Hubbard and the extended Hubbard models have $E_p=E_d$ and $U_p=U_d$. The one-band Hubbard model additionally has $V=0$.

The model of Eq. (1) with $T(\Phi)=0$ is exactly solvable for arbitrary L in 1D by the transfer-matrix method straightforwardly[10] ("atomic limit"); in the most general case it can be mapped onto a 1D classical $S=\frac{15}{2}$ Ising chain. The free energy and static charge-correlation functions can be calculated from the eigenvalues and eigenvectors of the transfer matrix. In the thermodynamic limit, the results further simplify in that only the largest (nondegenerate) eigenvalue, λ_M, is needed. The transfer matrix of the VSA atomic chain is given by

$$\begin{aligned}T_{i,i+1}&=e^{G_{i,i+1}}\ ,\\ G_{i,i+1}&=U_p\sum_i n_{p,i}+U_d\sum_i n_{d,i}\\ &\quad+V\sum_i n_{d,i}[n_{p,i}+n_{p,i-1}]\ ,\end{aligned} \tag{3}$$

and the free energy is given by

$$f=-\frac{1}{\beta}\ln\lambda_M\ , \tag{4}$$

when the maximum eigenvalue λ_m of the transfer matrix $T_{i,i+1}$ is assumed to be nondegenerate.

In the above "atomic" limit, it was found that for large values of U_d compared to U_p and Δ, and density away from half-filling, increasing V to $\mathcal{O}(\Delta)$ leads to a combined charge-transfer and phase-separation instability. In this instability, the average charge on the p orbitals increases at the expense of charge on the d orbitals. The former are either nearly doubly occupied or empty, as reflected by the compressibility tending to infinity. Mean-field calculations also show such instabilities with finite kinetic energy,[11] but in addition reveal a region of parameters where s-wave superconductivity exists without being preempted by phase separation. A central question is whether one can see in exact calculations that kinetic energy favors superconductivity over charge-transfer or phase-separation instabilities for any filling N and in any region of the parameter space with purely repulsive bare interactions. [We define the parameter

space of the VSA model as $\Lambda=(U_d,U_p,V,\Delta,t_{pd},N)$.] The possibility of superconducting pairing in a model with purely repulsive interactions is of fundamental interest independent of its applicability to the high-T_c oxides.

To explore these issues, we have considered the ground-state energy $E_0(\Phi)$ of the Hamiltonian of Eq. (1), in a ring geometry with $L/2$ number of Cu-O unit cells (L even, is the total number of sites in the problem). The ring is threaded with a flux Φ by applying a constant vector potential of magnitude

$$A=\frac{\hbar c}{e}\frac{\Phi}{L}\ , \tag{5}$$

along its circumference. The effect of such a vector potential is included by a gauge transformation (taking $\hbar=e=c=1$), $c_{\alpha,m,\sigma}\rightarrow c_{\alpha,m,\sigma}\exp(im\Phi/L)$; Φ is measured in units of 2π throughout. Thus, we have

$$T(\Phi)=-t_{pd}\sum_{i,\sigma}[e^{i\Phi/L}c^{\dagger}_{d,i,\sigma}c_{p,i,\sigma} +e^{-i\Phi/L}c^{\dagger}_{d,i,\sigma}c_{p,i-1,\sigma}+\text{H.c.}]\ . \tag{6}$$

The usefulness of threading the ring with a flux will become apparent shortly.

A remark on our choices of parameters in the model Eq. (1) is appropriate here. We are basically interested in providing an existence proof for dominant superconducting pairing fluctuations *in any parameter regime* of this model with purely repulsive Coulomb interactions. We are willing to abandon a so-called "realistic" region of the parameter space in order to possibly capture some of the basic physics of 2D in our 1D model. Our choices for parameter ranges are as follows: most calculations have fixed $U_d=10$, $U_p=0$, $\Delta=1$, and $t_{pd}=1$, while we choose $V\in[1,4]$. The large value of $U_d=10$ is chosen to effectively eliminate the possibility of doubly occupied Cu sites. The small value of U_p is chosen to facilitate an attraction on oxygen sites induced by a nearest-neighbor Coulomb interaction V when this becomes of order the oxide gap Δ. Increasing U_p to a more "realistic" value requires larger values for V to produce attraction on oxygen sites; however, the essential mechanism for pairing is qualitatively the same. We have fixed $\Delta=1$ throughout the calculations in order to produce a charge-transfer insulator at half-filling. (Recall that half-filling is defined to be one hole per unit cell.) In Sec. VI we do, however, consider the effect on the regime of parameters V on increasing the values of U_p. We also consider longer-range Coulomb interactions. These perturbations to the model Eq. (1) do not change our main conclusion that a sizeable $V\sim\Delta$ is the essential component necessary to produce "superconductivity" in this 1D lattice model.

III. TWISTED BOUNDARY CONDITIONS

From the ground-state energy $E_0(\Phi)$ one obtains information about flux quantization and possible superconductivity: In a normal one-dimensional ring, the ground-state energy is a periodic, even function of Φ with period $\Phi_0\equiv hc/e$. If the flux Φ is measured in units of the flux quantum Φ_0, we then have

$$E_0(\Phi)=E_0(\Phi+n),\quad n=0,\pm1,\pm2,\ldots\ . \tag{7}$$

Hence, for a normal metallic phase, the system has stable phases at particular values of the flux, $\Phi=0,\pm1,\pm2\ldots$, leading to flux quantization in units of hc/e.[12] In a superconducting state, the system also has

$$E_0(\Phi)=E_0\left[\Phi+\frac{n}{2}\right] \tag{8}$$

in the thermodynamic limit $L\rightarrow\infty$, showing that new stable phases appear also at $\Phi=\pm1/2,\pm3/2,\ldots$. In systems exhibiting superconductivity flux is thus quantized in units of $\Phi_0/2=hc/2e$,[12] hereafter referred to as anomalous flux quantization. Although superconducting pairing undoubtedly will give anomalous flux quantization, such flux quantization appears to be a necessary, but not sufficient requirement for the existence of *singlet* superconductivity in a system. This will be discussed further in the next section.

Another quantity of interest that should be considered in conjunction with Eq. (8) for the purpose of detecting superconductivity is the charge stiffness D of a 1D system, defined via the real part of the frequency-dependent conductivity in a translationally invariant system:

$$\sigma_r(\omega)=D\delta(\omega)+\frac{\pi e^2}{L}\sum_{m\neq0}\frac{|\langle m|j_p|0\rangle|^2}{E_m-E_0}\times\delta(\omega-(E_m-E_0))\ , \tag{9}$$

where the paramagnetic current in the presence of a flux Φ piercing the ring is given by

$$j_p(\Phi)=-it_{pd}\sum_{i,\sigma}[e^{i\Phi/L}c^{\dagger}_{d,i+1,\sigma}c_{p,i,\sigma} +e^{i\Phi/L}c^{\dagger}_{p,i,\sigma}c_{d,i,\sigma}-\text{H.c.}]\ . \tag{10}$$

Remarkably, the transport coefficient D may be obtained from the ground-state energy by considering the change under an infinitesimal twist in boundary conditions in the many-body wave function as one fermion is moved once around the ring[13,14] thereby acquiring a phase Φ:

$$\Psi(x_1,\ldots,x_{i+L},\ldots,x_N)=\exp(i\Phi)\Psi(x_1,\ldots,x_i,\ldots,x_N)\ . \tag{11}$$

Using arguments originally due to Kohn,[13] and refined by Shastry and Sutherland,[14]

$$D(L)=\left.\frac{\partial^2[LE_0(\Phi)]}{\partial\Phi^2}\right|_{\Phi=0}\ . \tag{12}$$

A necessary requirement for considering the system as superconducting or perfectly conducting is that $\lim_{L\rightarrow\infty}D(L)\neq0$. This is a minimal requirement for having zero resistivity in the system, which should be the case both for a superconductor and a perfect conductor. (Even if $D=0$, the regular part of the conductivity [the second term on the right-hand side of Eq. (9)] could ap-

proach a finite constant as $\omega \to 0$ in which case the system would be an ordinary dirty metal and not an insulator.) Equations (8)–(12) are useful diagnostic tools when looking for superconductivity in the VSA model Eq. (1). Note, however, that the quantity D in a 1D system cannot under any circumstance be interpreted as a Meissner fraction of the system; the Meissner effect is not operative in 1D and thus unfortunately does not lend itself as a useful diagnostic tool when trying to distinguish between perfect conductivity and superconductivity in 1D systems. Nevertheless, by utilizing the Luttinger-liquid framework in 1D, an alternative diagnostic tool for detecting dominant superconducting fluctuations is available to us. This will be discussed in Sec. V.

IV. PAIRING IN NONSUPERCONDUCTING GROUND STATES

In numerical approaches that necessarily are limited in system size L, one should bear in mind that nonsuperconducting states may produce anomalous flux quantization. In some cases, this turns out to be a pure finite size effect, in other cases it may be indicative of a paired state that is not superconducting, such as charge-density waves (CDW) that are pinned by commensuration effects (such commensuration effects are forced upon us in small systems), or paired but phase-separated states.

A surprising feature is, for instance, that even *repulsive* one-band Hubbard chains of finite length may show anomalous flux quantization, a feature which has also been noted by others.[15] Such a situation might at first seem to pose serious problems for an interpretation of anomalous flux quantization in terms of a paired state of some kind: In a Bethe-ansatz solution, bound two-particle states require complex pseudomomenta to appear as solutions to the Bethe-ansatz equations in the ground-state manifold. For the repulsive one-band Hubbard model, it is well known[2] that such complex solutions only appear in the excitation spectrum when $L \to \infty$, and correspond to antibound states. In the attractive Hubbard model, they do appear in the ground-state manifold, and in this case lead to dominant superconducting fluctuations even when $L \to \infty$. We have verified that no anomalous flux quantization occurs in the repulsive Hubbard model when states of a given total spin S are considered for all Φ. Were we not to work in a subspace of fixed S, we would find a level crossing between states with $S=0$ and $S=1$, and hence $E_0(\Phi)=E_0(\Phi+n/2)$.[8] The crossing in energy of states of different spin S occurs due to degeneracies in finite systems, and associated Hund's rule effects. More recently, this has also been confirmed on the 2D repulsive and attractive Hubbard model.[16]

A tendency to anomalous flux quantization in CDW ground states in finite rings was pointed out in Refs. 17 and 18. The competition between CDW and singlet superconductivity will be discussed further below, when considering correlation functions. At a phase-separation instability, the compressibility of the system diverges, i.e.,

$$\kappa^{-1}=\frac{N^2}{L}\left[\frac{E_0(N+2)+E_0(N-2)-2E_0(N)}{4}\right]=0 . \tag{13}$$

In the context of the VSA model Eq. (1), one would conclude (see below) that a near-phase separation would put the physical system in a region of parameters V that should be favorable for producing superconductivity. Indeed this was found in mean-field calculations on a 2D analog of the lattice model of Eq. (1).[11] A near-"pinning" of the chemical potential as a function of doping may have been observed in photoemission and inverse photoemission experiments.[19]

The most direct way to look for phase separation is through the consideration of multibody bound states. As mentioned above, a finite-size scaling analysis of the charge stiffness as a function of system would also yield useful information on this. Due to limitations in system size, neither of these methods are practical for our purposes. We therefore proceed by another route. Using Eq. (13) and the above considerations in conjunction with the first of Eqs. (24) (see below), it is clear that a reasonable idea of the differentiation between superconductivity and phase separation may be obtained by considering the divergence of the Luttinger-liquid correlation exponent K_ρ, which we discuss next. The parameter regime leading to either dominant superconducting pairing fluctuations, or phase separation, may thus be considered with the same method.

V. PAIRING CORRELATORS AND CORRELATION EXPONENTS

To investigate the possibility of dominant superconducting fluctuations at $T=0$ in a 1D model, we consider the expectation value in the ground state of the equal time singlet superconductivity (SS) pairing correlation function:

$$\begin{aligned} &C_{\mathrm{SS}}(|i-j|)=\langle \Delta_i^{+}\Delta_j \rangle , \\ &\Delta_i=\frac{1}{\sqrt{2}}[c_{p,i,\uparrow}c_{p,i,\downarrow}-c_{p,i,\downarrow}c_{p,i,\uparrow}] , \end{aligned} \tag{14}$$

as well as the correlation function for formation of charge density waves (CDW):

$$\begin{aligned} &C_{\mathrm{CDW}}(|i-j|)=\langle n_{p,i}n_{p,j} \rangle , \\ &n_{p,i}=\sum_{\sigma} c^{\dagger}_{p,i,\sigma}c_{p,i,\sigma} . \end{aligned} \tag{15}$$

We consider these correlation functions defined on oxygen sites, and not on Cu sites, due to the large onsite Coulomb repulsion we impose on the Cu sites. The above correlators are certainly the dominant ones in the problem. For zero pairing amplitude on Cu, the mean-field gap must satisfy $\sum_k \Delta(k)=0$. This means that we are examining the instability towards extended even-parity pairing in 1D.

In the Luttinger liquid,[20] the correlation functions for singlet superconductivity and charge-density waves decay asymptotically as power laws:

$$\begin{aligned} &C_{\mathrm{SS}}(x)=\frac{A}{x^{\alpha_{\mathrm{SS}}}} , \\ &C_{\mathrm{CDW}}(x)=\frac{B}{x^2}+C\frac{\cos(2k_F x)}{x^{\alpha_{\mathrm{CDW}}}} , \end{aligned} \tag{16}$$

up to logarithmic corrections. The exponents α_{SS} and α_{CDW} are nonuniversal; they are determined by the interactions in the problem. A, B, and C are model-dependent constants, and k_F is the Fermi wave vector. The correlation function with the slowest decay will determine which instability dominates. Hence, if $\alpha_{SS} < \alpha_{CDW}$, the dominant diverging fluctuations will be singlet superconducting fluctuations. We define in the standard way generalized susceptibilities associated with the correlator Eqs. (16), as

$$\chi(q,\omega) = \int\int dx\, dt\, C(x,t) \exp[i(qx - \omega t)] . \tag{17}$$

Due to the formal Lorentz invariance of the Luttinger liquid, we find $\lim_{q\to 0}\chi(q,\omega) \sim \omega^{\alpha-2}$, and hence

$$\lim_{T\to 0}\chi(T) \sim T^{\alpha-2} . \tag{18}$$

Furthermore, α_{SS} and α_{CDW} are related in a way that depends on whether the spin excitation spectrum is gapped or not. For ungapped spin excitations,

$$\alpha_{SS} = 1 + K_\rho^{-1}; \quad \alpha_{CDW} = 1 + K_\rho . \tag{19}$$

In contrast, when the spin-excitation spectrum is gapped,

$$\alpha_{SS} = K_\rho^{-1}; \quad \alpha_{CDW} = K_\rho , \tag{20}$$

where K_ρ is a model-dependent constant which sets the scaling dimension of all correlation functions.[20] A gap in the spin-excitation spectrum is seen in the 1D VSA model using the bosonization technique in the weak-coupling regime $[U_d, U_p, V] \ll t_{pd}$. The criterion for opening up such a gap in this weak-coupling regime is given by[8]

$$\tfrac{1}{2}[U_d + U_p] + 2V\cos(2k_F) < 0 . \tag{21}$$

This criterion demonstrates a generic feature in this model, namely that when the system is doped beyond half-filling, a positive critical value $V \geq V_c$ is required to open up a spin gap. We do not expect the precise value of V_c to be accurately determined from bosonization in the strong-coupling regime considered numerically in this paper.

Assuming a gapped spin-excitation spectrum for the 1D VSA model, we get from Eqs. (16) and (20) that the criterion for having dominant diverging superconducting fluctuations as $T \to 0$ in the system is given by

$$K_\rho > 1 . \tag{22}$$

This is a more unambiguous criterion for dominant superconductive pairing fluctuations than Eq. (8), on which emphasis was put.[8]

In the spin-gapped situation, divergent SS and CDW fluctuations may coexist. Without a spin gap in the excitation spectrum, the SS and CDW fluctuations are mutually exclusive. Note also that phase separation, using the results of the previous section, is signaled by the condition

$$K_\rho \to \infty , \tag{23}$$

regardless of the structure of the spin-excitation spectrum. Similar equations have been used to study the differentiation between superconductivity and phase separation in the 1D t-J model.[21]

A suitable algorithm is needed for the computation of the correlation exponent K_ρ, valid also in the strong-coupling regime. A method to do this was pioneered many years ago for the spinless problem,[22,23] and recently revived by Schulz[24] for the Hubbard model. The idea is to extract information about the power-law decay of correlation functions in the Luttinger liquid avoiding the formidable task of their direct calculation. K_ρ is obtained from $E_0(\Phi, N)$ via the two relations

$$\begin{aligned} \frac{\partial^2[LE_0(N)]}{\partial^2 N^2} &= \frac{\pi}{2}\frac{u_\rho}{K_\rho} = \kappa^{-1} , \\ \frac{\partial^2[LE_0(\Phi)]}{\partial^2 \Phi^2} &= 2u_\rho K_\rho = D . \end{aligned} \tag{24}$$

The first relation is the inverse compressibility, the second relation will be recognized as the charge stiffness. As mentioned above, it cannot be interpreted as the superfluid stiffness since the Meissner effect is absent in 1D. (For an appropriate method of extracting the Meissner fraction in 2D, see Ref. 25.) The above two equations essentially provide the substitute for the Meissner effect in 1D as a diagnostic tool in looking for dominant superconducting fluctuations.

We now concentrate on deriving information about dominant superconducting fluctuations from a calculation of K_ρ rather than a direct calculation of $C_{SS}(x)$ and $C_{CDW}(x)$. The reason for this is that finite-size effects affect K_ρ less dramatically than $C_{SS}(x)$ and $C_{CDW}(x)$. This is because K_ρ is determined only be the ground-state energy (see below) and not by the ground-state wave function. We, however, have no proof of this for the present model since no exact solution exists that would make it possible to determine the $L \to \infty$ limit. Nonetheless, the Hubbard chain with $L = 8, N = 6$ gives the value for K_ρ to within 5% of the thermodynamic limit.[24] The supersymmetric t-J model produces similar results.[4]

For the Luttinger liquid one can make the following general statement: Since the first relation in Eq. (24) is precisely the inverse compressibility of the system, a small K_ρ simultaneously suppresses the tendency towards superconductivity and towards phase separation, whereas large K_ρ enhances both tendencies. Consequently, in a Luttinger liquid, superconducting and phase-separation instabilities will be found in the same general region of parameter space.

VI. PAIRING CORRELATIONS IN THE 1D VSA MODEL

It is instructive to first give the result for the correlation exponent K_ρ obtained for the 1D VSA model, Eq. (1), using the weak-coupling bosonization technique, where K_ρ is found to be given by

$$K_\rho = \left[\frac{v_F}{v_F + \alpha_+ U/\pi + \alpha_- 4V/\pi + 2\alpha\Delta U/\pi - 2V\cos(2k_F)/\pi} \right]^{1/2},$$

$$\alpha_\pm = 1 \pm \frac{\Delta^2}{e_{k_F}^2 + \Delta^2}, \tag{25}$$

$$\alpha = \frac{\Delta}{\sqrt{e_{k_F}^2 + \Delta^2}},$$

where we have introduced $v_F = t_{pd}^2 \cos k_F \sin k_F / \sqrt{e_{k_F}^2 + \Delta^2}$, $U = (U_d + U_p)/2$, and $\Delta U = (U_d - U_p)/2$, and e_{k_F} is the Fermi energy of the noninteracting case. At half-filling, $k_F = \pi/4$. Beyond half-filling, such that $\cos(2k_F) > 0$, i.e., $\pi/4 < k_F < 3\pi/4$, and $U_d > U_p$, we see immediately that in the weak-coupling regime, where the bosonization approach is reliable, $K_\rho < 1$. In this weak-coupling regime, the 1D VSA model thus does not exhibit dominant superconducting pairing fluctuations. This is consistent with our numerical findings, to be presented below, where sizeable values $V \sim \Delta$, as well as an essential suppression of doubly occupied Cu sites in order to induce an effective attraction on oxygen sites, are required to produce $K_\rho > 1$. This puts the model in its strong-coupling regime.

We next consider numerical results obtained for the strong-coupling regime by Lanczos-diagonalization of finite chains. In Fig. 1, we show the correlation exponent K_ρ as a function of the parameter V for the system $L = 12, N = 10$, found via $E_0(\Phi, N)$ using Eqs. (24). It is seen to exceed the value $K_\rho = 1$ at a critical value $V \sim 2$. The result $K_\rho > 1$ implies that the generalized CDW susceptibility is less divergent at $T = 0$ than that of SS. Singlet superconductivity is thus found to be the dominating instability in a narrow region of parameter space where at least it is not obvious that the system has yet phase separated. Similar results have recently been reported.[26]

Since pairing in this model crucially depends on an effective attraction on oxygen sites, it is of interest to consider the effect of a nonzero on-site Coulomb repulsion U_p on oxygen sites. This is shown in Figs. 1(a) and 1(b). It is clear that an increase in U_p up to as large values as ~ 3 still allows pairing, provided that V is also increased. As expected, increasing U_p tends to suppress K_ρ and superconductive pairing. Note, however, that an increase of U_p to large values will ultimately destroy the spin gap in the system and replace Eq. (20) with Eq. (19). In this case, SS and CDW are strictly mutually exclusive.

In order to mimick the effect of longer-range Coulomb interactions, we have also considered the effect of adding a next-nearest-neighbor term to the Hamiltonian

$$H = H_{\mathrm{CuO}} + V_d' \sum_i n_{d,i} n_{d,i+1} + V_p' \sum_i n_{p,i} n_{p,i+1}, \tag{26}$$

where, again, $\sum_i$ is taken to run over unit cells. We will for simplicity consider the case $V_d' = V_p' = V'$. With increasing V', we find that the critical value of V where the compressibility tends to diverge rapidly is pushed to larger values. For given V, the inverse compressibility $\pi u_\rho / 2K_\rho$ increases with V'. Hence, the long-range part of the Coulomb interaction tends to reduce the compressibility and thus frustrate a tendency to static phase separation. Computing also the charge stiffness as a function of V with various V', we again extract the correlation exponent K_ρ. Fixing V and increasing V', it is clear that K_ρ *decreases,* as illustrated in Fig. 2. Longer-range Coulomb interactions as modeled here thus do not appear to promote singlet superconducting pairing correlations in the 1D copper-oxide model.[27] In our picture, this follows naturally from the fact that the third term in Eq.

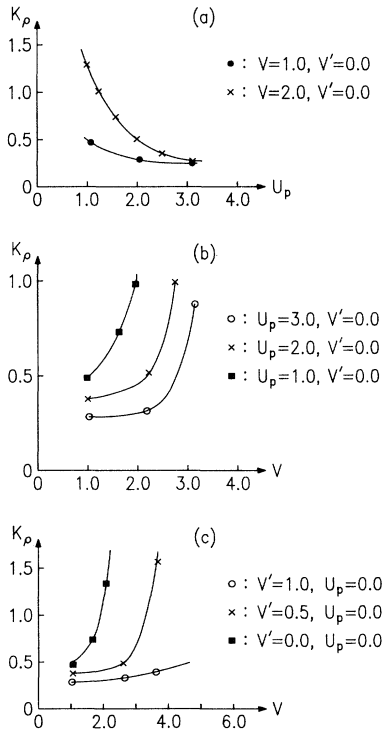

FIG. 1. Correlation exponent for the VSA model at fixed filling $N/L = 10/12$. (a) K_ρ as a function of U_p for various values of V, V'. Note that $K_\rho > 1$ for nonzero values of U_p. (b) K_ρ as a function of V for various values of U_p at fixed value $V' = 0$. Again, a value $K_\rho > 1$ is evident. (c) K_ρ as a function of V for various values of V' at fixed $U_p = 0$. K_ρ in this case typically becomes larger than 1 at smaller values of V than for finite U_p, as expected.

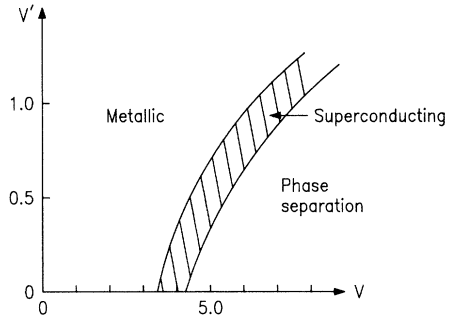

FIG. 2. Schematic phase diagram for the 1D copper-oxide model of Eq. (1), at fixed filling $\rho = L/N > 1/2$.

(26) in particular tends to suppress configurations which are dominated by doubly occupied oxygen sites. However, as seen from the curves for K_ρ in Fig. 1, the curves generally pass through the value $K_\rho = 1$ with *decreasing* slope as V' increases. This means that the region of superconductivity in the parameter space (V, V'), located between the metallic state at small V and the paired, but phase-separated state at larger V, at given filling becomes broader as V' increases. The resulting phase diagram in the parameter space (V, V') at fixed filling, is shown schematically in Fig. 2.

VII. CONCLUSION

The possibility of dominant divergent superconducting pairing fluctuations as $T \to 0$ has been investigated in a 1D copper-oxide model including two orbitals per unit cell, with a nearest-neighbor Coulomb repulsion V between copper and oxygen sites. Pairing in this 1D CuO model Eq. (1) is induced by V of the order of the charge transfer gap $\Delta \equiv (E_p - E_d)/2$. Similar results were found in 2D by approximate methods.[11] The ground state of the model in the relevant parameter regime has total spin $S = 0$, and the intersite interaction V effectively produces an attraction on oxygen sites, leading to pairing. To investigate the nature of the paired state, we calculated the Luttinger-liquid correlation exponent K_ρ as a function of the intersite Coulomb interaction V. The evaluation of K_ρ provides a substitute to distinguish between perfect conductivity and superconductivity in a 1D system, where the Meissner effect is not operative. Moreover, since K_ρ is calculated from the ground-state energies, without explicit use of any wave functions, we expect finite-size effects to be small. This would not be the case if K_ρ was extracted directly from calculations of correlation functions.

We find slow algebraic decay of the correlator for superconductivity on oxygen sites as well as a slow algebraic decay of the CDW correlator. In the 1D VSA model at $T = 0$ the dominant instability has been shown to be due to superconducting pairing by a detailed analysis of the correlation exponent K_ρ. These dominant superconducting fluctuations are found in a parameter regime (Δ, V, N) that locates the system close to a phase-separation instability of the model. Including longer-range Coulomb interactions $V' \lesssim 1.0$, as well as a finite on-site correlation energy on oxygen sites $U_p \lesssim 1.0$ tends to enhance the critical value V above which superconductivity occurs, but broadens the regime of the parameter V where the model shows dominant superconducting fluctuations.

The model of Eq. (1), although intended primarily to describe the 2D CuO_2 planes, is also relevant for realistic 1D systems, such as the alloy $[(TMTSF)_{0.5}(TMTTF)_{0.5}]_2RO_4$.[28] The "copper" and the "oxygen" used here would now represent the TMTTF and TMTSF molecules, respectively. These molecules have band structures and interactions similar to the ones discussed in this paper, but with a nonzero repulsion on the "oxygen." Unfortunately, the above compound is chemically constrained to half-filling and is thus an insulator. Our results tend to suggest that doping, if it becomes feasible in this or similar 1D compounds, should produce interesting effects and possibly superconductivity.

ACKNOWLEDGMENTS

E.B.S. acknowledges support from DOE-BES, Contract No. DE-AC04-76-DP00789, and A.S. acknowledges support from the Norges Forskningsråd, Grant No. 101172-432. E.B.S. acknowledges useful discussions with R. M. Fye.

[1]P. W. Anderson, Science **235**, 1196 (1987).
[2]E. H. Lieb and F. Wu, Phys. Rev. Lett. **21**, 112 (1968).
[3]B. Sutherland, Phys. Rev. B **12**, 3795 (1975).
[4]P. A. Bares and G. Blatter, Phys. Rev. Lett. **64**, 2231 (1990); P. A. Bares, G. Blatter, and M. Ogata, Phys. Rev. B **44**, 130 (1992).
[5]C. M. Varma, S. Schmitt-Rink, and E. Abrahams, Solid State Commun. **62**, 681 (1987).
[6]V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987).
[7]A. E. Ruckenstein and C. M. Varma, Physica C **185-189**, 134 (1991).
[8]A. Sudbø, C. M. Varma, T. Giamarchi, E. B. Stechel, and R. T. Scalettar, Phys. Rev. Lett. **70**, 978 (1993); C. M. Varma and A. Sudbø, J. Phys. I (France) **3**, 585 (1993).
[9]M. Grilli, R. Raimondi, C. Castellani, C. Di Castro, and G. Kotliar, Phys. Rev. Lett. **67**, 259 (1991).
[10]A. Sudbø, S. Schmitt-Rink, and C. M. Varma, Phys. Rev. B **46**, 5548 (1992).
[11]P. B. Littlewood, Phys. Rev. B **42**, 10075 (1990); S. N. Coppersmith and P. B. Littlewood, *ibid.* **41**, 2646 (1990), and Ref. 9.
[12]N. Byers and C. N. Yang, Phys. Rev. Lett. **7**, 46 (1961).
[13]W. Kohn, Phys. Rev. **133**, A171 (1964).
[14]B. S. Shastry and B. Sutherland, Phys. Rev. Lett. **65**, 243

(1990).
[15]R. M. Fye, M. J. Martins, D. J. Scalapino, J. Wagner, and W. Hanke, Phys. Rev. B **44**, 6909 (1991).
[16]F. Assaad, W. Hanke, and D. J. Scalapino, Phys. Rev. Lett. **71**, 1915 (1993).
[17]E. N. Bogachek, I. V. Krive, I. O. Kulik, and A. S. Rozhavsky, Phys. Rev. B **42**, 7614 (1990).
[18]A. Feretti, I. O. Kulik, and A. Lami, Phys. Rev. B **45**, 5486 (1992).
[19]J. W. Allen *et al.* (unpublished).
[20]J. Solyom, Adv. Phys. **28**, 209 (1979).
[21]M. Ogata, M. U. Luchini, S. Sorella, and F. F. Assaad, Phys. Rev. Lett. **66**, 2388 (1991).
[22]A. Luther and I. Peschel, Phys. Rev. B **12**, 3908 (1975).
[23]F. D. M. Haldane, Phys. Rev. Lett. **45**, 1358 (1980); **47**, 1840 (1981).
[24]H. J. Schulz, Phys. Rev. Lett. **64**, 2831 (1990).
[25]D. Scalapino, S. White, and S. Zhang, Phys. Rev. Lett. **68**, 2830 (1992).
[26]K. Sano and Y. Ono, Physica C **205**, 170 (1993).
[27]Recently, a Lanczos calculation was presented which used a $1/r$ potential added to H_{CuO}. J. Riera and E. DaGotto (unpublished).
[28]V. Ilakovac *et al.*, Phys. Rev. Lett. **50**, 7136 (1994).