Flux Quantization and Pairing in One-Dimensional Copper-Oxide Models

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We obtain the ground-state energy $E_0(\Phi)$ exactly as a function of flux Φ in a one-dimensional "copper-oxide model" on rings of finite circumference L, including on-site interactions and a nearest-neighbor interaction V. For V of the order of the charge-transfer gap or larger, the model extrapolated to large L exhibits flux quantization with charge $2e$, and a slow algebraic decay of the singlet superconducting correlation function on oxygen sites. The extrapolated superfluid stiffness appears, however, finite only for not too large V. These results suggest a superconductive state at V of order the charge-transfer gap of the model, but a paired and phase-separated state at larger V.

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Shortly after the discovery of superconductivity in copper-oxide–based materials, three distinct electronic models were proposed, which have since been extensively investigated. Anderson suggested that the essential physical features of the materials can be modeled by the two-dimensional (2D) one-band Hubbard model [1]. Varma, Schmitt-Rink, and Abrahams (VSA) presented a 2D model consisting of three orbitals per unit cell [2], namely, the Cu $3d_{x^2-y^2}$, and oxygen $2p_x, 2p_y$ with hopping between them, a repulsive interaction on Cu sites, U_d, and on oxygen sites, U_p, as well as a nearest-neighbor copper-oxygen interaction V. Independently, Emery presented a closely related three-band model [3], in which the parameter V was assumed to play no role. In Ref. [2], it was argued that the three-band model with V included (hereafter denoted as the VSA model) is the minimum model necessary to characterize the essential properties of the materials. In particular, the parameter V was shown to be important in inducing low-energy charge fluctuations in the metallic state. It was also argued that such fluctuations promote a superconducting instability and more recently that they may also lead to the anomalous normal metallic-state properties of the high-T_c cuprates [4], which at half filling are charge-transfer insulators. In this paper, we demonstrate that the parameter V is central in inducing pairing at $T=0$ in the one-dimensional (1D) version of the three-band model.

The 1D version of the VSA model may be written as $H=H_0+H_U+H_V$, where

$$
\begin{aligned}
H_0 &= T(\Phi)+\Delta\sum_i [n_{p,i}-n_{d,i}]\,,\\
H_U &= U_d\sum_i n_{d,i,\uparrow}n_{d,i,\downarrow}+U_p\sum_i n_{p,i,\uparrow}n_{p,i,\downarrow}\,, \qquad (1)\\
H_V &= V\sum_i n_{d,i}[n_{p,i-1}+n_{p,i}]\,.
\end{aligned}
$$

Here, $n_{\alpha,i}=\sum_\sigma n_{\alpha,i,\sigma}=\sum_\sigma c^\dagger_{\alpha,i,\sigma}c_{\alpha,i,\sigma}$, where α denotes an orbital index [$\alpha\in$ (Cu,O)], 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 $(E_p+E_d)/2$. Furthermore, 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 of Eq. (1) with $T(\Phi)=0$ is exactly solvable for arbitrary L in 1D by the transfer-matrix method [5]. For U_d large 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 the 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 [6], 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, through exact calculations, that kinetic energy favors superconductivity over the charge-transfer/phase-separation instabilities for any filling N and in *any* region of the parameter space (U_d,U_p,V,Δ), with *purely repulsive* bare interactions.

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 being an even integer representing the total number of sites in the problem). The ring is threaded with a flux Φ by applying a constant vector potential of magnitude $A=(\hbar c/e)\Phi/L$ along its circumference. The effect of the vector potential $A=(\hbar c/e)\Phi/L$ 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

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

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 $E_0(\Phi)=E_0(\Phi+n)$; $n=0,\pm 1,\pm 2,\ldots$. Hence, for a normal metallic phase, one then has *stable phases* at particular values of the flux, $\Phi=0,\pm 1,\pm 2,\ldots$, leading to flux quantization in units of hc/e [7]. In a *superconducting* state one further has $E_0(\Phi)=E_0(\Phi+n/2)$ in the thermodynamic limit $L\to\infty$, showing that *new* stable phases appear also at $\Phi=\pm\frac{1}{2},\pm\frac{3}{2},\ldots$, in addition to the ones at $\Phi=0,\pm 1,\pm 2,\ldots$ in the normal metallic state. In systems exhibiting superconductivity, flux is thus quantized in units of $\Phi_0/2=hc/2e$ [7], hereafter referred to as *anomalous flux quantization.*

Recently, the ground-state energy $E_0(\Phi)$ for the repulsive and attractive one-band Hubbard ring with finite circumference L and on-site interactions only, was considered in detail [8]. This model is exactly integrable for arbitrary flux Φ, and exact results for ground-state properties are thus available for arbitrary L. For the attractive case, which is known to exhibit singlet superconductivity, it was found that the results for this particular case may be written as

$$E_0\left(\Phi+\frac{n}{2}\right)-E_0(\Phi)=\Lambda\left(\frac{L}{\xi}\right)^{1/2}\exp\left(-\frac{L}{\xi}\right). \quad (2)$$

For the attractive Hubbard model, ξ is a length associated with a gap of spin excitations in the system, $\Lambda=\Lambda(U,N)$ is a coefficient which depends on details of the model, U is the on-site interaction, and N is the number of particles on the ring. Another quantity of interest, which should be considered in conjunction with $E_0(\Phi+n/2)-E_0(\Phi)$ for the purpose of detecting superconductivity, is the superfluid stiffness $\rho_s(L)=\partial^2[L\times E_0(\Phi)]/\partial\Phi^2|_{\Phi=0}$. This quantity should approach a *finite* constant as $L\to\infty$ in a superconducting or perfectly conducting state $\lim_{L\to\infty}\rho_s(L)\neq 0$. Equation (2) and $\lim_{L\to\infty}\rho_s(L)$ are diagnostic tools when looking for superconductivity in the VSA model Eq. (1), with $\Lambda=\Lambda(U_p,U_d,V,\Delta,N)$.

We use Lanczos diagonalization to obtain the $T=0$ eigenvalues and eigenvectors of the Hamiltonian Eq. (1). Considering numerical approaches of this kind, necessarily limited in system size L, one should bear in mind that also nonsuperconducting states may produce anomalous flux quantization. For instance, it was recently noted that $E_0(\Phi)=E_0(\Phi+n/2)$ is seen in exact diagonalization studies of small rings of the *repulsive* one-band Hubbard model [9]. We have, however, verified that *no anomalous flux quantization occurs* in this 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 $E_0(\Phi)=E_0(\Phi+n/2)$. The crossing in energy of states of different spin S occurs due to degeneracies in finite systems, and associated Hund's rule effects which are negligible in the thermodynamic limit $L\to\infty$. Furthermore, Bogachek *et al.* [10] have shown that a tendency to anomalous flux quantization also occurs in charge-density-wave (CDW) ground states in finite rings. The competition between CDW and singlet superconductivity will be discussed further below, when considering correlation functions. Paired states which are crystalline or phase separated will also tend to have $E_0(\Phi)=E_0(\Phi+n/2)$. In these cases ρ_s will decrease with L, whereas in a metallic or superconducting state ρ_s should approach a *finite* constant as $L\to\infty$. Hence, to test for superconductivity, one must calculate both $E_0(\Phi)$ *and* ρ_s, and consider their behavior with increasing L. In our computations, we have been limited in system sizes $L\leq 12$ sites for fillings $N>L/2$ of interest, i.e., systems doped beyond half filling. Our conclusion on the existence of superconductivity at $T=0$ in the 1D VSA model, based on finite-size scaling analysis alone, is therefore suggestive rather than final. Hence, we also consider pairing correlations explicitly, and discuss them within the general Luttinger liquid framework.

We now turn to the details of the calculations. The choice of the parameters is such that at half filling, the model is a charge-transfer insulator with a gap of about 2 (in units of t_{pd}), with 80% or more of the charge residing on the d orbitals (corresponding almost to a Cu^{++} state in the Cu-O materials). With $U_d\approx 6$, this is ensured for both Δ and V, in a range between 0 and 4. For such parameters, as V increases, one obtains a rapid transfer of charge from copper orbitals to oxygen orbitals *for systems doped beyond half filling,* at the few fillings we can consider. This was also seen in mean-field calculations [6]. It is this region of parameters bordering on phase separation which is the region of interest to us when searching for superconducting ground states.

Figure 1 shows $E_0(\Phi)$ obtained in the VSA model with parameters $L=10$, $N=8$, $t_{pd}=1$, $U_d=10$, $U_p=0$, and $2\Delta\equiv E_p-E_d=2$ for three values, $V=1.0$, 3.0, and 4.0. For the latter two values, the system exhibits anomalous flux quantization, but not for $V=1.0$. *A critical value of V is thus needed to see pairing.* The filling in this case corresponds to 60% doping beyond half filling. For small $V<1$, $E_0(\Phi)$ is minimum at $\Phi=\frac{1}{2}$, and has period 1, characteristic of a normal metallic state. As V is increased, a local minimum develops at $\Phi=\frac{1}{2}$ as a result of level crossing between states of different total momenta $k=2\pi m/L$; $m=0,\pm 1,\pm 2,\ldots$. It is found that $E_0(\frac{1}{2})-E_0(0)$ decreases rapidly as V is increased, consistent with Eq. (2). As the on-site Coulomb repulsion on oxygen sites U_p is increased, the effective attraction induced on oxygen sites by the presence of V is reduced. On-site pairing is consequently suppressed, and is not present when $U_p\approx U_d$.

The 10-site chain with $N=8$ shows anomalous flux

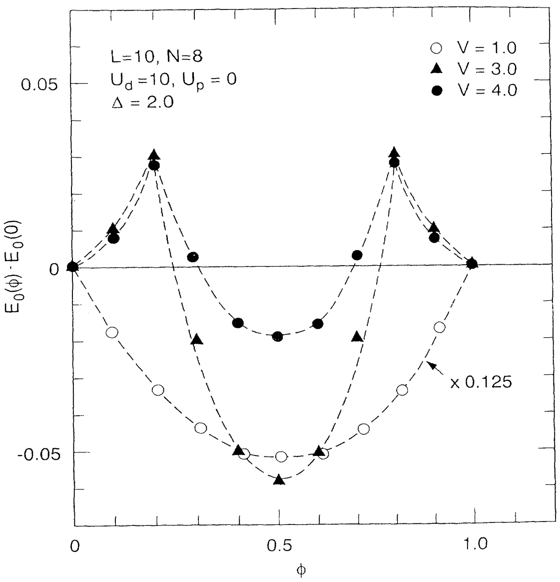

FIG. 1. Ground-state energy $E_0(\Phi)$ vs flux Φ for the 1D VSA model with $L=10$, $N=8$, $U_p=0$, $U_d=10$, $2\Delta=2$, and $t_{pd}=1$ for various values of V. Note the tendency to halve the periodicity of $E_0(\Phi)$, characteristic of flux quantization with charge $2e$, when $V=3.0$ and $V=4.0$ but not at $V=1.0$. Note also the rapid decrease of $E_0(\frac{1}{2})-E_0(0)$ as V increases, consistent with a reduction of the Cooper-pair size with increasing V. The thin broken lines are guides to the eye. Φ is measured in units of 2π.

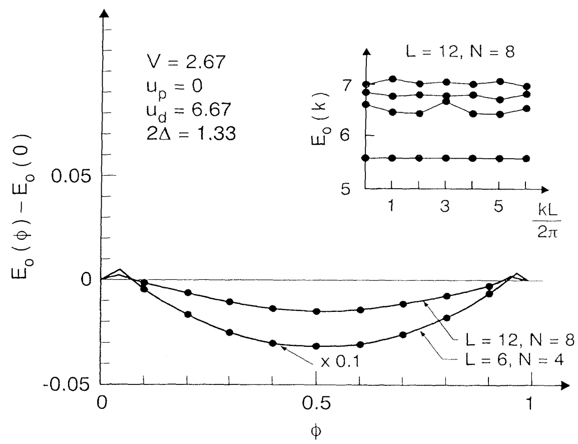

FIG. 2. Ground-state energy $E_0(\Phi)$ vs Φ for the 1D VSA model, with $U_{pd}=0$, $U_d=6.67$, $2\Delta=1.33$, $V=2.67$, and $t_{pd}=1$ for two values of L: $L=6$, $N=4$ and $L=12$, $N=8$. The inset shows $E_0(k)$ and a few excited states vs k for the 1D VSA model with $L=12$, $N=8$, with $U_p=0$, $U_d=6.67$, $2\Delta=1.33$, and $V=4.00$. The lowest energy is essentially dispersionless, consistent with a phase-separated state.

quantization for a large range of V. Furthermore, by inspecting the dispersion of the ground-state energy $E_0(k,\Phi=0)$, it is seen that the system maintains quasiparticles with mass within a factor of 2 [i.e., $E_0(k,\Phi=0)$ remains *dispersive*] from that at $V=0$ in the entire range of $2\leq V\leq 4$ we have considered, and where $\Phi_0/2$ quantization is observed. These are encouraging signs of a superconducting ground state. However, the 10-site chain is not convenient for carrying out the finite-size scaling analysis mentioned previously. We therefore consider next a 6-site and a 12-site chain, which also allows two systems with identical *fillings* to be investigated. For the 6-site chain we have used $N=4$, while for the 12-site chain, we have used $N=8$, which corresponds to 33% doping beyond half filling. The filling is lower than in the case of the 10-site chain; observation of anomalous flux quantization thus requires larger values of V [11].

In Fig. 2, we show $E_0(\Phi)$ for $L=6$ and $L=12$ with $N=4$ and $N=8$, respectively. For $U_d=6.67$, $U_p=0$, $2\Delta=1.33$, and $V=2.67$, we have $\Delta E_\Phi(L=6)/\Delta E_\Phi(L=12)=0.3$ and $\rho_s(L=12)/\rho_s(L=6)=0.67$, whereas for $V=4$, the former is 0.07 while the latter is 0.25. Here, we have defined $\Delta E_\Phi=E_0(\Phi=\frac{1}{2})-E_0(\Phi=0)$. Note the position of the *minima* at $\Phi=\pi$ in the curves $E_0(\Phi)$ between $L=10$ and $L=6,12$ [12]. For a superconductive ground state and for $L\gg\xi$, ρ_s should scale to a constant while ΔE_Φ should decrease exponentially with large L. For $V=2.67$ we find using Eq. (2) that $\xi\approx 6$, so we are not in the asymptotic regime and the small decrease of ρ_s with increasing L is consistent with a superconducting state. However, for $V=4$, we have $\xi\approx 2$; in this case the sharp decrease of ρ_s with L is suggestive of a paired, but nonsuperconducting state. In the inset of Fig. 2, we show $E_0(k,\Phi=0)$ for $L=12$, $N=8$ of such states, along with a few excited states. The lowest energy is seen to be essentially *dispersionless,* consistent with a pinned CDW or a paired/phase-separated state, the latter also previously indicated by mean-field calculations [6]. In this context, we note that for $L=12$ and $V\gtrsim 4$, we find that the chemical potential $\mu(N)=E_0(N+1)-E_0(N)$ at $N=8$ is close to its value at half filling, *a signature of phase separation.* These results, which will be elaborated on in a forthcoming paper, strongly suggest a superconducting state in a regime of parameters *locating the system close to a phase-separation instability.* The effect on longer-range Coulomb interaction (and the frustration of phase separation) [13] on the superconductivity will also be addressed.

To further investigate the possibilities of a superconducting state at $T=0$ in the 1D VSA model with purely repulsive interactions, we have considered the ground-state singlet-pairing correlation function $\Theta(i-j)\equiv\langle\Delta_i^+\Delta_j\rangle$, where $\Delta_i=c_{0,i,\downarrow}c_{0,i,\uparrow}$ within the Luttinger liquid framework [14]. In a Luttinger liquid, the correlation function for singlet superconductivity (SS) decays asymptotically as $1/x^{\alpha_{SS}}$, where α_{SS} is an exponent determined by the interactions in the problem. The correlation function for a charge-density wave decays asymptotically as $A/x^2+B\cos(2k_Fx)/x^{\alpha_{\rm CDW}}$ up to logarithmic corrections, where A,B are model-dependent constants, and k_F is the Fermi wave vector. The dominating instability is associated with the correlation function with the slowest decay, which is seen to be that of SS when $\alpha_{\rm SS}<\alpha_{\rm CDW}$. Furthermore, $\alpha_{\rm SS}$ and $\alpha_{\rm CDW}$ are related in a way which depends on whether the spin-excitation spectrum is gapped or not. When the spin-excitation spectrum is gapped [15], we have $\alpha_{\rm SS}=1/K_\rho$ and $\alpha_{\rm CDW}=K_\rho$, where K_ρ is a model-dependent constant which sets the scaling dimension of *all* correlation functions [14].

We concentrate on obtaining K_ρ rather than $\Theta(i-j)$ directly: K_ρ is expected to exhibit only very modest finite-size effects. The Hubbard chain with $L=8$, $N=6$ gives the value for K_ρ obtained via the Bethe ansatz in the thermodynamic limit to within 5% [14,16]; similar results are found in the supersymmetric t-J model [17]. K_ρ is obtained from $E_0(\Phi,N)$ via $\partial^2[LE_0(N)]/\partial N^2=(\pi/2)\times u_\rho/K_\rho$ and $\partial^2[LE_0(\Phi)]/\partial\Phi^2|_{\Phi=0}=2u_\rho K_\rho$, where u_ρ is the velocity of charge excitations [14,16]. For $U_d=6.7$, $U_p=0.0$, $2\Delta=1.33$, and $V=2.67$, we obtain $K_\rho=1.3$, and hence $\alpha_{\rm SS}<1$. The results $K_\rho>1$ implies that the generalized CDW susceptibility is *less* divergent at $T=0$ than that of SS. *Singlet superconductivity is thus the dominanting instability.* (Note that in our calculations, we cannot resolve the logarithmic corrections that distinguish triplet pairing from singlet pairing.) We note also that the effective attraction on oxygen sites induced by V *may* be simulated by a $U<0$ oxygen-band Hubbard model. For such a model, one has $K_\rho=1-U/v_F\pi>1$ with $v_F=2\sin k_F$ in the weak-coupling limit [14,16], and $K_\rho>1$ quite generally. This again implies that superconductivity is favored over CDW.

In conclusion, flux quantization has been used as a diagnostic tool to investigate the existence of superconducting pairing in a fermion system with purely repulsive interactions. The VSA model, Eq. (1), promotes superconductive pairing in 1D at $T=0$. The pairing is induced by an intersite Coulomb interaction V between the copper and oxygen sites of order the charge transfer gap. 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. To investigate the nature of the paired state, we have obtained the Luttinger liquid correlation exponent K_ρ, showing 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, however, been shown to be due to superconducting pairing by a detailed analysis of the correlation exponents. The superconducting phase is located close to a phase-separation instability of the model.

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