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Symmetric Hubbard systems with superconducting magnetic response

A. Callegari, M. Cini[a], E. Perfetto, and G. Stefanucci

Istituto Nazionale per la Fisica della Materia, Dipartimento di Fisica, Università di Roma Tor Vergata, Via della Ricerca Scientifica, I-00133 Roma, Italy

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Abstract. In purely repulsive, C_{4v}-symmetric Hubbard clusters a correlation effect produces an effective two-body attraction and pairing; the key ingredient is the availability of $W = 0$ pairs, that is, two-body solutions of appropriate symmetry. We study the tunneling of bound pairs in rings of 5-site units connected by weak intercell links; each unit has the topology of a CuO_4 cluster and a repulsive interaction is included on every site. Further, we test the superconducting nature of the response of this model to a threading magnetic field. We present a detailed numerical study of the two-unit ring filled with 6 particles and the three-unit ring with 8 particles; in both cases a lower filling yields normal behavior. In previous studies on $1d$ Hubbard chains, level crossings were reported (half-integer or fractional Aharonov-Bohm effect) which however cannot be due to superconducting pairs. In contrast, the nontrivial basis of clusters carrying $W = 0$ pairs leads to genuine Superconducting Flux Quantization (SFQ). The data are understood in terms of a cell-perturbation theory scheme which is very accurate for weak links. This low-energy approach leads to an effective hard core boson Hamiltonian which naturally describes itinerant pairs and SFQ in mesoscopic rings. For the numerical calculations, we take advantage of a recently proposed exact diagonalization technique which can be generally applied to many-fermion problems and drastically reduces the size of the matrices to be handled.

PACS. 71.27.+a Strongly correlated electron systems; heavy fermions – 74.20.Mn Nonconventional mechanisms – 73.22.-f Electronic structure of nanoscale materials: clusters, nanoparticles, nanotubes, and nanocrystals

1 Introduction

Low-dimensional systems with strong electron-electron correlations may lead to an anomalous Aharonov-Bohm (AB) effect [1] with ground-state energy oscillations *versus* flux ϕ having a period shorter than the fundamental one, given by $\phi_0 = hc/e$. However, as we shall see below, a fractional period ϕ_0/N does not generally mean that the current is carried by particles with an effective charge $e^* = Ne$. In particular, if $N = 2$ the half-integer AB effect is not equivalent to the superconducting flux quantization (SFQ) and pairing is not necessarily implied.

The repulsive Hubbard ring in the presence of a magnetic flux has been studied by several authors. At half filling it was inferred by numerical evidence [2] that the period of the ground state energy $E^{(0)}(\phi)$ as a function of the trapped flux ϕ is a whole fluxon if U/t is in a physical parameter range. Away from half filling Kusmartsev [3] pointed out that for microscopic Hubbard rings with N particles the ground state energy has Néminima in the range $[0, \phi_0)$ for $U = \infty$ and at low density. (This result has been confirmed by Schofield *et al.* in Ref. [4]). These oscillations were originally explained in terms of spin-flip processes by the same author, so that the system varies its total spin as the flux changes by one flux quantum. However, when $U = \infty$ many degenerate ground states with different total spin S exist, and a more accurate explanation of the fractional AB effect has been provided by Yu and Fowler [5,6]. They studied the Lieb-Wu [7] equations for a chain with twisted boundary conditions (a flux ϕ corresponds to a twist of $2\pi\phi/\phi_0$) with leading t/U corrections. Increasing the flux the holon momenta get shifted and the energy of the holon sea grows; to counterbalance this effect the system generates a compensating momentum by creating a hole in the distribution of the spinon quantum numbers. This excitation in the spinon sea is not energetically suppressed as far as $Nt/LU \ll 1$ where L is the number of sites. The quantization of the spinon momenta does not allow a full compensation for the effect of a continuously varying flux ϕ and leads to the energy oscillations discussed above. As Nt/LU increases the spinon excitation energies are raised and beyond a critical value

[a] e-mail: cini@roma2.infn.it

$E_0(\phi)$ has only two minima at $\phi = 0$ and $\phi = \phi_0/2$ corresponding to the spinon excitations with momentum 0 and π, as numerically observed in references [2,5,8]. Hence, the half-integer AB effect is driven by level-crossing due to the spinon degrees of freedom and it is not SFQ.

Recently, an exact result on the infinite U Hubbard ring with twisted boundary conditions has been obtained by Nakano [9]. He proved that the ground state energy $E^{(0)}(\phi)$ with an even number of particles N is periodic with period $\phi_0/2$ if the z-component of the total spin $S_z = 0$ and with period ϕ_0/N if $M_\uparrow/M_\downarrow$ (with $M_\uparrow \geq M_\downarrow$) is not an integer; here M_σ is the number of particles with spin $\sigma = \uparrow, \downarrow$. We emphasize that the Nakano theorem is not in contrast with the results by Kusmartsev. Indeed, even if $E^{(0)}(\phi)$ has period $\phi_0/2$ it may exhibit other minima in the range $[0, \phi_0)$.

The half-integer AB effect caused by the existence of confined pairs has been observed in the framework of extended $1d$ Hubbard models. Sudbø *et al.* [10] studied an alternating Cu-O ring with a charge-gap between Cu and O (which favors the particles to occupy O sites) and an on-site repulsion is allowed on Cu's but not on O's. In this way a half-integer flux quantization needs a strong off-site repulsion; pair confinement is achieved by allowing for repulsion-free sites, and not by producing an effective attraction. Other authors considered modified $1d$ models with bond-charge interactions so that the number of doubly occupied sites is an extra conserved quantity [11]. Turning on a term breaking the extra symmetry gives rise to an effective attractive interaction and to the SFQ for moderate on-site repulsion. However, the pairing mechanism is not driven by the Hubbard interaction as witnessed by the presence of SFQ even at $U = 0$ [12,13].

Few data are available in $2d$ Hubbard systems, since no exact solutions exist in this case and numerical explorations are possible only for small clusters. Long ago Canright and Girvin [14] discussed the magnetic response of the Hubbard model showing SFQ in the *attractive* case by threading a magnetic field into a cylindrical probe. Assaad *et al.* [15] computed numerically the magnetic response of the repulsive Hubbard model in the same geometry at quarter filling, but the flux quantization was found to be normal. Signatures of anomalous flux quantization in a 4×4 geometry have been provided by Arrachea *et al.* [16]; however they studied an *extended* Hubbard model with nearest-neighbour correlated, *e.g.* occupation-dependent, hopping.

All these results would suggest that the half-integer AB effect cannot be interpreted as SFQ in the context of repulsive Hubbard systems. However, Anderson [17] first advocated the non-conventional superconductivity arising from repulsive interactions, proposing the one-band Hubbard Hamiltonian as a prototype model. Evidence for pairing has then been obtained by several authors by a variety of methods. Analytic approaches based on a renormalization method [18,19] and on various implementations of the renormalization group technique [20–22], generalized conserving approximation theories like FLEX [23], as well as Quantum Monte Carlo studies on supercells [24] lead to this conclusion. In references [25–28] we show that pairing occurs also in purely repulsive, C_{4v}-symmetric Hubbard clusters.

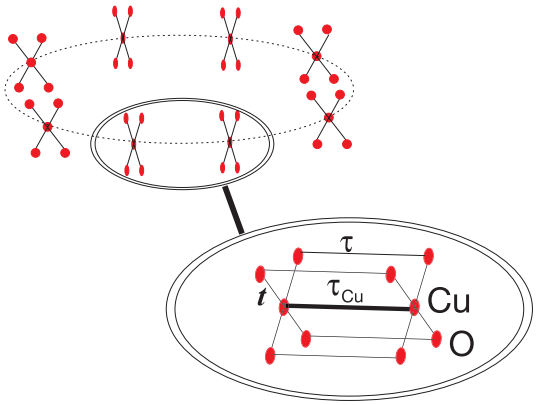

Fig. 1. Illustration of the ring topology described in the main text. τ and $\tau_{\rm Cu}$ represent O-O and Cu-Cu links, respectively, as explained in detail in Section 3 below.

In this paper we wish to study the tunneling of bound pairs in rings of 5-site units with a CuO_4 topology, see Figure 1.

In the following we shall refer to the central site as Cu and to the four external sites as O just to distinguish their position in the unit cell. We shall see that numerical solutions of such a model clearly show superconducting pair hopping if the total number of particles is $2|\Lambda| + 2p$ where $|\Lambda|$ is the number of units and $0 < p < |\Lambda|$; in particular, once a magnetic field is switched on into the ring, SFQ is unambiguously observed. We note that in our model no superconducting response is obtained with less than 2 particles per 5-site unit [CuO_4]. This means that the Zhang-Rice picture [29] for the two-dimensional $d-p$ model does not work in the present context and we wish to explore a scenario with a larger number of particles. The data are interpreted by implementing a cell-perturbation theory which is very accurate for weak links. This low-energy approach leads to an effective hard core boson Hamiltonian which naturally describes itinerant pairs and SFQ in mesoscopic rings as well. We feel that SFQ from purely repulsive Hubbard models is interesting by itself even if it may have no direct relevance for high-T_c cuprates. The tunneling of pairs has been studied in the context of the t-J model too [30], but here we wish to study symmetric Hubbard clusters for a broad range of U/t including the weak coupling limit.

The plan of the paper is the following. In Section 2 we recall that the CuO_4 cluster has two-body singlet eigenstates without double occupation called $W = 0$ pairs. By exploiting a symmetry driven configuration interaction mechanism they get bound once dressed by the virtual electron-hole excitations; the binding is due to an effective attraction among the particles of the $W = 0$ pair. In Section 3 we introduce the model Hamiltonian with symmetric clusters, as units of an arbitrary graph, linked by intercell hoppings. For any given graph, we deduce a low-energy effective Hamiltonian in Section 4. Partial results

presented elsewhere [31] are extended to any number of conducting pairs and we show that the effective Hamiltonian is equivalent to the $1d$ antiferromagnetic Heisenberg-Ising model for a ring topology. In Section 5 we recall a recently proposed spin-disentangled diagonalization technique that allowed us to carry out the numerical calculations. We also give practical details on the performance of this novel approach. Results are presented and interpreted physically in Section 6 for the two-unit ring and in Section 7 for the three-unit ring and compared with the analytic predictions. For the larger ring, after reviewing from reference [31] the flux dependence of the energy levels in the case of O-O intercell bonds we analyze the current and show that it is a discontinuous function of the flux and can be paramagnetic as well as diamagnetic. Novel results for the case of Cu-Cu bonds are presented, and this case is definitely more exotic: the bound pairs have an infinite effective mass and the flux quantization is normal. Our main conclusions are summarized in Section 8.

2 W = 0 pairing in Hubbard models

The repulsive Hubbard Hamiltonian has *two-body* singlet eigenstates without double occupation [25–28] called $W = 0$ pairs. Such solutions are also allowed in the fully symmetric clusters $\mathcal{C}$. In the *many-body* ground state these pairs get dressed and bound, and this is signaled by $\Delta_{\mathcal{C}}(N) < 0$ where $\Delta_{\mathcal{C}}(N) = E_{\mathcal{C}}^{(0)}(N) + E_{\mathcal{C}}^{(0)}(N-2) - 2E_{\mathcal{C}}^{(0)}(N-1)$; $E_{\mathcal{C}}^{(0)}(N)$ is the interacting ground state energy of the cluster $\mathcal{C}$ with N particles. By means of a non-perturbative canonical transformation [18,19], it can also be shown that $\Delta_{\mathcal{C}}(N) < 0$ is due to an attractive effective interaction and at weak coupling $|\Delta_{\mathcal{C}}(N)|$ is just the binding energy of the pair. The extension of the theory to the full plane was also put forth in reference [18].

The C_{4v} symmetric 5-site cluster is the smallest one where the $W = 0$ pairing mechanism works. We have already described $W = 0$ pairing in great detail as a function of the one-body and interaction parameters on all sites; the study was extended to larger clusters too [27,32]. The 5-site unit has the same topology of the CuO_4 cluster; thus, we label the central site by the Cu symbol and the four external ones by the O symbol. The 5-site cluster will be also called CuO_4. In order to simplify the analytical formulas, we neglect the O-O hopping term and the only nonvanishing hopping matrix elements are those between an O site and the central Cu site; they are all equal to t. For the sake of simplicity, we parametrize the Hubbard model in such a way that actually everything depends only on the ratio U/t. Thus, we consider the Hubbard Hamiltonian

$$H_{\mathrm{CuO_4}} = t \sum_{i\sigma} \left(d_\sigma^\dagger p_{i\sigma} + p_{i\sigma}^\dagger d_\sigma \right) + U \left(\sum_i \hat{n}_{i\uparrow}^{(p)} \hat{n}_{i\downarrow}^{(p)} + \hat{n}_\uparrow^{(d)} \hat{n}_\downarrow^{(d)} \right) \quad (1)$$

Table 1. Character table of the S_4 group. Each quatern (n_1, n_2, n_3, n_4) labels a class of S_4.

S_4	$(4,0,0,0)$	$(2,1,0,0)$	$(0,2,0,0)$	$(1,0,1,0)$	$(0,0,0,1)$
$\mathcal{A}_1$	1	1	1	1	1
$\mathcal{B}_2$	1	-1	1	1	-1
$\mathcal{E}$	2	0	2	-1	0
$\mathcal{T}_1$	3	1	-1	0	-1
$\mathcal{T}_2$	3	-1	-1	0	1

Table 2. Character table of the C_{4v} symmetry group. Here **1** denotes the identity, C_2 the 180 degrees rotation, $C_4^{(+)}$, $C_4^{(-)}$ the counterclockwise and clockwise 90 degrees rotation, σ_x, σ_y the reflection with respect to the $y = 0$ and $x = 0$ axis and σ_+, σ_- the reflection with respect to the $x = y$ and $x = -y$ diagonals. In the last column we show typical basis functions.

C_{4v}	**1**	C_2	$C_4^{(+)}$, $C_4^{(-)}$	σ_x, σ_y	σ_+, σ_-	Symmetry
A_1	1	1	1	1	1	$x^2 + y^2$
A_2	1	1	1	-1	-1	$(x/y) - (y/x)$
B_1	1	1	-1	1	-1	$x^2 - y^2$
B_2	1	1	-1	-1	1	xy
E	2	-2	0	0	0	(x, y)

where $p_{i\sigma}^\dagger$ and $p_{i\sigma}$ are the creation and annihilation operators onto the O $i = 1, .., 4$ with spin $\sigma = \uparrow, \downarrow$, $d_\sigma^\dagger$ and d_σ are the creation and annihilation operators onto the Cu site, while $\hat{n}_{i\sigma}^{(p)} = p_{i\sigma}^\dagger p_{i\sigma}$ and $\hat{n}_\sigma^{(d)} = d_\sigma^\dagger d_\sigma$ are the corresponding number operators. $H_{\mathrm{CuO_4}}$ is invariant under the permutation group S_4. The classes of S_4 can be labelled with the quatern (n_1, n_2, n_3, n_4). Each class contains all the permutations where n_i is the maximum number of sets of i elements that remain unchanged after the permutation. For example (4,0,0,0) contains all the permutations such that 4 sets containing one element remain unchanged, that is the identity. On the other hand (2,1,0,0) contains all the permutations such that 2 sets containing one element and one set containing 2 elements remain unchanged. Starting from the configuration 1234, this class contains the permutations 1243, 1432, 1324, 4231, 3214, 2134. S_4 has the irreducible representations (*irreps*) $\mathcal{A}_1$ (total-symmetric), $\mathcal{B}_2$ (total-antisymmetric), $\mathcal{E}$ (self-dual), $\mathcal{T}_1$ and its dual $\mathcal{T}_2$, of dimensions 1, 1, 2, 3 and 3, respectively, see Table 1. The model admits a $W = 0$ pair belonging to the irrep $\mathcal{E}$ and formed by mixing degenerate one-body states.

For later use, we recall how the irrep $\Gamma \in \{\mathcal{A}_1, \mathcal{T}_1, \mathcal{E}, \mathcal{T}_2, \mathcal{B}_2\}$ of S_4 breaks in C_{4v}, that is the point symmetry group of the square. C_{4v} is a subgroup of S_4 and its Character Table is shown in Table 2. From Tables 1 and 2 we have

$$\mathcal{A}_1 = A_1, \quad \mathcal{T}_1 = B_1 \oplus E, \quad \mathcal{T}_2 = A_2 \oplus E, \quad \mathcal{B}_2 = B_2, \quad \mathcal{E} = A_1 \oplus B_2 \,. \quad (2)$$

From equation (2) we see that we may label the two components of the $W = 0$-pair irrep $\mathcal{E}$ in terms of the

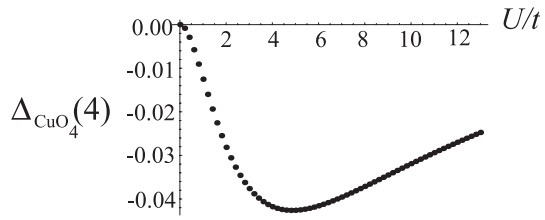

Fig. 2. $\Delta_{\mathrm{CuO_4}}(4)$ (in t units) as a function of U/t. The maximum binding occurs at $U \sim 5t$ where $\Delta_{\mathrm{CuO_4}}(4) \approx -0.042\ t$. For $U > 34.77\ t$ (not shown), $\Delta_{\mathrm{CuO_4}}(4)$ becomes positive and pairing disappears.

irreps A_1 and B_2 of C_{4v}. For example, defining by $p^\dagger_{x,\sigma} = \frac{1}{\sqrt{2}}(p^\dagger_{1,\sigma} - p^\dagger_{3,\sigma})$ and $p^\dagger_{y,\sigma} = \frac{1}{\sqrt{2}}(p^\dagger_{2,\sigma} - p^\dagger_{4,\sigma})$ two of the three degenerate eigen-operators of the kinetic term in $H_{\mathrm{CuO_4}}$, the B_2 component of the $W = 0$ pair is obtained by acting with the two-body singlet operator

$$\frac{1}{\sqrt{2}}\left(p^\dagger_{x,\uparrow}p^\dagger_{y,\downarrow} + p^\dagger_{y,\uparrow}p^\dagger_{x,\downarrow}\right) \tag{3}$$

on the vacuum.

The ground state of CuO_4 [2] (*i.e.* CuO_4 with 2 particles) belongs to ${}^1\mathcal{A}_1$ and that of CuO_4 [4] is in ${}^1\mathcal{E}$; both are singlets, as the notation implies. The ground state of CuO_4 [3] is a ${}^2\mathcal{T}_1$ doublet. $\Delta_{\mathrm{CuO_4}}(4)$ has a minimum at $U \approx 5\ t$ for this model, as shown in Figure 2, and it is negative when $0 < U < 34.77\ t$. We emphasize that $\Delta_{\mathrm{CuO_4}}(4)$ becomes positive for large values of U/t and hence pairing disappears in the strong coupling regime. In the present problem U must exceed several tens of times t before the asymptotic *strong coupling regime* sets in. A perturbation theory will strictly apply at *weak coupling* where the second derivative of the curve is negative; however, qualitatively a weak coupling approach is rewarding in all the physically interesting range of parameters. The above pairing mechanism does not work in the neighborhood of the infinite U limit.

We analyzed the pairing mechanism in detail in reference [28]; for the sake of simplicity here we report in Figure 3 the leading, second-order two-body amplitude for particles of opposite spins in the degenerate (x, y) orbitals of CuO_4. We demonstrated [28] that this produces an effective interaction, which pushes down the singlet in equation (3) and up the triplet by $|\Delta_{\mathrm{CuO_4}}(4)|$. In this way, $\Delta_{\mathrm{CuO_4}}(4)$ can be redefined without any reference to the ground state of clusters with a different number of particles, and we are free from the objections based on a possible Jahn-Teller distortion of odd-N clusters [33].

The formation of bound pairs from purely repulsive interactions was first proposed in a pioneering paper [34] by Kohn and Luttinger. They showed that any three-dimensional Fermi liquid undergoes a superconducting transition by Cooper pairs of very large angular momentum l. A simplified view of the Kohn-Luttinger effect is given by considering one particle of the pair as an external charge. Then, the screening gives rise to a long-range oscillatory potential (Friedel oscillations) due to the singularity of the longitudinal dielectric function at $2k_{\mathrm{F}}$;

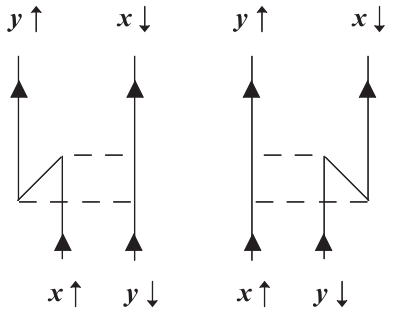

Fig. 3. The second order spin-flip diagrams for the two-body amplitude.

here k_{F} is the Fermi wavevector. The strict reasoning exploits the fact that the Legendre expansion coefficients of any regular direct interaction between particles of opposite momentum drops off exponentially in l. On the other hand, the second-order contribution to the scattering amplitude falls as $1/l^4$ and at least for odd l leads to an attractive interaction. In the modern renormalization group language [35], the second-order correction is obtained by summing up the marginal scattering amplitudes of the isotropic Fermi liquid coming from the so-called Forward channels, including, for antiparallel spins, a spin-flip diagram. This scenario does not work in the two-dimensional Fermi liquid, but going beyond the second-order perturbation theory the Kohn-Luttinger effect is recovered [36]. In the Hubbard model, there is first-order interaction only for antiparallel spins, but it vanishes for $W = 0$ pairs; in second-order, in the singlet channel, the spin-flip diagram is the only one that survives. We found pairing in the singlet channel in a variety of models including carbon nanotubes [37]. Hence, the $W = 0$ pairing mechanism in the Hubbard model belongs to the broad category of Kohn-Luttinger effects with no direct interaction and a second-order correction coming from the spin-flip channel only, as shown in Figure 3.

3 Modelling intercell hopping

We use CuO_4 units as nodes of a graph Λ. The total Hamiltonian is

$$H_{\mathrm{tot}} = H_0 + H_\tau, \tag{4}$$

with

$$H_0 = \sum_{\alpha\in\Lambda}\left[t\sum_{i\sigma}\left(d^\dagger_{\alpha\sigma}p_{\alpha,i\sigma} + p^\dagger_{\alpha,i\sigma}d_{\alpha\sigma}\right) + U\left(\hat{n}^{(d)}_{\alpha\uparrow}\hat{n}^{(d)}_{\alpha\downarrow} + \sum_i \hat{n}^{(p)}_{\alpha,i\uparrow}\hat{n}^{(p)}_{\alpha,i\downarrow}\right)\right] \tag{5}$$

where $p^\dagger_{\alpha,i\sigma}$ is the creation operator onto the O $i = 1, .., 4$ of the α-th cell and so on, while H_τ is an intercell hopping Hamiltonian. The point symmetry group of H_0 includes $S_4^{|\Lambda|}$, with $|\Lambda|$ the number of nodes.

There are many different ways to add an intercell hopping. Nevertheless, to preserve the symmetry that produces the $\Delta_{\mathrm{CuO_4}}(4) < 0$ property, we take H_τ invariant under the S_4 subgroup of $S_4^{|\Lambda|}$. In the following we shall consider a hopping term that allows a particle in the ith O site of the αth unit to move towards the ith O site of the βth unit with hopping integral $\tau_{\alpha\beta} \equiv |\tau_{\alpha\beta}| e^{i\theta_{\alpha\beta}}$:

$$H_\tau = \sum_{\alpha,\beta\in\Lambda} \sum_{i\sigma} \left[\tau_{\alpha\beta} p^\dagger_{\alpha,i\sigma} p_{\beta,i\sigma} + \mathrm{h.}c. \right]. \tag{6}$$

For $N = 2|\Lambda|$ and $\tau_{\alpha\beta} \equiv 0$, the unique ground state consists of 2 particles in each CuO_4 unit. Section 4 (theory) and Section 7.1 (numerical) are devoted to the intercell hopping produced by small $|\tau_{\alpha\beta}| \ll |\Delta_{\mathrm{CuO_4}}(4)|$; to study the propagation of p pairs we consider a total number of $N = 2|\Lambda| + 2p$ particles. When U/t is such that $\Delta_{\mathrm{CuO_4}}(4) < 0$, each pair prefers to lie on a single CuO_4 and for $N = 2|\Lambda| + 2p$ the unperturbed ground state is $2^p \times \binom{|\Lambda|}{p}$ times degenerate (since ${}^1\mathcal{E}$ has dimension 2). On the other hand, Section 7.2 reports the effects of an intercell hopping τ_{Cu} between Cu sites only; this does not break the $S_4^{|\Lambda|}$ symmetry and therefore its consequences on pair propagation and SFQ are drastically different. By this sort of models one can study the interaction of several pairs in the same system. We are using CuO_4 as the unit just for the sake of simplicity, but the $W = 0$ mechanism produces bound pairs at different fillings for larger clusters [28] too. By replacing CuO_4 by larger units one can model other ranges of filling fraction.

4 Low-energy effective Hamiltonian for O-O intercell hopping

In order to study the propagation of the p added pairs, we obtain an effective Hamiltonian by the cell-perturbation method with H_0, equation (5), the "cell-Hamiltonian" and H_τ, equation (6), the "intercell perturbation" and by taking into account only the low-energy singlet sector. We note that the cell-perturbation method was already used in reference [38] and in reference [39] to support the original Anderson's conjecture [17] on the "low-energy equivalence" between the $d-p$ model (proposed by Emery [40]) and the single-band Hubbard model. Despite the analogies with reference [39] (like the same cell-Hamiltonian and weak O-O links between different cells) our intercell perturbation is different and, more important, it is the low-energy sector which differs (one needs to consider CuO_4 units with 2, 3 and 4 bodies, in contrast with 0, 1 and 2 bodies of Ref. [39]).

Let us introduce some useful notation. Let $|\Psi_0^{(N)}(\alpha)\rangle$, $\alpha = 1 \ldots |\Lambda|$ be the ground state of the $\alpha-$th CuO_4 unit with $2 \le N \le 4$ particles and $E^{(0)}(N)$ the corresponding energies. Let $\mathcal{S} \subset \Lambda$, with $|\mathcal{S}| = p$, be the set of p CuO_4 units occupied by four particles and $\bar{\mathcal{S}}$ its complement in Λ, that is $\bar{\mathcal{S}} \equiv \Lambda \setminus \mathcal{S}$. When $\Delta_{\mathrm{CuO_4}}(4) < 0$, the unperturbed ground state with $2|\Lambda| + 2p$ particles can be written as

$$|\Phi_0^{\mathcal{S}}\rangle = \prod_{\alpha\in\mathcal{S}} |\Psi_0^{(4)}(\alpha)\rangle \prod_{\beta\in\bar{\mathcal{S}}} |\Psi_0^{(2)}(\beta)\rangle \tag{7}$$

and its unperturbed eigenenergy is given by

$$H_0|\Phi_0^{\mathcal{S}}\rangle = \left[pE^{(0)}(4) + (|\Lambda| - p)E^{(0)}(2) \right] |\Phi_0^{\mathcal{S}}\rangle \equiv E_p^{(0)} |\Phi_0^{\mathcal{S}}\rangle. \tag{8}$$

The energies needed to excite the CuO_4 cluster from the ground state for $U = 5 \div 6\ t$ (when $\Delta_{\mathrm{CuO_4}}(4) \approx -0.04\,t$, see Fig. 2) is $\approx t$ with 2 bodies and $\approx 0.1\ t$ with 4 bodies; both are large compared with $|\Delta_{\mathrm{CuO_4}}(4)|$ and no level crossings take place if $|\tau_{\alpha\beta}| \ll |\Delta_{\mathrm{CuO_4}}(4)|$.

The perturbation H_τ in second order will remove part of the $2^p \times \binom{|\Lambda|}{p}$ degeneracy. Let $|\Phi_0\rangle$ be an exact eigenstate with eigenenergy E. Expanding $|\Phi_0\rangle$ as

$$|\Phi_0\rangle \simeq \sum_{\mathcal{S}'} a_{\mathcal{S}'} |\Phi_0^{\mathcal{S}'}\rangle \tag{9}$$

one gets

$$(E - E_p^{(0)}) a_{\mathcal{S}} = \sum_{\mathcal{S}'} \left[\sum_m \frac{\langle \Phi_0^{\mathcal{S}} | H_\tau | \Phi_m \rangle \langle \Phi_m | H_\tau | \Phi_0^{\mathcal{S}'} \rangle}{E - E_m^{(0)}} \right] a_{\mathcal{S}'} \tag{10}$$

where $\{|\Phi_m\rangle\}$ is a complete set of excited eigenstates of H_0 and $\{E_m^{(0)}\}$ their eigenenergies.

Our crucial approximation is now to truncate the sum over the excited states $\{|\Phi_m\rangle\}$ considering only the low-energy states of the form

$$|\Phi_0^{\mathcal{T},\mathcal{D}}\rangle = \prod_{\alpha\in\mathcal{T}} |\Psi_0^{(4)}(\alpha)\rangle \prod_{\gamma\in\mathcal{D}} |\Psi_0^{(3)}(\gamma)\rangle \prod_{\beta\in\overline{\mathcal{T}\cup\mathcal{D}}} |\Psi_0^{(2)}(\beta)\rangle, \tag{11}$$

where $\mathcal{T} \subset \Lambda$ is the set of $|\mathcal{S}| - 1 \equiv |\mathcal{T}|$ CuO_4 units with 4 particles, obtained by removing one particle in one of the previous $|\mathcal{S}|$ units with 4 particles; in this way we get $|\mathcal{D}| = 2$ cells with 3 particles; the remaining $|\Lambda| - |\mathcal{S}| - 1 \equiv |\overline{\mathcal{T}\cup\mathcal{D}}|$ cells have 2 particles. This approximation is legitimated by the fact that the first excited state with 3 particles is $\approx t$ above the ground state for U in the range $5 \div 6\ t$.

The energy of the excited states in equation (11) is

$$\tilde{E}_p^{(0)} = (|\mathcal{S}| - 1)E^{(0)}(4) + 2E^{(0)}(3) + (|\Lambda| - |\mathcal{S}| - 1)E^{(0)}(2)$$

and does not depend on the sets $\mathcal{T}$ and $\mathcal{D}$. Within this approximation the Schrödinger equation (10) reduces to

$$\frac{1}{\Delta_{\mathrm{CuO_4}}(4)} \sum_{\mathcal{T},\mathcal{D}} \sum_{S'} \langle \Phi_0^{\mathcal{S}} | H_\tau | \Phi_0^{\mathcal{T},\mathcal{D}} \rangle \langle \Phi_0^{\mathcal{T},\mathcal{D}} | H_\tau | \Phi_0^{\mathcal{S}'} \rangle\, a_{\mathcal{S}'} = \varepsilon a_{\mathcal{S}}, \tag{12}$$

where $\varepsilon \equiv E - E_p^{(0)}$ and we have disregarded contributions of higher order in ε.

The amplitude $a_{\mathcal{S}} \equiv a(\alpha_1, \ldots, \alpha_p)$ is totally symmetric with respect the permutations of the distinct indices $\alpha_1, \ldots, \alpha_p$. Letting $\mathcal{K}(\alpha) = \{\beta \in \Lambda : \tau_{\alpha\beta} \neq 0\}$, after

some algebra equation (12) may be written in the form:

$$\sum_{j=1}^{p}\sum_{\beta\in\mathcal{K}(\alpha_j)}\prod_{i\neq j}(1-\delta_{\beta\alpha_i})\mathcal{J}_{\beta,\alpha_j}[a(\alpha_1,\ldots,\alpha_p) + e^{2i\theta_{\beta\alpha_j}}a(\alpha_1,..,\alpha_{j-1},\beta,\alpha_{j+1},..,\alpha_p)] = \varepsilon a(\alpha_1,\ldots,\alpha_p). \quad (13)$$

This is a Schrödinger equation for p hard-core bosons with a complex effective hopping integral; below the $\mathcal{J}$ coefficients will be calculated analytically and studied as a function of the ratio U/t. In equation (13), the second term in the l.h.s. describes pair propagation, *e.g.* from unit α_j to an *unoccupied* unit β; in the first term, the system gets back to the initial state after virtually exploring unit β; $\prod_{i\neq j}(1-\delta_{\beta\alpha_i})$ takes into account that if β is one of the *occupied* units, the particle cannot move toward it.

4.1 Evaluation of the effective hopping integral and selection rules

In equations (7–11) we omitted the irrep labels of $|\Psi_0^{(2)}\rangle$, $|\Psi_0^{(3)}\rangle$ and $|\Psi_0^{(4)}\rangle$ in order to avoid a proliferation of indices. Nevertheless, to calculate the $\mathcal{J}$'s we need to reintroduce them. The ground state with two particles is nondegenerate; it belongs to the irrep $\mathcal{A}_1$ of S_4 that coincides with A_1 in C_{4v}, and the change in notation is:

$$|\Psi_0^{(2)}\rangle \longrightarrow |\Psi_0^{(2),\mathcal{A}_1}\rangle = |\Psi_0^{(2),A_1}\rangle. \quad (14)$$

As far as the ground state with three particles is concerned, we recall that it is three times degenerate (apart from the trivial spin degeneracy) and belongs to the irrep $\mathcal{T}_1$ of S_4 that in C_{4v} breaks into $B_1 \oplus E$:

$$|\Psi_0^{(3)}\rangle \longrightarrow |\Psi_0^{(3),\mathcal{T}_1^{(r)}}\rangle \quad r=1,2,3 \quad (15)$$

where we may set up our basis such that $\mathcal{T}_1^{(1)} = B_1$, $\mathcal{T}_1^{(2)} = E_x$ and $\mathcal{T}_1^{(3)} = E_y$.

Finally, the ground state with four particles is two times degenerate and belongs to the irrep $\mathcal{E}$ of S_4 that in C_{4v} breaks into $A_1 \oplus B_2$:

$$|\Psi_0^{(4)}\rangle \longrightarrow |\Psi_0^{(4),\mathcal{E}^{(s)}}\rangle \quad s=1,2 \quad (16)$$

where $\mathcal{E}^{(1)} = A_1$ and $\mathcal{E}^{(2)} = B_2$. Useful selection rules may be obtained using group theory. By exploiting the invariance of H_τ under the group S_4 and omitting, for the sake of clarity, the spin indices in the states $|\Psi_0^{(3)}\rangle$, it follows that

$$\langle\Psi_0^{(4),\mathcal{E}^{(s)}}(\alpha)|\langle\Psi_0^{(2),A_1}(\beta)|H_\tau|\Psi_0^{(3),\mathcal{T}_1^{(r_\alpha)}}(\alpha)\rangle|\Psi_0^{(3),\mathcal{T}_1^{(r_\beta)}}(\beta)\rangle \quad (17)$$

is non-vanishing if and only if

$$\mathcal{T}_1^{(r_\alpha)} = \mathcal{T}_1^{(r_\beta)} \quad (18)$$

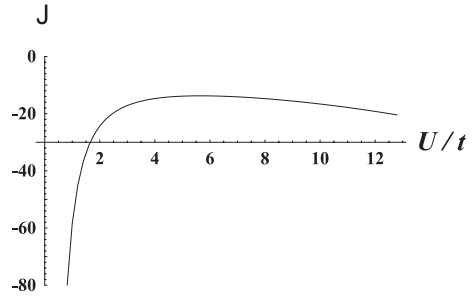

Fig. 4. $\mathcal{J}$ in units of $|\tau|^2$ *versus* U/t. The formal divergence as $U \to 0$ is not serious since the effective theory holds for intermediate U/t, when $|\Delta_{\mathrm{CuO_4}}(4)|$ is large enough.

for $\mathcal{E}^{(s)} = A_1$; instead for $\mathcal{E}^{(s)} = B_2$,

$$\mathcal{T}_1^{(r_\alpha)} = E_x, \;\; \mathcal{T}_1^{(r_\beta)} = E_y \quad (19)$$

or

$$\mathcal{T}_1^{(r_\alpha)} = E_y, \;\; \mathcal{T}_1^{(r_\beta)} = E_x. \quad (20)$$

In the case $s=1$, we have $\mathcal{E}^{(1)} = A_1$ and hence by using the selection rules in equation (18), the matrix element in equation (17) consists of three different contributions coming from the virtual 3-body states of symmetry $B_1 \otimes B_1$, $E_x \otimes E_x$ and $E_y \otimes E_y$:

$$\tau^{\mathrm{eff}}_{\alpha\beta}[B_1,B_1] \equiv -\tau_{\alpha\beta}\sum_i \langle\Psi_{0,\uparrow}^{(3),B_1}(\alpha)|p^\dagger_{\alpha,i\uparrow}|\Psi_0^{(2),A_1}(\alpha)\rangle \times \langle\Psi_{0,\downarrow}^{(3),B_1}(\beta)|p_{\beta,i\uparrow}|\Psi_0^{(4),A_1}(\beta)\rangle;$$

$$\tau^{\mathrm{eff}}_{\alpha\beta}[E_\mu,E_\mu] \equiv -\tau_{\alpha\beta}\sum_i \langle\Psi_{0,\uparrow}^{(3),E_\mu}(\alpha)|p^\dagger_{\alpha,i\uparrow}|\Psi_0^{(2),A_1}(\alpha)\rangle \times \langle\Psi_{0,\downarrow}^{(3),E_\mu}(\beta)|p_{\beta,i\uparrow}|\Psi_0^{(4),A_1}(\beta)\rangle,$$

with $\mu = x,y$. Therefore one can solve the Schrödinger equation (13) with

$$\mathcal{J}_{\alpha,\beta} = 2\times\frac{|\tau^{\mathrm{eff}}_{\alpha\beta}[B_1,B_1]|^2 + |\tau^{\mathrm{eff}}_{\alpha\beta}[E_x,E_x]|^2 + |\tau^{\mathrm{eff}}_{\alpha\beta}[E_y,E_y]|^2}{\Delta_{\mathrm{CuO_4}}(4)}, \quad (21)$$

where the factor 2 comes from the spin degeneracy. In Figure 4 we show the trend of $\mathcal{J}$ in units of $|\tau|^2$ *versus* U/t. The case $\mathcal{E}^{(2)} = B_2$ is similar and may be obtained by group theory.

The above treatment holds for any Λ; in the next section we shall specialize to the case of a one-dimensional chain with hopping integrals $\tau_{\alpha\beta}$ only between nearest neighbors units.

4.2 Ring shaped system

In order to discuss the propagation of bound pairs and the quantization of a magnetic flux, we use a chain with periodic boundary conditions and nearest neighbors hopping

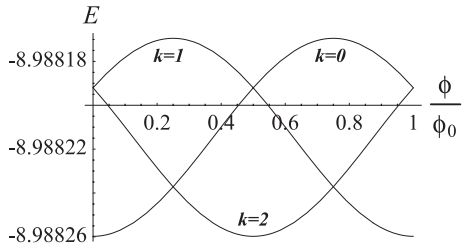

Fig. 5. Results of equation (13) for the three-unit ring with $|\tau| = 0.001\ t$, $U = 5\ t$. Lowest-energy eigenvalues labelled by their intercell quasi-momentum are shown *versus* flux ϕ. All energies are in t units.

matrix elements $\tau_{\alpha\beta}$:

$$\tau_{\alpha\beta} = \begin{cases} \tau & \text{if } \beta = \alpha + 1, \\ \tau^* & \text{if } \beta = \alpha - 1, \\ 0 & \text{otherwise} \end{cases} \qquad \tau = |\tau| e^{\frac{2\pi i}{|\Lambda|}\frac{\phi}{\phi_0}}. \quad (22)$$

For the sake of simplicity we first analyze the case with just one added pair (p=1) in detail. If the pair belongs to the A_1 component of the $\mathcal{E}$ irrep the zeroth-order ground-state is $|\Lambda|$ times degenerate. The effective Schrödinger equation (13) reads

$$\varepsilon a(\alpha) = \mathcal{J}\left[2a(\alpha) + e^{\frac{4i\pi}{|\Lambda|}\frac{\phi}{\phi_0}} a(\alpha+1) + e^{-\frac{4i\pi}{|\Lambda|}\frac{\phi}{\phi_0}} a(\alpha-1)\right]$$

which is readily solved by Fourier transforming and yields the following eigenvalues

$$\varepsilon_k = 2\mathcal{J}\left[1 + \cos\frac{2\pi}{|\Lambda|}\left(k + 2\frac{\phi}{\phi_0}\right)\right], \quad k = 1, \ldots, |\Lambda|\,. \quad (23)$$

The presence of the factor 2 in front of ϕ/ϕ_0 implies that the model quantizes the flux in units of $\phi_0/2$, like superconducting pairs do. Indeed, the ground state energy $E_\Lambda^{(0)}(2|\Lambda|+2) = \min_k \varepsilon_k$ is strictly periodic in ϕ with period $\phi_0/2$ for any $|\Lambda| > 2$.

The case $|\Lambda| = 3$ will be used below for a numerical test of equation (23). The lowest state energies for every quasimomentum in the three-unit ring with 8 particles are plotted in Figure 5 *versus* ϕ/ϕ_0. It can be shown, see below, that $|\Lambda| = 3$ is the shortest ring showing this effect.

In the case of p pairs, equation (13) yields

$$\sum_{j=1}^{p}\sum_{\beta=\pm1}\prod_{i\neq j}(1-\delta_{\alpha_j+\beta,\alpha_i})\mathcal{J}[a(\alpha_1,\ldots,\alpha_p) + e^{\beta\frac{4i\pi}{|\Lambda|}\frac{\phi}{\phi_0}} a(\alpha_1,..,\alpha_j+\beta,..,\alpha_p)] = \varepsilon a(\alpha_1,\ldots,\alpha_p) \quad (24)$$

and the model is equivalent to the Heisenberg-Ising spin chain governed by the Hamiltonian

$$H_{\rm HI} = \sum_{\alpha=1}^{|\Lambda|}\mathcal{J}[2\eta\sigma_\alpha^z\sigma_{\alpha+1}^z + e^{\frac{4i\pi}{|\Lambda|}\frac{\phi}{\phi_0}}\sigma_{\alpha+1}^+\sigma_\alpha^- + e^{-\frac{4i\pi}{|\Lambda|}\frac{\phi}{\phi_0}}\sigma_\alpha^+\sigma_{\alpha+1}^-] \quad (25)$$

where the σ's are Pauli matrices, spin up represents an empty site and spin down represents a pair. η is the so called anisotropy parameter and to reproduce equation (24) we must choose $\eta = -1$. For $\eta = 1$, we have the isotropic Heisenberg interaction. By performing a Jordan-Wigner transformation, the Hamiltonian in equation (25) can also be mapped into a model of spinless fermions on the ring. In the absence of a threading magnetic field ($\phi = 0$) the problem was originally studied by Bloch [41] and then exactly solved by Hulthen [42] (in the case $\eta = -1$) and Orbach [43] (in the case $\eta \leq -1$) using the Bethe's hypothesis [44]. A systematic analysis in the whole range of parameters was given by Yang and Yang in a self-contained series of papers [45]. Here we just recall that the model has a gapless phase if $|\eta| \leq 1$, corresponding to the conducting state, while an insulating phase sets in for $\eta < -1$. As in the $1d$ Hubbard model, the "magnetic perturbation" ($\phi \neq 0$) does not spoil the integrability and the Heisenberg-Ising Hamiltonian remains exactly solvable by the Bethe-ansatz method. Let us write an eigenfunction of $H_{\rm HI}$ as

$$a(\alpha_1, ..., \alpha_p) = \sum_P A_P e^{i\sum_j k_{Pj}\alpha_j} \quad (26)$$

where P is a permutation of the integers $1, \ldots, p$ and A_P are $p!$ coefficients. Shastry and Sutherland [46] have shown that the variables k_j are given by

$$|\Lambda| k_j = 2\pi I_j + 4\pi\frac{\phi}{\phi_0} - \sum_{l\neq j}\theta(k_j, k_l) \quad (27)$$

with a phase shift

$$\theta(k,q) = 2\tan^{-1}\left[\frac{\eta\sin[(k-q)/2]}{\cos[(k+q)/2] - \eta\cos[(k-q)/2]}\right]. \quad (28)$$

From equations (25–27) we readily see that the ground state energy of the low-energy effective Hamiltonian $H_{\rm HI}$ is periodic with period $\phi_0/2$, independent of the number of added pairs. Moreover $H_{\rm HI}$ is also the appropriate effective model for the strong-negative U Hubbard model [47], for which evidence of superconductivity is clear [48]. Thus we conclude that the purely repulsive CuO_4-Hubbard ring threaded by a magnetic field quantizes the flux in a superconducting fashion if the number of particles is $2|\Lambda| + 2p$ with $0 \leq p \leq |\Lambda|$.

5 Spin-disentangled diagonalization

In order to find the lowest energy eigenvalues and eigenfunctions when the dimension $\mathcal{N}$ of the Hilbert space is very large one must avoid storing the $\mathcal{N}\times\mathcal{N}$ Hamiltonian matrix $\mathcal{H}_{\mathcal{N}\times\mathcal{N}}$. The obvious recipe for sparse matrices, which are best handled by the Lanczos method, prescribes storing the nonzero elements and their row and column addresses in arrays. However for big problems this process is slow, since the matrix elements must be referenced to their position in $\mathcal{H}_{\mathcal{N}\times\mathcal{N}}$ and must be retrieved each time

for later use. One can try to improve the situation by projecting on the irreps of the symmetry group in order to reduce $\mathcal{N}$; however this involves building the projected basis and then new Hamiltonian matrix elements, and the new Hamiltonian is much less sparse than before, which destroys much of the benefit gained by the symmetry.

Here we exactly diagonalize the $|\Lambda| = 2$ and $|\Lambda| = 3$ ring Hamiltonian by the *Spin-Disentangled* technique, which we briefly introduced recently [31], but deserves a fuller illustration. This allows to solve the $\mathcal{N} \times \mathcal{N}$ many-electron problem by storing and handling $\sqrt{\mathcal{N}} \times \sqrt{\mathcal{N}}$ matrices. One of its clear advantages is that it *does not require the Hamiltonian to be sparse*. The method is also much more convenient than the usual one, since the $\sqrt{\mathcal{N}} \times \sqrt{\mathcal{N}}$ matrices are directly used by matrix multiplication, which is a fast process, and no mapping back onto $\mathcal{H}_{\mathcal{N}\times\mathcal{N}}$ is involved. All the advantages of symmetry are gained simply by using a projected starting state of the Lanczos chain. To the best of our knowledge, the *Spin-Disentangled* technique was not invented earlier, which is somewhat surprising, being a very general method.

We let $M_\uparrow + M_\downarrow = N$ where M_σ is the number of particles of spin σ; $\{|\phi_{\alpha\sigma}\rangle\}$ is a real orthonormal basis, that is, each vector is a homogeneous polynomial in the $p^\dagger$ and $d^\dagger$ of degree M_σ acting on the vacuum. We write the ground state wave function in the form

$$|\Psi\rangle = \sum_{\alpha\beta} L_{\alpha\beta} |\phi_{\alpha\uparrow}\rangle \otimes |\phi_{\beta\downarrow}\rangle \tag{29}$$

which shows how the $\uparrow$ and $\downarrow$ configurations are entangled. The particles of one spin are treated as the "bath" for those of the opposite spin: this form also enters the proof of a famous theorem by Lieb [49]. In equation (29) $L_{\alpha\beta}$ is a $m_\uparrow \times m_\downarrow$ rectangular matrix with $m_\sigma = \binom{5|\Lambda|}{M_\sigma}$. We let K_σ denote the kinetic energy $m_\sigma \times m_\sigma$ square matrix of $H_{\rm tot}$ in the basis $\{|\phi_{\alpha\sigma}\rangle\}$, and $N_s^{(\sigma)}$ the spin-σ occupation number matrix at site s in the same basis ($N_s^{(\sigma)}$ is a symmetric matrix since the $|\phi_{\alpha\sigma}\rangle$'s are real). Then, L is acted upon by the Hamiltonian $H_{\rm tot}$ according to the rule

$$H_{\rm tot}[L] = [K_\uparrow L + L K_\downarrow] + U \sum_s N_s^{(\uparrow)} L N_s^{(\downarrow)} \,. \tag{30}$$

In particular for $M_\uparrow = M_\downarrow$ ($S_z = 0$ sector) it holds $K_\uparrow = K_\downarrow$ and $N_s^{(\uparrow)} = N_s^{(\downarrow)}$. Thus, the action of H is obtained in a spin-disentangled way. The generality of the method is not spoiled by the fact that it is fastest in the $S_z = 0$ sector, because it is useful provided that the spins are not totally lined up; on the other hand, $S_z = 0$ can always be assumed, as long as the Hamiltonian is $SU(2)$ invariant.

For illustration, consider the Hubbard model with two sites a and b and two electrons (H_2 molecule) each in the ϕ_a or ϕ_b orbital. The intersite hopping is t and the on-site repulsion U. In the standard method, one sets up basis vectors for the $S_z = 0$ sector

$$|\psi_1\rangle = |\phi_{a\uparrow}\rangle \otimes |\phi_{a\downarrow}\rangle, \qquad |\psi_2\rangle = |\phi_{a\uparrow}\rangle \otimes |\phi_{b\downarrow}\rangle,$$
$$|\psi_3\rangle = |\phi_{b\uparrow}\rangle \otimes |\phi_{a\downarrow}\rangle, \qquad |\psi_4\rangle = |\phi_{b\uparrow}\rangle \otimes |\phi_{b\downarrow}\rangle.$$

One then looks for eigenstates (three singlets and one triplet)

$$|\Psi\rangle = \sum_{i=1}^{4} \psi_i |\psi_i\rangle \tag{31}$$

of the Hamiltonian

$$H_{\rm H_2} = \begin{pmatrix} U & t & t & 0 \\ t & 0 & 0 & t \\ t & 0 & 0 & t \\ 0 & t & t & U \end{pmatrix}. \tag{32}$$

Instead of working with 4×4 matrices, we can cope with 2×2 by the spin-disentangled method using the form in equation (29) with

$$L = \begin{pmatrix} \psi_1 & \psi_2 \\ \psi_3 & \psi_4 \end{pmatrix}, \qquad K_\sigma = \begin{pmatrix} 0 & t \\ t & 0 \end{pmatrix},$$
$$N_a^{(\sigma)} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad N_b^{(\sigma)} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Using equation (30), one finds

$$H_{\rm H_2}|\Psi\rangle = \sum_{\alpha=a,b} \sum_{\beta=a,b} (H_{\rm H_2}[L])_{\alpha\beta} |\phi_{\alpha\uparrow}\rangle \otimes |\phi_{\beta\downarrow}\rangle \tag{33}$$

with

$$H_{\rm H_2}[L] = \begin{pmatrix} U\psi_1 + t(\psi_2 + \psi_3) & t(\psi_1 + \psi_4) \\ t(\psi_1 + \psi_4) & U\psi_4 + t(\psi_2 + \psi_3) \end{pmatrix}. \tag{34}$$

The reader can readily verify that this is the same as applying $H_{\rm H_2}$ in the form of equation (32) to the standard wave function in equation (31) and then casting the result in the form of equation (29). Since we can apply $H_{\rm H_2}$ we can also diagonalize it.

$\mathcal{N} = 4$ for the H_2 toy model, but in the $S_z = 0$ sector for the $|\Lambda|$=3 ring, $\mathcal{N} = 1863225$ and $\sqrt{\mathcal{N}} = 1365$, which is a clear advantage. Here we have implemented this method for the Hubbard Hamiltonian. We emphasize, however, that this approach will be generally useful for the many-fermion problem, even with a realistic Coulomb interaction, which can be suitably discretized.

5.1 The practical numerical recipe

We put a symmetry-adapted trial wave function in the form in equation (29) and operate the Hamiltonian matrix by equation (30); each new application introduces a new Lanczos *site* and we can proceed by generating a Lanczos *chain*. To this end we need to orthogonalize to the previous *sites* by the scalar product given by $\langle\Psi_1|\Psi_2\rangle = {\rm Tr}(L_1^\dagger L_2)$. In this way we put the Hamiltonian matrix in a tri-diagonal form. This method is well suited since we are mainly interested in the low-lying part of the spectrum. A severe numerical instability sets in when the chain exceeds a few tens of *sites*, *i.e.* well before the Lanczos method converges. Therefore we use repeated two-site chains alternated with moderate-size ones.

In the basis of the sites (of the original cluster) the occupation matrices $N_s^{(\sigma)}$ are diagonal with elements equal to 0 or 1, simplifying the calculation of the interaction term. Moreover, in choosing the trial wave function for small τ we take full advantage from our knowledge of the S_4 irrep of the $\tau = 0$ ground state. This speeds the calculation by a factor of the order of 2 or 3 compared to a random starting state (or even more, if U is large). Typically, starting from a $\tau = 0$ ground state for the three-unit ring, 24 short Lanczos *chains* were enough to obtain a roughly correct energy and a 20-*site chain* achieved an accurate eigenvalue and an already stabilized eigenvector. In limiting cases when the results could be checked against analytic ones, using double precision routines an accuracy better than 12 significant digits was readily obtained. On a personal computer with a Celeron CPU the three-unit ring with 8 particles required 40 minutes for the eigenvalue, and an accurate wave function required less than a hour.

6 Numerical results and discussion: the two-unit "ring"

In this section we analyze the two-unit ring with $\Delta_{\mathrm{CuO_4}}(4) < 0$. Here a complex τ is equivalent to a real one, *i.e.* no magnetic field can thread the system. This is peculiar of the ring with two clusters, since each CuO_4 is on the right as well as on the left of the other. Indeed, we have

$$H_\tau = (\tau + \tau^*) \sum_{j\sigma} \left(p^\dagger_{1,j\sigma} p_{2,j\sigma} + p^\dagger_{2,j\sigma} p_{1,j\sigma} \right) = 2|\tau| \cos\left(\frac{\pi\phi}{\phi_0}\right) \sum_{j\sigma} \left(p^\dagger_{1,j\sigma} p_{2,j\sigma} + p^\dagger_{2,j\sigma} p_{1,j\sigma} \right); \quad (35)$$

hence, the ground state energy $E^{(0)}(\phi, |\tau|)$ as a function of the flux ϕ and of the modulus of τ satisfies

$$E^{(0)}(\phi, |\tau|) = E^{(0)}\left(0, |\tau| \cos\frac{\pi\phi}{\phi_0}\right). \quad (36)$$

$E^{(0)}(\phi, |\tau|)$ has a local maximum at $\phi = \phi_0/2$ (a property which is independent of the number of particles in the two-unit ring) since H_τ in equation (35) vanishes; see Figure 6 for the case of $2|\Lambda| + 2 = 6$ particles.

The translational invariance allows to label any state by the *crystal momentum* $p \equiv \pi\hbar k$, $k = 0, 1$. We introduce the short-hand notation $|+\rangle$ and $|-\rangle$ for the components of the 6-body non-interacting ground-state multiplet with $k = 0$ and $k = 1$ respectively

$$|\pm\rangle = \frac{1}{\sqrt{2}} \left[|\Psi_0^{(4)}(1)\rangle |\Psi_0^{(2)}(2)\rangle \pm |\Psi_0^{(2)}(1)\rangle |\Psi_0^{(4)}(2)\rangle \right]. \quad (37)$$

We have

$$\langle \Psi_0^{(3)}(1)| \langle \Psi_0^{(3)}(2)| H_\tau |-\rangle = 0 \quad (38)$$

(the singlet projection of $|\Psi_0^{(3)}(1)\rangle |\Psi_0^{(3)}(2)\rangle$ has $k = 0$ quantum number) and there is no second order correction in the $k = 1$ subspace as shown in Figure 6. In the $k = 0$ subspace the correction is proportional to $|\tau|^2/\Delta_{\mathrm{CuO_4}}$ for small $|\tau|$, in agreement with the analytical predictions. As shown in Figure 6, the maximum at $\phi = \phi_0/2$ is not a cusp, as there no level crossing is found.

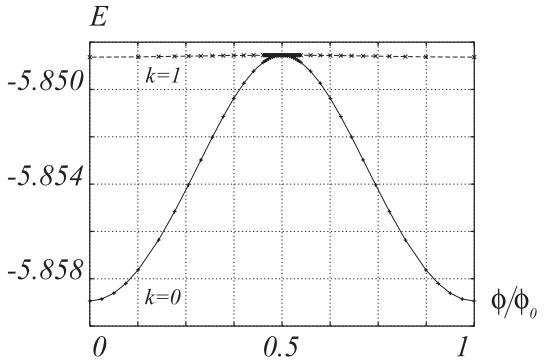

Fig. 6. Energy of the ground state ($k = 0$) and of the first excited state ($k = 1$) with $2|\Lambda|+2 = 6$ particles as a function of ϕ/ϕ_0. Here $U = 5t$, ($\Delta_{\mathrm{CuO_4}}(4) \approx -0.04258\,t$) and $|\tau| = 0.001\,t$. The energies are in units of t.

7 Numerical results and discussion: the three-unit ring

7.1 O-O intercell hopping

In this section we consider the three-unit ring focusing the attention on the case $\Delta_{\mathrm{CuO_4}}(4) < 0$ and total number of particles $2|\Lambda| + 2 = 8$. The switching on of the hopping τ between the O sites breaks the symmetry group $C_{3v} \otimes S_4^3$ into $C_{3v} \otimes S_4$ for real τ; in a magnetic field (complex τ), this further breaks into $C_3 \otimes S_4$. Real τ lifts the degeneracy between the $k = 0$ subspace and the subspaces $k = 1$ and $k = 2$ of C_3 (as usual k is related to the crystal momentum $p \equiv 2\pi\hbar k/3$ in this case), but cannot split $k = 1$ and 2 because they belong to the degenerate irrep of C_{3v}; complex τ resolves this degeneracy.

In Figure 7 we report the numerically exact results for a ring with three clusters, with $U = 5t$ and $|\tau|$ in the range from 0 to $0.006t$. The ground state energy and the first excited level depend quadratically on $|\tau|$ for small $|\tau|$. As expected from equation (23), the lower eigenspace has $k = 0$, while the first excited one contains the states with $k = 1$ and 2. Differently from the two-unit ring, the first excited level receives a second-order correction.

The three-unit ring is the smallest ring where we can insert a magnetic flux ϕ by $\tau = |\tau| e^{i\theta}$, $\theta = \frac{2\pi}{3}(\phi/\phi_0)$. The energies of the three ground-state multiplet components are reported in Figure 8 for $|\tau| \ll |\Delta_{\mathrm{CuO_4}}(4)|$ and $U = 5t$. At $\phi = 0$ the ground state belongs to the $k = 0$ subspace, while the first excited levels have $k = 1$ and 2. Their spatial degeneration is fully lifted: the $k = 1$ level increases while the $k = 2$ level decreases up to $\phi = \phi_0/2$. As ϕ increases, the ground state energy grows quadratically in ϕ (diamagnetic behaviour). Near $\phi = \phi_0/4$ we find a level crossing between $k = 0$ and $k = 2$, while at

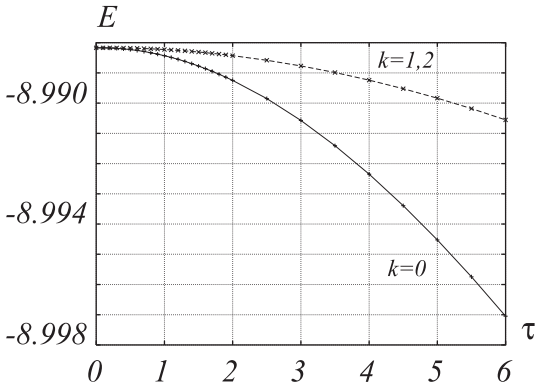

Fig. 7. Energies of the ground state ($k = 0$) and of the first excited state ($k = 1$ and 2) of the three-unit ring with 8 particles *versus* $|\tau|$ for $U = 5t$. The energies are in units of t, the parameter $|\tau|$ is in units of $10^{-3}t$.

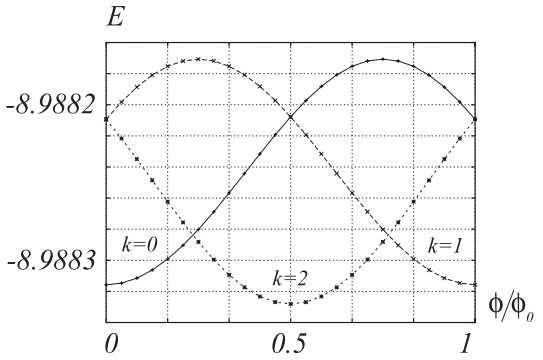

Fig. 8. Numerical results for the low energy states of the three-unit ring , as a function of the concatenated magnetic flux. Here $U = 5\ t$, ($\Delta_{\mathrm{CuO_4}}(4) \approx -0.04258\, t$) $|\tau| = 0.001\, t$. The energy is in units of t.

$\phi = \phi_0/2$, $k = 0$ becomes degenerate with $k = 1$ and the ground state energy is in a new minimum belonging to the $k = 2$ subspace: a sort of "restoring" of the $\phi = 0$ situation is taking place as in the BCS theory [50]. Indeed, at $\phi = \phi_0/2$ the symmetry group is $\tilde{C}_{3v} \otimes S_4$ where $\tilde{C}_{3v}$ is isomorphous to C_{3v} (reflections σ are replaced by σg, where g is a suitable gauge transformation). This feature was also found in other geometries [18,32]. In the region from $\phi = \phi_0/2$ and $\phi = \phi_0$ we numerically verified that $E_{k=2}(\phi) = E_{k=2}(\phi_0 - \phi)$, $E_{k=0}(\phi) = E_{k=1}(\phi_0 - \phi)$ and $E_{k=1}(\phi) = E_{k=0}(\phi_0 - \phi)$, where $E_k(\phi)$ is the ground state energy in the k sector. The comparison of the numerical results shown in Figure 8 with the analytic ones in Figure 5 supports the accuracy of the cell-perturbation scheme proposed in Section 4. Thus, the dressed $W = 0$ pair screens the vector potential as a particle with an effective charge $e^* = 2e$ does. At both minima of $E^{(0)}(\phi)$ we have computed $\Delta_{3-\mathrm{unit}}(8) \approx -10^{-2}t$. Here, the half-integer AB effect is actually SFQ.

Fulfilling the conditions $\Delta_{\mathrm{CuO_4}}(4) < 0$ and $|\tau| \ll |\Delta_{\mathrm{CuO_4}}(4)|$, we varied U and $|\tau|$ and found analogous trends for the ground state energy. Increasing $|\tau|$ with fixed $\Delta_{\mathrm{CuO_4}}(4)$ lowers the central minimum and depresses the two maxima. On the other hand, if $|\Delta_{\mathrm{CuO_4}}(4)|$ decreases at fixed $|\tau|$ the central minimum and the side peaks are affected in a similar way. This is reasonable since the perturbative parameter is $|\tau|/|\Delta_{\mathrm{CuO_4}}(4)|$.

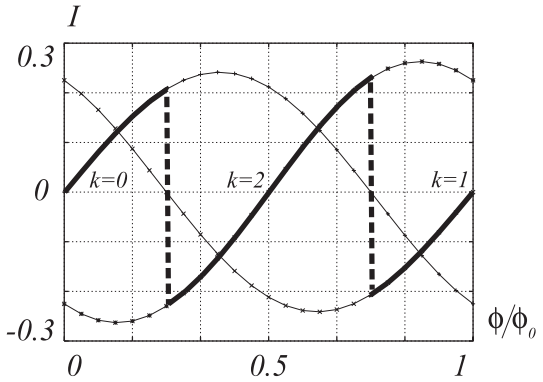

Fig. 9. Total current for the three-CuO_4 ring, as a function of the magnetic flux. Here $U = 5\ t$, $|\tau| = 0.001\, t$. The current is in units of $e|\tau|/h$. The thick line marks the ground state current.

The three-unit ring also enables us to study persistent diamagnetic currents carried by bound pairs screening the magnetic flux. We calculated the expectation value for each k of the total current operator as a function of the flux. The current operator [51]

$$\hat{I} = c\frac{\partial H_{\mathrm{tot}}}{\partial \phi} = \frac{e}{\hbar|\Lambda|}\sum_{i,\alpha,\sigma} i\left(\tau\, p^{\dagger}_{\alpha+1,i\sigma}p_{\alpha,i\sigma} - \tau^{*}p^{\dagger}_{\alpha,i\sigma}p_{\alpha+1,i\sigma}\right) \quad (39)$$

yields a gauge invariant average I. By expanding $\hat{I}$ in equation (39) in powers of ϕ near $\phi = 0$ one may identify the paramagnetic and the diamagnetic contributions with the zeroth and the first order terms respectively [52]. The results are reported in Figure 9; the current is proportional to the flux derivative of the ground-state energy (see Fig. 8) according to the Hellmann-Feynman theorem. Near $\phi = 0$ the system generates a diamagnetic current which screens the threaded magnetic field. When ϕ exceeds a critical value $\sim \phi_0/4$, a breakdown of the ground state occurs. This corresponds to a discontinuity of the current which changes sign; then the current enhances the external field. At $\phi = \phi_0/2$ the current vanishes again. Indeed, like at $\phi = 0$, the eigenfunctions may be chosen real (H_τ at $\phi = \phi_0/2$ is obtained from H_τ at $\phi = 0$ by reversing the sign of four O-O bonds connecting two nearest neighbours units). Thus, near $\phi_0/2$ the magnetic flux is still a small perturbation with respect to a new real intercell hopping Hamiltonian and the current correctly screens the new magnetic field. From Figure 9 we see that the maximum value of the diamagnetic current is of the order of $1 \div 10$ nano Ampere if $t = 1$ eV and the ratio $I/(\phi/\phi_0) \approx e|\tau|/h$ near $\phi = 0$.

In Figure 10 we show the trend of the ground state energy in each k sector for the non-interacting ($U = 0$) three-unit ring. In this case there is no pairing in CuO_4 and indeed the ground state energy is linear in the field at small fields (normal Zeeman effect). The lowest state is

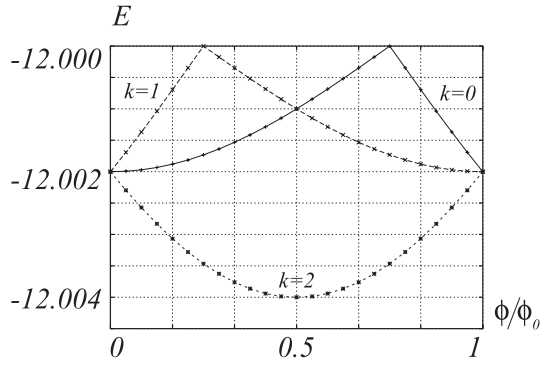

Fig. 10. Low energy states of the three-unit ring *versus* ϕ/ϕ_0. Here $U = 0$ and $|\tau| = 0.001\,t$. The energy is in units of t.

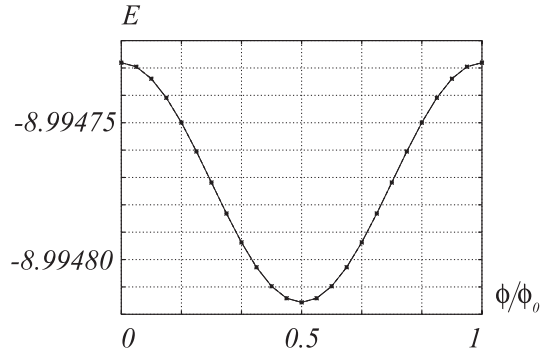

Fig. 11. Ground state energy E of the three-unit ring in units of t, as a function of the concatenated magnetic flux. E is k-independent (see text). Here $U = 5\ t$, $|\tau_{\rm Cu}| = 0.1t$.

$k = 2$ throughout. Interestingly, the three-unit ring *concatenated with half a flux quantum* would be diamagnetic, but the absence of a second minimum shows that it would be Larmor diamagnetism. The absence of SFQ in Figure 10 is a further evidence of the repulsion-driven pairing mechanism discussed in Section 2.

7.2 Cu-Cu intercell hopping

We can alternatively model the three-unit ring by connecting only the central Cu sites of the constituent CuO_4 units with a hopping term $\tau_{\rm Cu}$; in order to study the propagation of a bound pair we again assume the total number of particles $2|\Lambda| + 2 = 8$. The full system threaded by the flux has a $C_3 \otimes S_4^3$ symmetry because the O sites are not involved in the intercell Hamiltonian. Again, we consider the case $\Delta_{\rm CuO_4}(4) < 0$ and ask if now the $W = 0$ bound pair can screen out the magnetic flux.

We find that $\tau_{\rm Cu}$ produces much smaller effects than τ; for $|\tau_{\rm Cu}| \ll |\Delta_{\rm CuO_4}(4)|$ the energy eigenvalues are outright ϕ independent to great accuracy. Therefore we considered $|\tau_{\rm Cu}| = 0.1t$; still the dependence of the ground state energy is weak, see Figure 11. At $\phi = 0$, the correction [53] due to $|\tau_{\rm Cu}|$ to ground state energy is $\sim 10^{-3}t$. Moreover, remarkably, the system behaves as a paramagnet.

The reason of this unusual behavior is the following. There is no flux-induced splitting of the three k levels because the $W = 0$ pair is strictly localized by the *local* symmetry. Indeed the S_4 label of each CuO_4 unit is a good quantum number. No SFQ is observed because the screening of the magnetic field by the bound pair is forbidden. The small correction to the ground state energy comes from a second-order process. Starting *e.g.* with an unperturbed state $|4, 2, 2\rangle$, in which the bound pair is localized on the first cluster, the correction involves virtual states $|3, 3, 2\rangle$ and $|3, 2, 3\rangle$ in which a totalsymmetric particle jumps forth and back on the nearby clusters. This process occurs with a small amplitude because of a severe energy misfit. This is particularly clear at weak coupling, when the lowest-energy A_1 particle of the first cluster must hop to antibonding A_1 orbitals of the nearby clusters; the amplitude of this process is further reduced by the overlap of these orbitals with the localized Cu one. However, such virtual processes are insensitive to the flux. Any ϕ dependence arises from third-order corrections (order $|\Lambda|$ in general). Indeed, the A_1 particle must go virtually around the trip clockwise or anticlockwise. In the ground state, of course, it chooses the wise in such a way to gain energy from the magnetic field. This is why a paramagnetic dependence on the flux is seen in Figure 11 and the correction goes like $-\phi^2$ at small ϕ. This is interesting because it shows how the local symmetry can hinder the tunneling of bound pairs carrying conserved quantum numbers; SFQ is not a necessary consequence of superconductivity if the pairs are not totalsymmetric.

8 Conclusions

We propose a Hubbard model with on-site repulsion defined on a graph Λ with 5-site C_{4v}-symmetric clusters as nodes in order to study the response of the system to a threading magnetic flux. For ring-shaped systems and weak O-O links we find a half-integer AB effect which is unambiguously interpreted as SFQ. The key ingredient is the $W = 0$ pair which is a two-body singlet eigenstate of $H_{\rm CuO_4}$ without double occupation and is formed by mixing degenerate one-body states. In the interacting problem the $W = 0$ pair becomes a bound pair when four particles lie in the CuO_4 cluster. The pairing mechanism is due to an effective attractive interaction mediated by repeated electron-hole exchanges with the *Fermi sea*. Thus, SFQ may be found in purely repulsive $1d$ Hubbard models if the nodes are represented by a non-trivial basis. Focusing on the low-energy sector, we find a simplified description of the model in terms of an effective hard-core boson Hamiltonian that can be solved exactly for ring-shaped systems and arbitrary filling. Further, we show that the boson Hamiltonian is equivalent to the well-known [42] Heisenberg-Ising spin chain with an antiferromagnetic anisotropy parameter $\eta = -1$.

The analytic results are well confirmed by the numerical findings for the two- and three-unit ring (14,400 and 1,863,225 configurations). To this end, we have recently introduced a new exact-diagonalization technique. By disentangling spin-up and spin-down we reduce the size of

the matrices that must be handled considerably; for spin-unpolarized systems the matrix dimension is the square root of the overall size of the Hilbert space. The method allows large further reductions by exploiting the symmetry; this can be done in several ways. One can first diagonalize Dirac's characters and then apply the spin-disentangled technique with a smaller function space; alternatively, one can set up the spin-disentangled technique by a variational approach, a projection operator (H^n) or Lanczos method, starting with a trial state belonging to a well defined symmetry.

We have computed the ground state energy and the induced supercurrent as a function of the trapped flux in the case of weak O-O links. We have also studied the effect of direct intercell Cu-Cu links; in this case, bound pair propagation is hindered by symmetry, because each unit must keep its own S_4 irrep. Hence, the unusual situation arises when the threading flux is not screened by the superconducting pairs and a paramagnetic response prevails.

References

1. Y. Aharonov, D. Bohm, Phys. Rev. **115**, 485 (1959); R.G. Chambers, Phys. Rev. Lett. **5**, 3 (1960)
2. R.M. Fye, M.J. Martins, D.J. Scalapino, J. Wagner, W. Hanke, Phys. Rev. B **44**, 6909 (1991)
3. F.V. Kusmartsev, J. Phys.: Condens. Matter **3**, 3199 (1991)
4. A.J. Schofield, J.M. Wheatley, T. Xiang, Phys. Rev. B **44**, 8349 (1991)
5. N. Yu, M. Fowler, Phys. Rev. B **45**, 11795 (1992)
6. F.V. Kusmartsev, J.F. Weisz, R. Kishore, M. Takahashi, Phys. Rev. B **49**, 16234 (1994); F.V. Kusmartsev, Phys. Rev. B **52**, 14445 (1995)
7. E.H. Lieb, F. Wu, Phys. Rev. Lett. **20**, 1445 (1968)
8. A. Ferretti, I.O. Kulik, A. Lami, Phys. Rev. B **45**, 5486 (1992)
9. F. Nakano, J. Phys. A **33**, 5429 (2000)
10. A. Sudbø, C.M. Varma, T. Giamarchi, E.B. Stechel, R.T. Scalettar, Phys. Rev. Lett. **70**, 978 (1993); E.B. Stechel, A. Sudbø, T. Giamarchi, C.M. Varma, Phys. Rev. B **51**, 553 (1995)
11. L. Arrachea, A.A. Aligia, Phys. Rev. Lett. **73**, 2240 (1994)
12. L. Arrachea, A.A. Aligia, E. Gagliano, Phys. Rev. Lett. **76**, 4396 (1996)
13. A. Ferretti, I.O. Kulik, A. Lami, Phys. Rev. B **47**, 12235 (1993)
14. G.S. Canright, S.M. Girvin, Int. J. Mod. Phys. B **3**, 1943 (1989)
15. F.F. Assaad, W. Hanke, D.J. Scalapino, Phys. Rev. Lett. **71**, 1915 (1993)
16. L. Arrachea, A.A. Aligia, Phys. Rev. B **61**, 9686 (2000)
17. P.W. Anderson, Science **235**, 1196 (1987)
18. M. Cini, G. Stefanucci, A. Balzarotti, Eur. Phys. J. B **10**, 293 (1999)
19. M. Cini, G. Stefanucci, A. Balzarotti, Solid State Commun. **109**, 229 (1999)
20. D. Zanchi, H.J. Schulz, Z. Phys.: Condens. Matter B **103**, 339 (1997); D. Zanchi, H.J. Schulz, Europhys. Lett. **44**, 235 (1998)
21. C.J. Halboth, W. Metzner, Phys. Rev. B **61**, 7364 (2000)
22. C. Honerkamp, M. Salmhofer, N. Furukawa, T.M. Rice, Phys. Rev. B **63**, 035109 (2001); C. Honerkamp, Eur. Phys. J. B **21**, 81 (2001)
23. N.E. Bickers, D.J. Scalapino, S.R. White, Phys. Rev. Lett. **62**, 961 (1989); N.E. Bickers, S.R. White, Phys. Rev. B **43**, 8044 (1991); G. Esirgen, N.E. Bickers, Phys. Rev. B **57**, 5376 (1998) and references therein
24. W. Fettes, I. Morgensten, Eur. Phys. J. B **9**, 635 (1999) and references therein
25. M. Cini, A. Balzarotti, Il Nuovo Cimento D **18**, 89 (1996)
26. M. Cini, A. Balzarotti, J. Phys. C **8**, L265 (1996)
27. M. Cini, A. Balzarotti, Solid State Comm. **101**, 671 (1997); M. Cini, A. Balzarotti, J. Tinka Gammel, A.R. Bishop, Il Nuovo Cimento D **19**, 1329 (1997)
28. M. Cini, A. Balzarotti, Phys. Rev. B **56**, 14711 (1997)
29. F.C. Zhang, T.M. Rice, Phys. Rev. B **37**, 3759 (1988)
30. M. Arjunwadkar, G. Baskaran, R. Basu, V.N. Mathumukar, Phys. Rev. Lett. **70**, 674 (1993)
31. M. Cini, G. Stefanucci, E. Perfetto, A. Callegari, J. Phys.: Cond. Matt. **14**, L709 (2002)
32. M. Cini, A. Balzarotti, G. Stefanucci, Eur. Phys. J. B **14**, 269 (2000)
33. S. Mazumdar, F. Guo, D. Guo, K.C. Ung, J.T. Gammel, *Proceeding of the Discussion meeting on strongly correlated electron systems in chemistry, Bangalore, India* (Springer Verlag 1996)
34. W. Kohn, J. Luttinger, Phys. Rev. Lett. **15**, 524 (1965)
35. R. Shankar, Rev. Mod. Phys. **66**, 129 (1994)
36. A.V. Chubukov, Phys. Rev. B **48**, 1097 (1993)
37. E. Perfetto, G. Stefanucci, M. Cini, Phys. Rev. B **66**, 165434 (2002)
38. H.B. Schttler, A.J. Fedro, Phys. Rev B **45**, 7588 (1992)
39. J.H. Jefferson, H. Eskes, L.F. Feiner, Phys. Rev. B **45**, 7959 (1992); L.F. Feiner, J.H. Jefferson, H. Eskes, Phys. Rev. B **53**, 8751 (1996)
40. V.J. Emery, Phys. Rev. Lett. **58**, 2794 (1987)
41. F. Bloch, Z. Physik **61**, 206 (1930); F. Bloch, Z. Physik **74**, 295 (1932)
42. L. Hulthen, Arkiv. Mat. Astron. Fysik **26** A, No. 11 (1938)
43. R. Orbach, Phys. Rev. **112**, 309 (1958)
44. H.A. Bethe, Z. Physik **71**, 205 (1931)
45. C.N. Yang, C.P Yang, Phys. Rev. **147**, 303 (1966); C.N. Yang, C.P. Yang, Phys. Rev. **150**, 321 (1966); C.N. Yang, C.P. Yang, Phys. Rev. **150**, 327 (1966); C.N. Yang, C.P. Yang, Phys. Rev. **151**, 258 (1966)
46. B.S. Shastry, B. Sutherland, Phys. Rev. Lett. **65**, 243 (1990); B. Sutherland, B.S. Shastry, Phys. Rev. Lett. **65**, 1833 (1990)
47. R. Micnas, J. Ranninger, S. Robaszkiewicz, Rev. Mod. Phys. **62**, 113 (1990)
48. A.A. Aligia, Phys. Rev. B **61**, 7028 (2000)
49. E.H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989)
50. W.A. Little, R.D. Parks, Phys. Rev. Lett. **9**, 9 (1962)
51. W. Kohn, Phys. Rev. **133**, A171 (1964)
52. E. Dagotto, Rev. Mod. Phys. **66**, 763 (1994)
53. Using as above $U = 5t$ one finds $E^{(0)}_{\mathrm{CuO_4}}(2) = -3.13962t$, and $E^{(0)}_{\mathrm{CuO_4}}(4) = -2.708931t$