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LETTER TO THE EDITOR

'Spin-disentangled' exact diagonalization of repulsive Hubbard systems: superconducting pair propagation

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Abstract

By means of a novel exact-diagonalization technique, we show that bound pairs propagate between repulsive Hubbard clusters in a superconducting fashion. The size of the matrices that must be handled depends on the number of fermion configurations *per spin*, which is of the order of the square root of the overall size of the Hilbert space. We use CuO_4 units connected by weak O–O links to model the interplanar coupling and *c*-axis superconductivity in cuprates. The numerical evidence on Cu_2O_8 and Cu_3O_{12} prompts the proposal of a new analytic scheme describing the propagation of bound pairs and also the superconducting flux quantization in a 3D geometry.

(Some figures in this article are in colour only in the electronic version)

Evidence for pairing in the repulsive Hubbard and related models has been reported by several authors. Analytic approaches [1, 2], even at strong coupling [3], generalized conserving approximation theories like FLEX [4], as well as quantum Monte Carlo studies on supercells [5] lead to this conclusion. However, we want more evidence about the real nature of the pairing interactions. Su and co-workers [6] have reported that in narrow-band one- and two-dimensional Hubbard models, no kind of superconducting long-range order holds at any non-zero temperature. Here we wish to explore the possibility that the Hubbard model can show superconductivity in the ground state when interplanar coupling is allowed. Since one cannot master the problem with an infinite stack of infinite planes, some economy is needed. However, in high-T_c superconductors the coherent length is approximately a few lattice constants, and Cu–O planes can be approximately represented by clusters that are large enough to host a bound pair. The *interplanar* hopping does not dissolve pairs and superconducting flux quantization is their clear signature. The magnetic properties of *attractive* Hubbard models have been studied by Canright and Girvin [7]; here we propose a gedanken experiment very much in the spirit of Little and Parks [8], in the *repulsive* case.

The repulsive Hubbard Hamiltonian of fully symmetric clusters $\mathcal{C}$ has two-body singlet eigenstates without double occupation [9–12] called $W = 0$ pairs. The presence of such

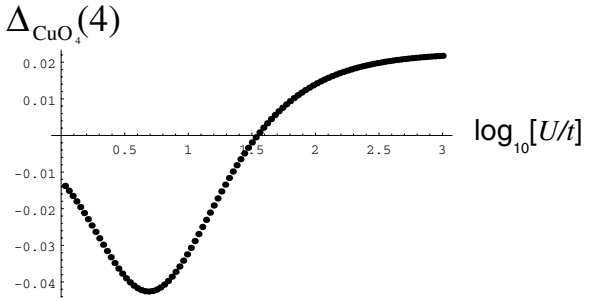

Figure 1. The trend of $\Delta_{CuO_4}(4)$ in t units versus $\log[U/t]$.

solutions at the highest occupied level of the non-interacting (Hubbard $U \to 0$) system is necessary to allow $\Delta_{\mathcal{C}}(N) < 0$ where $\Delta_{\mathcal{C}}(N) = E_{\mathcal{C}}^{(0)}(N) + E_{\mathcal{C}}^{(0)}(N-2) - 2E_{\mathcal{C}}^{(0)}(N-1)$, and $E_{\mathcal{C}}^{(0)}(N)$ is the interacting ground state energy of the cluster $\mathcal{C}$ with N fermions. By means of a non-perturbative canonical transformation [2] [13], it can also be shown that $\Delta_{\mathcal{C}}(N) < 0$ is due to an attractive pairing effective interaction and at weak coupling $|\Delta_{\mathcal{C}}(N)|$ is just the binding energy of the pair.

CuO_4 is the smallest cluster which fully preserves the point symmetry of the copper oxide planes of high-T_c materials. 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 [1, 11]. $W = 0$ bound pairs in the CuO_4 cluster are found to exist in the physical region of the parameter space. However, since it is the symmetry that produces the pairing force, we use the simplest working model to study bound pair propagation. Here, in order to simplify the analytical formulae, we neglect the O–O hopping term and also any distinction between Cu and O sites (except as regards geometry, of course). The only non-vanishing hopping matrix elements are those between an oxygen site and the central copper 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; the important thing is that in this way we still have access to the part of the parameter space where pairing occurs [9]. Thus, we consider the Hubbard Hamiltonian

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

where $p_{i\sigma}^\dagger$ and $p_{i\sigma}$ are the creation and annihilation operators on the oxygen $i = 1, \ldots, 4$ with spin $\sigma = \uparrow, \downarrow$, $d_\sigma^\dagger$ and d_σ are the creation and annihilation operators on the copper 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_{CuO_4} is invariant under the permutation group $S[4]$, which has the irreducible representations (*irreps*) $\mathcal{A}_1$ (totally symmetric), $\mathcal{B}_2$ (totally antisymmetric), $\mathcal{E}$ (self-dual), $\mathcal{T}_1$ and its dual $\mathcal{T}_2$, of dimensions 1, 1, 2, 3 and 3, respectively. The ground state of $CuO_4[2]$ (i.e. CuO_4 with two fermions) 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. $\Delta_{CuO_4}(4) < 0$ for this model when $0 < U \lesssim 34.77t$, as shown in figure 1.

Thus, we introduce a graph Λ with CuO_4 units as nodes. The total Hamiltonian is

$$H_{tot} = H_0 + H_\tau \tag{2}$$

with

$$H_0 = \sum_{\alpha\in\Lambda}\left[t\sum_{i\sigma}(d^\dagger_{\alpha\sigma}p_{\alpha,i\sigma} + p^\dagger_{\alpha,i\sigma}d_{\alpha\sigma}) + U\left(\sum_i \hat{n}^{(p)}_{\alpha,i\uparrow}\hat{n}^{(p)}_{\alpha,i\downarrow} + \hat{n}^{(d)}_{\alpha\uparrow}\hat{n}^{(d)}_{\alpha\downarrow}\right)\right], \quad (3)$$

where $p^\dagger_{\alpha,i\sigma}$ is the creation operator on the oxygen $i = 1,\ldots,4$ of the αth cell and so on. Hence, the point symmetry group of H_0 is $S[4]^{|\Lambda|}$, with $|\Lambda|$ the number of nodes. There are many different ways to model an *interplanar* hopping. Nevertheless, to preserve the symmetry that produces the $\Delta_{CuO_4}(4) < 0$ property, H_τ must be invariant under the $S[4]$ diagonal subgroup of $S[4]^{|\Lambda|}$. In the following we shall consider a hopping term allowing a particle in the ith oxygen site of the αth unit to move towards the ith oxygen site of the βth unit with hopping integral $\tau_{\alpha\beta}$:

$$H_\tau = \sum_{\alpha,\beta\in\Lambda}\sum_{i\sigma}[\tau_{\alpha\beta}p^\dagger_{\alpha,i\sigma}p_{\beta,i\sigma} + \text{h.c.}]. \quad (4)$$

For $N = 2|\Lambda|$ and $\tau_{\alpha\beta} \equiv 0$, the unique ground state consists of two fermions in each CuO_4 unit. This letter is devoted to the interplanar hopping produced by small $\tau_{\alpha\beta} \ll |\Delta_{CuO_4}(4)|$ with a total number of particles $N = 2|\Lambda|+2p$; p represents the number of added pairs. When U/t is such that $\Delta_{CuO_4}(4) < 0$, 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).

Using such models, one can study the interaction of several fermion pairs in the same system. The simplest topologically non-trivial graph is the ring, with a set $\Lambda = \{1, 2, \ldots, |\Lambda|\}$ and

$$\tau_{\alpha\beta} = \begin{cases} \tau & \text{if } \beta = \alpha + 1, \\ \tau^* & \text{if } \beta = \alpha - 1, \\ 0 & \text{otherwise,} \end{cases} \qquad \tau = |\tau|\exp\left(\frac{2\pi\mathrm{i}}{|\Lambda|}\frac{\phi}{\phi_0}\right), \quad (5)$$

where ϕ is the magnetic flux concatenated by the ring and $\phi_0 = hc/e$. In the absence of magnetic field, τ will be taken to be real.

Note that for $p = 0$ the concentration (number of holes per atom) is $2/5 = 0.4$; this is somewhat more than half-filling ($1/3 \approx 0.33$) but still reasonable. 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 [12] and the full plane [1, 2] too. By replacing CuO_4 by larger units, one can model other ranges of the hole concentration.

We exactly diagonalize the $|\Lambda| = 2$- and 3-ring Hamiltonians; to this end we introduce the *spin-disentangled* technique. 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 wavefunction in the form

$$|\Psi\rangle = \sum_{\alpha\beta} L_{\alpha\beta}|\phi_{\alpha\uparrow}\rangle \otimes |\phi_{\beta\downarrow}\rangle \quad (6)$$

which shows how the $\uparrow$ and $\downarrow$ configurations are entangled. The electrons of one spin are treated as the 'bath' for those of the opposite spin: this form also enters the proof of a famous theorem of Lieb [14]. In equation (6) $L_{\alpha\beta}$ 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_{tot} in the basis $\{|\phi_{\alpha\sigma}\rangle\}$, and $N^{(\sigma)}_s$ the spin-σ occupation number matrix at site s in the same basis ($N^{(\sigma)}_s$ is a symmetric matrix since the $|\phi_{\alpha\sigma}\rangle$s are real). Then, L is acted upon by the Hamiltonian H_{tot} according to the rule

$$H_{\text{tot}}[L] = [K_\uparrow L + LK_\downarrow] + U\sum_s N^{(\uparrow)}_s L N^{(\downarrow)}_s. \quad (7)$$

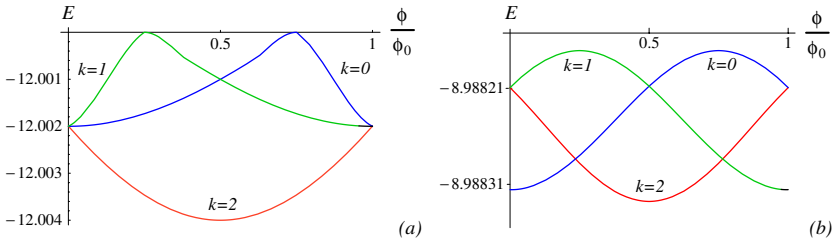

Figure 2. Numerical results for Cu_3O_{12} with $\tau = 0.001$. Lowest-energy eigenvalues labelled by their interplanar quasi-momentum are shown versus flux ϕ. The pattern is periodic (a flux quantum can be gauged away). (a) $U = 0$. A paramagnetic current is excited by the field and the system is utterly normal. (b) $U = 5$. The ground state shows a clear superconducting pattern, with a minimum at $\phi = \phi_0/2$. All energies are in t units.

In particular for $M_\uparrow = M_\downarrow$ ($S_z = 0$ sector) it holds that $K_\uparrow = K_\downarrow$ and $N_s^{(\uparrow)} = N_s^{(\downarrow)}$. Thus, the action of H is obtained in a spin-disentangled way. In the $S_z = 0$ sector for $|\Lambda| = 3$, the size of the problem is 1863 225 and the storage of the Hamiltonian matrix requires a lot of space; by the above device, we can work with matrices whose dimension is the square root of those of the Hilbert space: 1365×1365 matrices solve the $1863\,225 \times 1863\,225$ problem, and are not even required to be sparse. We believe that this approach will be generally useful for the many-fermion problem. Since we are mainly interested in getting the low-lying part of the spectrum as fast as possible, we opted for the Lanczos method, taking advantage of our knowledge of the $S[4]$ irrep of the $\tau = 0$ ground state; the scalar product is given by $\langle\Psi_1|\Psi_2\rangle = \mathrm{Tr}(L_1^\dagger L_2)$. In this way, the Hamiltonian matrix takes the tri-diagonal form; however, a numerical instability sets in well before convergence is achieved if one uses chains longer than a few tens of sites. Therefore we use repeated two-site chains alternated with moderate-size ones.

The two-CuO_4 ring (14 400 configurations in the $S_z = 0$ sector) is readily solved by a *Mathematica* code on a personal computer; however, this cluster is not adequate for studying the quantization (superconducting or otherwise) of a magnetic flux by the bound pair. The reason is that the two units are each at the left *and* at the right of each other; any vector potential perpendicular to the CuO_4s can always be gauged away. However, we have verified that the ground state energy with six holes is $E^{(0)}_{Cu_2O_8}(6) = E^{(0)}_{CuO_4}(4) + E^{(0)}_{CuO_4}(2)$ for $\tau = 0$ and it receives a negative correction $\propto \tau^2/|\Delta_{CuO_4}(4)|$ for small τ, which is consistent with the presence of a bound pair.

The three-CuO_4 ring behaves similarly, but can also concatenate a flux. In figures 2(a) and (b) we show the lowest eigenvalues versus ϕ for $U = 0$ and $5t$, respectively; k denotes the interplanar quasi-momentum quantum label. At $\tau = 0$ the ground state energy is $E^{(0)}_{Cu_3O_{12}}(8) = E^{(0)}_{CuO_4}(4) + 2E^{(0)}_{CuO_4}(2)$ and the low-energy sector derives mainly from the tensor product of the ground states of three independent CuO_4s with four, two and two holes (which is the fundamental multiplet) and three, three and two holes (which is the lowest-lying excited multiplet separated by a gap $\Delta_{CuO_4}(4)$). For $U = 0$—see figure 2(a)—there is no pairing in CuO_4 and indeed the ground state energy is linear in the field at small fields (the normal Zeeman effect). The lowest state is $k = 2$ throughout. Interestingly, Cu_3O_{12} *concatenated with half a flux quantum* would be diamagnetic, but the absence of a second minimum shows that this would be Larmor diamagnetism. By contrast, at $U = 5t$, when pairing in CuO_4 is about optimum—see figure 1)—the $k = 2$ state is lowest in the central sector, $k = 0$ is the ground state at $\phi \to 0$ while $k = 1$ is lowest as $\phi \to \phi_0$—see figure 2(b); this produces level crossings and the superconducting flux quantization; there is a central minimum when the system swallows a half-quantum of flux while, as we verified, $\Delta_{Cu_3O_{12}} < 0$. Remarkably, one

also observes superconducting quantization of a magnetic flux orthogonal to the plane [12]. With increasing U/t, the binding energy of the pair starts decreasing and eventually vanishes for $U \approx 34.77t$; we have found that at this point the flux quantization returns to normal and the system behaves like a paramagnet. Even at optimal U, the side barriers are depressed by increasing τ; at $\tau \sim 0.1t$ only small remnants remain; for still larger interplanar hoppings, the superconductivity is removed and a pattern similar to that of figure 2(a) prevails. For larger $|\Lambda|$, a smaller supercurrent would be necessary to screen the half-quantum of flux and the critical τ which kills the superconductivity should be expected to grow larger.

In order to better analyse the results physically and extend them qualitatively to arbitrary graphs, we obtained an effective Hamiltonian by the cell-perturbation method with H_0, equation (3), the 'cell Hamiltonian' and H_τ, equation (4), 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 [15] to support the original Anderson conjecture [16] on the 'low-energy equivalence' between the d–p model (proposed by Emery [17]) and the single-band Hubbard model. Despite the similarities with [15] (like having 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 two, three and four holes to get bound pairs, in contrast to the ones with zero, one and two holes of [15]).

For a general graph Λ, with $2|\Lambda| + 2p$ holes, we treat H_τ using a simplified second-order degenerate perturbation theory, since H_τ is a one-body operator. Each degenerate unperturbed ground state $|\Phi_0^{\mathcal{S}}\rangle$ may be labelled by a set $\mathcal{S} \subset \Lambda$ of units occupied by four holes; $|\mathcal{S}| = p$. The secular problem yields the eigenvalue equation

$$\frac{1}{\Delta_{CuO_4}(4)} \sum_q \sum_{\mathcal{S}'} \langle \Phi_0^{\mathcal{S}} | H_\tau | \Phi_q \rangle \langle \Phi_q | H_\tau | \Phi_0^{\mathcal{S}'} \rangle a_{\mathcal{S}'} = \varepsilon a_{\mathcal{S}} \tag{8}$$

where the sum has been truncated to the low-energy excited eigenstates involving CuO_4 units with $2 \leqslant n \leqslant 4$ holes, all taken in their ground states $|\Psi_0^{(n)}(\alpha)\rangle, \alpha = 1, \ldots, |\Lambda|$. The amplitude $a_{\mathcal{S}} \equiv a(\alpha_1, \ldots, \alpha_p)$ is totally symmetric with respect to permutations of the distinct indices $\alpha_1, \ldots, \alpha_p$. Letting $\mathcal{C}(\alpha) = \{\beta \in \Lambda : \tau_{\alpha\beta} \neq 0\}$, after some algebra equation (8) may be written in the form

$$\varepsilon a(\alpha_1, \ldots, \alpha_p) = \sum_{j=1}^{p} \sum_{\beta \in \mathcal{C}(\alpha_j)} \Bigg[\mathcal{T}^{\text{Bose}}_{\beta,\alpha_j} a(\alpha_1, \ldots, \alpha_{j-1}, \beta, \alpha_{j+1}, \ldots, \alpha_p) - |\mathcal{T}^{\text{Bose}}_{\beta,\alpha_j}| \prod_{i \neq j} (1 - \delta_{\beta\alpha_i}) a(\alpha_1, \ldots, \alpha_p) \Bigg]. \tag{9}$$

This is a Schrödinger equation for p hard-core bosons hopping with an effective hopping integral $\mathcal{T}^{\text{Bose}}_{\alpha,\beta} \equiv (\tau^{\text{eff}}_{\alpha\beta})^2 / \Delta_{CuO_4}(4)$, with

$$\tau^{\text{eff}}_{\alpha\beta} = \langle \Psi_0^{(2)}(\alpha)| \otimes \langle \Psi_0^{(4)}(\beta)| H_\tau |\Psi_0^{(3)}(\alpha)\rangle \otimes |\Psi_0^{(3)}(\beta)\rangle. \tag{10}$$

In figure 3(a) we show the trend of $(|\tau^{\text{eff}}_{\alpha\beta}|/|\tau_{\alpha\beta}|)^2$ versus U/t; we note that the ratio decreases monotonically. In equation (9), the first term in the rhs describes hole pair propagation, e.g. from unit α_j to an unoccupied unit β; in the second sum, the system gets back to the initial state after virtually exploring unit β; the term $\prod_{i \neq j}(1 - \delta_{\beta\alpha_i})$ takes into account that if β is one of the occupied units, the particle cannot move toward it. Due to the minus sign, the term in $|\mathcal{T}^{\text{Bose}}_{\beta,\alpha_j}|$ represents pair–pair repulsion.

In figure 3(b) the superconducting flux quantization for the $|\Lambda| = 3$ ring is reported as reproduced by solving equation (9); it agrees well both qualitatively and quantitatively with the numerical results of figure 2(b), thus confirming the above approximation. More data and a fuller account of the low-energy theory will be presented elsewhere.

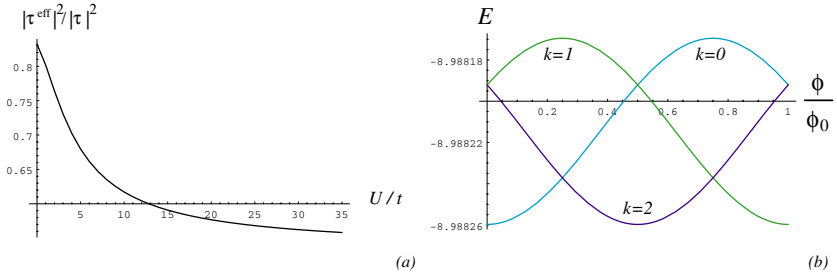

Figure 3. (a) $(|\tau^{\mathrm{eff}}_{\alpha\beta}|/|\tau_{\alpha\beta}|)^2$ versus U/t. (b) Results of equation (9) for Cu_3O_{12} with $\tau = 0.001t$, $U = 5t$. Lowest-energy eigenvalues labelled by their interplanar quasi-momentum are shown versus flux ϕ. All energies are in t units.

In conclusion, we used a set of CuO_4 units connected by weak O–O links to model the interplanar coupling and c-axis superconductivity in cuprates. The results show that the system with two holes in each unit is a background such that inserting $2p$ holes one gets p pairs, bound by the repulsive interaction. The bound pair propagation is well described by equation (9). We found analytically superconducting flux quantization in the ring-shaped systems and confirmed this finding numerically for the three-unit ring (1863 225 configurations). To this end, we introduced a novel exact-diagonalization technique, which reduces the size of the matrices that must be handled to the square root of the overall size of the Hilbert space. In fact, real systems also contain vertical links via the orbitals of the apical oxygens. We expect that the inclusion of these hoppings will not change the results qualitatively, since they do not contribute to the propagation of the bound pair in the lowest-order approximation.

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