PAIRING AND TUNNELING IN REPULSIVE MODELS

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Abstract

The $W = 0$ pairs are two-body singlet eigenstates of the Hamiltonian with vanishing on-site repulsion; they exist in square and hexagonal lattices. Therefore, in such geometries many-body models with purely repulsive Hubbard interactions on all sites and appropriate fillings show pairing; the screened interaction is attractive due to a symmetry driven correlation effect. We can set up gedanken experiments with these bound pairs. Chains of CuO$_4$ units connected by weak links provide a test case which displays bound pair hopping and Superconducting Flux Quantization (SFQ). Focussing on the low-energy sector, one obtains an accurate description in terms of 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 spin-disentangled diagonalization technique which can be generally applied to many-fermion problems and drastically reduces the size of the matrices to be handled. Remarkably, the very same pairing mechanism also works neatly with the wrapped honeycomb lattice, suitable for armchair carbon nanotubes; the binding energy of $W = 0$ pairs depends strongly on the filling and decreases towards a small but nonzero value in the graphite limit.
1 Introduction

In this paper we wish to explore a recently proposed electronic pairing mechanism focussing the attention on repulsive Hubbard square and hexagonal geometries. Any proposal for a pairing mechanism in low-dimensional systems, like the cuprates and carbon nanotubes, must overcome somehow the problem of the repulsion between confined charges. This is an obvious difference compared to the traditional superconductors where pairs have hundreds of Angstrom of space to delocalize. In our approach the first-order Hubbard repulsion is removed by a proper choice of the pair symmetry since the Hamiltonian allows for two-body singlet eigenstates without double occupation, called $W = 0$ pairs\(^1\). The presence of such solutions at the highest occupied level of the non-interacting (Hubbard $U \rightarrow 0$) system is necessary to allow $\Delta(N) < 0$, where $\Delta(N) = E(N) + E(N - 2) - 2E(N - 1)$, and $E(N)$ is the interacting ground state energy with $N$ particles. By means of a non-perturbative canonical transformation\(^3\), one can show that $\Delta(N) < 0$ is due to a genuine attraction.

In Refs.\(^5\)\(^6\)\(^7\) we find that pairing occurs in purely repulsive, $C_{4v}$-symmetric Hubbard clusters and that $|\Delta(N)|$ is just the binding energy of the $W = 0$ pair. CuO\(_4\) is the smallest cluster where the $W = 0$ pairing mechanism works. In Section 2 we provide further evidence for pairing by studying the magnetic response of rings having CuO\(_4\) as units. We show that the low-energy physics is well described by a hard-core boson (fermion-pair) Hamiltonian and that the elementary excitations quantize the magnetic flux in a superconducting fashion\(^8\). For the numerical calculations, Section 3, we take advantage of a new exact-diagonalization technique\(^8\). 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 analytic results agree with the exact diagonalization data for weak CuO\(_4\)-CuO\(_4\) links. Next, in Section 4 we show that the $W = 0$ pairing mechanism works in hexagonal geometries too. We study the Hubbard model on wrapped honeycomb lattices describing armchair single wall carbon nanotubes (SWNT)\(^9\)\(^10\). We calculate the binding energy as a function of the length and the radius of the tube for various filling fractions. Our main conclusions are summarized in Section 5.
2 \( W = 0 \) Pair Tunneling and SFQ in CuO\(_4\) rings

In this Section we wish to study the tunneling of \( W = 0 \) bound pairs in rings of CuO\(_4\) units connected by weak links. We shall see that such a model clearly shows superconducting pair hopping and in particular, once a magnetic field is switched on into the ring, Superconducting Flux Quantization (SFQ) obtains. This implies that the field is screened by carriers of charge \( e^* = 2e \) and the system swallows up half of the flux quantum \( \phi_0 = \frac{hc}{e} \).

Below we shall arrive at a quite clear-cut diagnosis of SFQ, but in general one must be careful to avoid a confusion with other magnetic behaviour. Low-dimensional systems with strong electron-electron correlations may lead to an anomalous Aharonov-Bohm (AB) effect with ground-state energy oscillations versus flux \( \phi \) having a period \( \phi_0/N \) but this does not generally mean that the current is carried by particles with an effective charge \( e^* = Ne \). As an example, the ground state energy of a repulsive Hubbard ring threaded by a magnetic flux has 2 minima in the range \( [0, \phi_0] \) at low density and below a critical \( U/t \) value. However, as pointed out by Yu and Fowler[11], such an AB effect is driven by level-crossing due to the spinon degrees of freedom. The half-integer AB effect caused by the existence of confined pairs has been observed in the framework of extended 1\( d \) Hubbard models. Sudbo et al.[12] studied an alternating Cu-O ring with a charge-gap between Cu and O 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; hole pair confinement is achieved by providing repulsion-free sites, and not by producing an effective attraction. Other authors[13] considered modified 1\( d \) models with bond-charge interactions and found an effective attraction 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 \( U = 0 \)[14][15].

These results show that the half-integer AB effect in itself cannot be interpreted as SFQ, unless one can show that at both minima at \( \phi = 0 \) and \( \phi_0/2 \) the ground state of the system has bound pairs; the pair symmetries at both minima must be different, as in the BCS case. On the other hand, evidence for pairing in the context of repulsive Hubbard systems has been obtained by a variety of methods. Analytic approaches based on a renormalization method[3][4] and on various implementations of the renormalization group technique[16][17][18], generalized conserving approximation theories like FLEX[19], as well as Quantum Monte Carlo studies on supercells[20] lead to this conclusion.
Bound-pair solutions can also be found in $C_{4v}$-symmetric Hubbard clusters, as the CuO$_4$ governed by the Hamiltonian

$$H_{\text{CuO}_4} = t \sum_{i,\sigma}(d^\dagger_{i\sigma} p_{i\sigma} + p^\dagger_{i\sigma} d_{i\sigma}) +$$

$$+U \left( \sum_i \hat{n}^{(p)}_{i\uparrow} \hat{n}^{(p)}_{i\downarrow} + \hat{n}^{(d)}_{i\uparrow} \hat{n}^{(d)}_{i\downarrow} \right), \ U > 0 \quad (1)$$

where $p^\dagger_i$ creates a hole on the $i$-th O site, $d^\dagger$ on the Cu site and so on. For the sake of simplicity, in Eq.(1) we have neglected the O-O hopping term and also any distinction between Cu and O sites. However, we emphasize that this simplified model contains all the essential features of a CuO$_4$ system with more realistic parameters\cite{5}. $H_{\text{CuO}_4}$ is invariant under the permutation group $S_4$ and admits a $W=0$ pair solution belonging to a two-dimensional irreducible representation (irrep). In Ref.\cite{5}\cite{6} we have shown that the $W=0$ pair gets dressed and bound when four holes lie in the cluster, as signaled by $\Delta(4) < 0$, see Fig.(1). We emphasize that $\Delta(4)$ becomes positive for large values of $U/t$ and hence pairing disappears in the strong coupling regime. The above pairing mechanism does not work in the neighborhood of the infinite $U$ limit.

Next, we use CuO$_4$ units as nodes of a ring. The total Hamiltonian is $H_{\text{tot}} = H_0 + H_\tau$, with

$$H_0 = \sum_{\alpha=1}^L \left[ t \sum_{i,\sigma}(d^\dagger_{\alpha\sigma} p_{\alpha,i\sigma} + p^\dagger_{\alpha,i\sigma} d_{\alpha\sigma}) +$$

$$+U \left( \hat{n}^{(d)}_{\alpha\uparrow} \hat{n}^{(d)}_{\alpha\downarrow} + \sum_i \hat{n}^{(p)}_{\alpha,i\uparrow} \hat{n}^{(p)}_{\alpha,i\downarrow} \right) \right] \quad (2)$$
where $p_{\alpha,i\sigma}^\dagger$ is the creation operator for a hole onto the O site $i = 1, \ldots, 4$ of the cell $\alpha = 1, \ldots, L$ and so on, while

$$H_\tau = \sum_\alpha \sum_{i\sigma} \left[ \tau p_{\alpha,i\sigma}^\dagger p_{\alpha+1,i\sigma} + h.c. \right],$$

with $\tau = |\tau| \exp\left(\frac{2\pi i}{L} \phi\right)$, is an intercell hopping Hamiltonian chosen in such a way to preserve the $S_4$ symmetry that produces the $\Delta(4) < 0$ property.

For $N = 2L$ and $\tau \equiv 0$, the unique ground state consists of 2 holes in each CuO$_4$ unit[8]. To study the propagation of $p$ pairs we consider a total number of $N = 2L + 2p$ holes. When $U/t$ is such that $\Delta(4) < 0$, each pair prefers to lie on a single CuO$_4$ and for $N = 2L + 2p$ the unperturbed ground state is $2^p \times \binom{L}{p}$ times degenerate (since the $W = 0$ pair irrep has dimension 2). By this sort of models one can study the interaction of several hole pairs in the same system. Note that for $p=0$ the concentration (number of holes per site) is $2/5 = 0.4$; this is somewhat more than half-filling in the Copper-Oxide planes ($1/3 \approx 0.33$) 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[6] and the full plane[4][7] too. By replacing CuO$_4$ by larger units one can model other ranges of the hole concentration.

In order to study the propagation of the $p$ added pairs, we obtain an effective Hamiltonian by the cell-perturbation method with $H_0$, Eq.(2), the “cell-Hamiltonian” and $H_\tau$, Eq.(3), the “intercell perturbation” and by taking into account only the low-energy singlet sector. Each degenerate unperturbed ground state $|\Phi_0^S\rangle$ may be labelled by a set $S$ of units occupied by four holes; $|S| = p$. The secular problem yields the eigenvalue equation

$$\frac{1}{\Delta(4)} \sum_q \sum_{S'} \langle \Phi_0^S | H_\tau | \Phi_q \rangle \langle \Phi_q | H_\tau | \Phi_0^{S'} \rangle a_{S'} = \varepsilon a_S$$

where the sum over $q$ runs on the low-energy excited eigenstates involving CuO$_4$ units with 2, 3 or 4 holes, all taken in their ground states. The amplitude $a_S \equiv a(\alpha_1, \ldots, \alpha_p)$ is totally symmetric with respect to the permutations of the distinct indices $\alpha_1, \ldots, \alpha_p$. After some algebra Eq.(4) may be written in the form:

$$\sum_{j=1}^p \sum_{\beta=\pm 1} \prod_{i \neq j} (1 - \delta_{\alpha_j + \beta, \alpha_i}) J[a(\alpha_1, \ldots, \alpha_p)] +$$

$$+ e^{\beta \frac{2\pi i}{L} \phi} a(\alpha_1, \ldots, \alpha_j + \beta, \ldots, \alpha_p)] = \varepsilon a(\alpha_1, \ldots, \alpha_p).$$
This is a Schrödinger equation for $p$ hard-core bosons with a complex effective hopping integral. The $J$ coefficients have been numerically calculated as a function of the ratio $U/t[8]$; for $U/t \approx 5$ [where $\Delta(4)$ is minimum, see Fig.(1)] we found $J \approx -25$ in units of $|\tau|^2$. In Eq.(5), the second term in the l.h.s. describes hole pair propagation, e.g. from unit $\alpha_j$ to an unoccupied unit $\beta$; in the first term, the system gets back to the initial state after virtually exploring unit $\beta$; $\prod_{i \neq j} (1 - \delta_{\beta,\alpha_i})$ takes into account that if $\beta$ is one of the occupied units, the particle cannot move toward it.

In the case of just one added pair ($p=1$) the effective Schrödinger equation is readily solved by Fourier transforming and yields the following eigenvalues

$$
\varepsilon_k = 2J \left[ 1 + \cos \frac{2\pi}{L} \left( k + \frac{2\phi}{\phi_0} \right) \right], \quad k = 1, \ldots, L. \quad (6)
$$

The presence of the factor 2 in front of $\phi/\phi_0$ implies that the model quantizes the flux in units of $\phi_0/2$, like superconducting pairs do. Indeed, the ground state energy $E(2L+2) = \min_k \varepsilon_k$ is strictly periodic in $\phi$ with period $\phi_0/2$ for any $L > 2$. The case $L = 3$ will be used below for a numerical test of Eq.(6). The lowest state energies for any quasimomentum in $\text{Cu}_3\text{O}_{12}$ with 8 holes are plotted in Fig.(2) versus $\phi/\phi_0$. The low-energy effective model giving rise to Eq.(5) is equivalent to the Heisenberg - Ising spin chain governed by the Hamiltonian

$$
H_{\text{HI}} = \sum_{\alpha=1}^{L} J \left[ e^{\frac{4i\pi}{L} \frac{\phi}{\phi_0}} \sigma_{\alpha+1}^+ \sigma_{\alpha}^- + e^{-\frac{4i\pi}{L} \frac{\phi}{\phi_0}} \sigma_{\alpha}^+ \sigma_{\alpha+1}^- + 2\eta \sigma_{\alpha}^z \sigma_{\alpha+1}^z \right], \quad (7)
$$

where the $\sigma$’s are Pauli matrices, spin up represents an empty site and spin down represents a pair. $\eta$ is the so called anisotropy parameter and to
reproduce Eq.(5) we must choose $\eta = -1$. As in the 1$d$ 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[21]. The eigenenergies are given by (modulo an additive constant)

$$\varepsilon_{k_1...k_p} = 2J \sum_{j=1}^{p} \left[ 1 + \cos \frac{2\pi}{L} \left( k_j + 2\frac{\phi}{\phi_0} \right) \right]$$

(8)

where the variables $k_j$ satisfy the algebraic system

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

(9)

where $I_j$ are integers and the phase shift is given by

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

From Eqs.(7)-(9) we readily see that the ground state energy of the low-energy effective Hamiltonian $H_{\text{III}}$ is periodic with period $\phi_0/2$, independent of the number of added pairs. 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 $2L+2p$ with $0 \leq p \leq L$.

3 Spin Disentangled Exact Diagonalization Results

We exactly diagonalize the $L = 2$ and $L = 3$ CuO$_4$-ring Hamiltonian; to this end we introduce the Spin-Disentangled technique[8]. We let $M_\uparrow + M_\downarrow = N$ where $M_\sigma$ is the number of particles of spin $\sigma$; $\{ |\phi_{\alpha\sigma}\rangle \}$ is a real orthonormal basis, that is, each vector is a homogeneous polynomial in the $p^\dagger$ and $d^\dagger$ of degree $M_\sigma$ acting on the vacuum. We write the ground state wave function in the form

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

(10)

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. In Eq.(10) $L_{\alpha\beta}$ is a $m_\uparrow \times m_\downarrow$ rectangular matrix with $m_\sigma = (5L/M_\sigma)$. We let $K_\sigma$ denote the kinetic energy $m_\sigma \times m_\sigma$ square matrix of $H_{\text{tot}}$ in the basis $\{ |\phi_{\alpha\sigma}\rangle \}$, and $N_s^{(\sigma)}$ the spin-$\sigma$ 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 $H_{\text{tot}}$ according to the rule

$$H_{\text{tot}}[L] = [K_1 L + L K_1] + U \sum_s N_s^{(1)} L N_s^{(1)} .$$

(11)

In particular for $M_\uparrow = M_\downarrow$ ($S_z = 0$ sector) it holds $K_\uparrow = K_\downarrow$ and $N_s^{(1)} = N_s^{(1)}$. Thus, the action of $H$ is obtained in a spin-disentangled way. In the $S_z = 0$ sector for $L=3$ the size of the problem is 1,863,225 and the storage of the Hamiltonian matrix requires much space; by this device, we can work with matrices whose dimensions is the square root of those of the Hilbert space: 1,365 $\times$ 1,365 matrices solve the 1,863,225 $\times$ 1,863,225 problem, and are not even required to be sparse.

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.

### 3.1 Numerical Results and discussion: the Three CuO$_4$ Ring

In this section we consider the three-CuO$_4$ ring focusing the attention on the case $\Delta(4) < 0$ and total number of holes $2L + 2 = 8$. This is the smallest ring where we can insert a magnetic flux $\phi$ by $\tau = |\tau| e^{i\theta}$, $\theta = \frac{2\pi}{3} (\phi/\phi_0)$. The energies of the ground-state multiplet components are reported in Fig.(3) for $|\tau| \ll |\Delta(4)|$ and $U = 5t$. At $\phi = 0$ the ground state belongs to the $k = 0$ subspace (as usual $k$ is related to the crystal momentum $q = 2\pi \hbar k/3$ in this case), 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 $\phi$ increases, the ground state energy grows quadratically in $\phi$ (diamagnetic behaviour). Near $\phi = \phi_0/4$ we find a level crossing between $k = 0$ and $k = 2$, while at $\phi = \phi_0/2$, $k = 0$ 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[22]. The comparison of the numerical results shown in Fig.(3) with the analytic ones in Fig.(2) supports the accuracy of the cell-perturbation scheme proposed in Section 2. Thus, the dressed $W = 0$ pair screens the vector potential as a particle with an effective charge $e^* = 2e$ does. At both minima of the ground state energy we have computed $\Delta(8) \approx -10^{-2}t$. Here, the half-integer AB effect is actually SFQ.

Fulfilling the conditions $\Delta(4) < 0$ and $|\tau| \ll |\Delta(4)|$, we varied $U$ and $|\tau|$ and found analogous trends for the ground state energy. Increasing $|\tau|$ with fixed $\Delta(4)$ lowers the central minumum and depresses the two maxima. On the other hand, if $|\Delta(4)|$ 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 $|\tau|/|\Delta(4)|$.

The three-CuO$_4$ 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

$$\hat{I} = \frac{e}{c} \frac{\partial H_{\text{tot}}}{\partial \phi} = \frac{e}{\hbar L} \sum_{i,\alpha,\sigma} \tau p_{\alpha+1,i\sigma}^\dagger p_{\alpha,i\sigma} - \tau^* p_{\alpha,i\sigma}^\dagger p_{\alpha+1,i\sigma}$$

as a function of the flux. By expanding $\hat{I}$ in Eq.(12) in powers of $\phi$ near $\phi = 0$ one may identify the paramagnetic and the diamagnetic contributions with the zeroth and the first order terms respectively[23]. The results are reported in Fig.(4); the current is proportional to the flux derivative of the ground-state energy [see Fig.(3)] according to the Hellmann-Feynman theorem. Near $\phi = 0$ the system generates a diamagnetic current which screens the threaded magnetic field. When $\phi$ 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 eigenfuctions may be chosen real [$H_\tau$ at $\phi = \phi_0/2$ is obtained from $H_\tau$ at $\phi = 0$ by reversing the sign of four O-O bonds connecting two nearest neighbours CuO$_4$ 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 Fig.(4) 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 $\phi = 0$.

For the non-interacting ($U = 0$) Cu$_3$O$_{12}$ ring there is no pairing in CuO$_4$ and indeed the ground state energy is linear in the field at small fields (normal Zeeman effect)[8]. The absence of SFQ is a further evidence of the repulsion-driven pairing mechanism discussed in Section 2.

We can alternatively model the three-CuO$_4$ ring by connecting only the central Copper sites of the constituent CuO$_4$ units with a hopping term $\tau_{\text{Cu}}$; in order to study the propagation of a bound pair we again assume that the total number of holes is $2L + 2 = 8$. The whole system threaded by the flux has a $C_3 \otimes S_4^2$ symmetry because the Oxygen sites are not involved in the intercell Hamiltonian. 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[24]. 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 pairing if the pairs are not totalsymmetric.
4 \ W = 0 \ Pairing \ in \ Armchair \ Nanotubes

In this Section we use the Hubbard Hamiltonian $H$ on the honeycomb lattice to represent the valence bands of carbon single-wall $(N, N)$ nanotubes and study the $W = 0$ pairing mechanism. Using standard notation, the full Hamiltonian reads

$$H = t \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \sum_{\sigma} \left( c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}', \sigma} + h.c. \right) + U \sum_{\mathbf{r}} \hat{n}_{\mathbf{r}, \uparrow} \hat{n}_{\mathbf{r}, \downarrow},$$

(13)

where $\mathbf{r}$ denotes the honeycomb site, the sum runs over the pairs $\langle \mathbf{r}, \mathbf{r}' \rangle$ of nearest neighbour carbon atoms and $t$ is the hopping parameter. The one-body eigenvalues $\varepsilon^\pm(\mathbf{k})$, (- for the bonding and + for the antibonding bands) are readily obtained, and the Fermi line has $C_{2v}$ symmetry for the nanotubes ($C_{6v}$ for the graphite sheet). Here, we assume that the Fermi level $\varepsilon_F$ lies in the + band. The Hamiltonian in Eq.(13) admits $W = 0$ pairs; we find that in the vanishing quasi-momentum sector they only belong to the pseudoscalar irrep $A_2$ of $C_{2v}$. Let $(a, b)$ denote the basis of the Bravais lattice and $u(\mathbf{k}, \zeta)$ the periodic part of the Bloch function of quasi-momentum $\mathbf{k}$, with $\zeta = a, b$. The pair wavefunction reads

$$\psi_{[A_2]} = \frac{1}{\sqrt{2}} \left[ u^*(\mathbf{k}, \zeta_1) u^*(-\mathbf{k}, \zeta_2) e^{ik_y(Y_1-Y_2)} - u^*(\mathbf{k}, \zeta_2) u^*(-\mathbf{k}, \zeta_1) e^{-ik_y(Y_1-Y_2)} \right] \sin [k_x(X_1 - X_2)],$$

with $\mathbf{R}_i = (X_i, Y_i)$ the origin of the cell where the particle $i$ lies. We can verify by direct inspection that $\psi_{[A_2]}$ vanishes for $X_1 = X_2$, that is the two-body singlet wavefunction vanishes if the particles lie on the same annulus of the $(N, N)$ tube. As a consequence $\psi_{[A_2]}$ is an eigenstate of the kinetic energy [with eigenvalue $2\varepsilon(\mathbf{k})$] and of the on-site Hubbard repulsion $W$ with vanishing eigenvalue of the latter, that is $\psi_{[A_2]}$ is a $W = 0$ pair. Remarkably, $\psi_{[A_2]} = 0$ when the transverse component $k_y = 0$. The effective interaction $W_{\text{eff}}$ between the particles of a $W = 0$ pair can be obtained analytically by a canonical transformation in the spirit of Ref.[3]. Letting $n_{\nu}^{(0)}(\mathbf{p})$ denote the non-interacting occupation number in band $\nu$ with wavevector $\mathbf{p}$, we find

$$W_{\text{eff}}(\mathbf{k}, \mathbf{k}', E) = 2 \sum_{\hat{O} \in C_{2v}} \chi^{(A_2)}(\hat{O}) \sum_{\mathbf{p}, \nu} n_{\nu}^{(0)}(\mathbf{p})
\left[1 - n_+^{(0)}(\hat{O}\mathbf{k}' + \mathbf{k} + \mathbf{p})\right] U_{\nu}(\hat{O}\mathbf{k}' + \mathbf{k} + \mathbf{p}, -\mathbf{k}, \hat{O}\mathbf{k}', \mathbf{p})
\frac{U_{\nu}(\mathbf{k}, \mathbf{p}, \hat{O}\mathbf{k}' + \mathbf{k} + \mathbf{p}, -\hat{O}\mathbf{k})}{\varepsilon^+(\hat{O}\mathbf{k}' + \mathbf{k} + \mathbf{p}) - \varepsilon^-(\mathbf{p}) + \varepsilon^+(\mathbf{k}') + \varepsilon^+(\mathbf{k}) - E}$$

(14)
where $\chi^{(n)}(\hat{O})$ is the character in $\eta$ of the operation $\hat{O}$ of $C_{2v}$, $E$ is the interacting pair energy and $U_\nu(k_1, k_2, k_3, k_4)$ is the interaction vertex, with incoming legs $k_3$ and $k_4$ in band $+$ and outgoing $k_1$ in band $+$ and $k_2$ legs in band $\nu$. The effective Schrödinger equation for the pair reads

$$[2\varepsilon(k) + W_F + F(k, E)] a_k + \sum_{k' \in \mathcal{D}} W_{\text{eff}}(k, k', E) a_{k'} = E a_k,$$

where $W_F$ is the first-order self-energy shift and

$$F(k, E) = -2 \sum_{p, \nu} \sum_q |U_\nu(k, p, k + p - q, q)|^2 \times$$

$$\frac{[1 - n_\nu^{(0)}(k + p - q)] [1 - n_\nu^{(0)}(q)] n_\nu^{(0)}(p)}{\varepsilon^+(k + p + q) - \varepsilon^\nu(p) + \varepsilon^+(q) + \varepsilon^+(k) - E}$$

is the forward scattering term which does not contain any direct interaction between the particles of the pair but renormalizes the Fermi energy. Eq.(15) requires a self-consistent calculation of $E$ (since $W_{\text{eff}}$ and $F$ are $E$-dependent). The indices $k$ and $k'$ run over $1/4$ of the empty part of the FBZ and we denoted such a set of wavevectors as $\mathcal{D}$. We show below that $E = 2\varepsilon_F + W_F + F_{\text{min}}(k_F) + \Delta$, with a positive binding energy $-\Delta$ of the $W = 0$ pair; here $F_{\text{min}}(k_F)$ is the minimum value of $F(k, E)$ among the $k_F$-wavevectors on the Fermi line.

We considered supercells of $2N \times L = N_C$ cells, where $L$ is the length of the $(N, N)$ nanotube in units of the lattice spacing. We solved the Cooper-like equation in a virtually exact way for $N$ up to 6 and $L$ up to 25, using $U/t = 2.5$ (which is of the correct order of magnitude for graphite[25]). The canonical transformation overestimates $\Delta$ in this range of $U/t$, but remains qualitatively correct. The calculations are performed with the Fermi energy $\varepsilon_F$ varying between $0.8 \, t$ and $1.1 \, t$ (half filling corresponds to $\varepsilon_F = 0$). The binding energy $-\Delta$ of the pairs decreases monotonically both with the radius and the length of the tube.

With supercell sizes $N_C > 300$ numerical calculations become hard. Since we are concerned with the asymptotic behaviour for fixed $N$ and $L \to \infty$ and $\Delta$ depends on $N$ and $L$ in a complicated way, we need a method to make reliable extrapolations of the numerical results. To this end, like in previous work[3],[20] we define the Average Effective Interaction $V$. This is such that setting in Eq.(15) $W_{\text{eff}} = -\frac{V}{N_C}$, with a constant $V > 0$ for all $k$ and $k'$ in $\mathcal{D}$, one obtains the correct value of $\Delta$. In other terms,
once the binding energy $-\Delta$ is known, the constant $V$ must be chosen in such a way that

$$\frac{1}{V} = \frac{1}{N_C} \sum_{\mathbf{k} \in \mathcal{D}} \frac{1}{2[\varepsilon(k) - \varepsilon_F] + F(k) - F_{\min}(k_F) - \Delta}.$$ 

We found that $V$ remain fairly stable around $\approx 1.5 \div 2 \ t$ for $N > 2$ with increasing $L[10]$. Therefore $V$ is largely independent on the Fermi energy and on the radius and this allows us to extrapolate to $\Delta_{\text{asympt}} = \lim_{L \to \infty} \Delta$. For $N = 4, 6, 10$ the results are shown in Fig.(5). We found that $\Delta_{\text{asympt}}$ is strongly dependent on the filling at fixed $N$; the sharp maximum at the optimal doping $\varepsilon_F \approx t$ (which corresponds to a number of electrons per C atom of 1.25) can be understood in terms of a corresponding peak in the density of states. We note that high metal concentration samples such as C$_2$Li (where the electron concentration per C atom is $\approx 1.15 \div 1.2$) have been synthesized[26] and a net charge transfer was observed between the alkali-metal and the carbon atoms. The alkali-metals cause little structural deformation, but increase the filling of the original bands.

In the optimally doped case $-\Delta_{\text{asympt}}$ decreases monotonically as the radius of the tube increases[9]. The decreasing of the binding energy with $N$ is suggested by recent measurements on nanotubes with diameter of few Angstrom[27]. However, in the limit of large $N$, $\Delta_{\text{asympt}}$ remains stable around 0.0028 $t$ and may be interpreted as the binding energy of the $W = 0$ pair in an optimally doped graphite sheet.

The paired state we have obtained here is essentially two-dimensional, that is the transverse direction is crucial to have a non-Abelian symmetry group and hence $W = 0$ pairs; the pairing mechanism uses degenerate electronic states that exist in 2d and works away from half filling.

## 5 Conclusions

Within the repulsive Hubbard Model, we propose a purely electronic pairing mechanism based on the spatial symmetry of the lattice. The key ingredient is the $W = 0$ pair which is a two-body singlet eigenstate of the Hubbard Hamiltonian without double occupation and is formed by mixing degenerate one-body states. In the interacting problem the $W = 0$ pair gets dressed in part of the parameter space by virtual electron-hole exchanges with the Fermi sea; at appropriate fillings the effective interaction is attractive in the square (CuO$_4$) and in the hexagonal (nanotube) geometry.
Figure 5: Results of the canonical transformation approach with $U/t = 2.5$. $-\Delta_{\text{asympt}}$ as a function of the Fermi energy $\varepsilon_F$ for $N = 4$ (black boxes), $N = 6$ (empty triangles) and $N = 10$ (grey diamonds). The Fermi energy varies in the range $0.8 \div 1.1 t$. $\Delta_{\text{asympt}}$ is in units of $10^{-3} t$.

For CuO$_4$-rings and weak O-O links we find a half-integer AB effect which is the unambiguous signature of the SFQ. Indeed, SFQ was long sought in purely repulsive Hubbard chains; we present evidence that it can prevail only provided that the nodes are fully symmetric clusters.

The analytic results are confirmed and extended by the numerical findings for the two- and three-CuO$_4$ ring (14,400 and 1,863,225 configurations). Large diagonalizations are easily done by our novel technique, based on a suitable disentanglement of the up and down spin configurations; we wish to advertise it specially to the benefit of the more numerically-oriented people.

By manipulating matrices whose dimension is the square root of the overall size of the Hilbert space, we were able to exactly diagonalize the Hamiltonian: $\sqrt{M} \times \sqrt{M}$ matrices solve the $M \times M$ problem. The spin-disentangled exact-diagonalization technique is a general method for many-electron problems that allows to manipulate with matrices whose dimension is the square root of the overall size of the Hilbert space. In the present case, $1,365 \times 1,365$ matrices solve the $1,863,225 \times 1,863,225$ problem with 12-digit precision and unprecedented efficiency. 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; by the way, $S_z = 0$ can always be assumed, as long as the hamiltonian is $SU(2)$ invariant.

We have also shown that the $W = 0$ pairing mechanism works in hexagonal geometries too, as in the case of carbon nanotubes. Away from half filling, we have obtained stronger binding in nanotubes than in graphite sheets and this suggests a higher critical temperature for the former. This is also supported by the measurements of a $T_c \approx 15$ K in the 4 Angstrom single-wall nanotube (SWNT) by Tang et al.[27].

Currently, intercalated graphite and carbon nanotubes superconduct at
much lower temperatures than high-$T_c$ Cuprates and the two kinds of materials are apparently quite different. However, symmetry arguments tell us that, despite the obvious differences, the pairs get bound by a mechanism which is basically the same: for some symmetries the on-site Coulomb interaction is utterly turned off from the start, and there is no repulsion to overcome.

References


