Density of states width-parity effect in *d*-wave superconducting quantum wires

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We calculate the density of states (DOS) in a clean mesoscopic *d*-wave superconducting quantum wire, i.e., a sample of in®nite length but ®nite width*N*. For open boundary conditions and half-®lling, the DOS at zero energy is found to be zero if *N* is even and nonzero if *N* is odd. At ®nite chemical potential, all chains are gapped but the qualtitative differences between even and odd *N* remain.

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I. INTRODUCTION

In recent years the fabrication of nanoscale devices has heightened interest in solid-state quantum systems where the discreteness of the level spacing plays an important role. Originally discussed only in semiconductor quantum dots and quantum wires, following the work of Ralph *et al.*[1] many fascinating consequences of the level discreteness were also observed in ultrasmall metal particles. These included the observation of a spectroscopic gap attributed to pair correlations in the small grains, which depended on the so-called number parity of the sample, i.e., whether the number of electrons in the grain was even or odd. The physics of the levels in such grains has been quite well understood.[2] Superconducting systems extended in one dimension but mesoscopic in another have also been studied.[3]

In most of these studies, a gap with A_{1g} or s-wave symmetry has been assumed. However, for some practical purposes it may be of interest to use cuprate samples, which are known to have $d_{x^2-y^2}$ symmetry. From a fundamental point of view it is also expected that these systems will be different because already in the bulk state there are states below the maximum gap scale; the pure *d*-wave bulk density of states (DOS) is linear in energy, $\rho(E)\sim|E|$. We have studied the DOS of mesoscopic *d*-wave quantum wires and found a new kind of parity effect, not related to the number of particles in the system, but to the parity of the number of chains across the mesoscopic sample. In some ways, the effect is reminiscent of a type of mesoscopic gap effect that has been recently discussed in the context of single-wall carbon nanotubes, where the existence or nonexistence of a gap depends on the intrinsic twist or chirality induced while forming the tube.[5] While the *d*-wave systems we discuss may be considered to be tubes if periodic boundary conditions are employed, they do not break either time-reversal symmetry or spatial parity. Nevertheless, at half-®lling, we observe that if the width of the system *N* is even, there is a gap in the DOS whereas if the width is odd the density of states at zero energy $\rho(0)$ is nonzero. As *N* is increased, both the even-*N* gap and the odd-*N* $\rho(0)$ vanish as they must to give the bulk *d*-wave result $\rho(E)\sim|E|$. Although the DOS vanishes at $E=0$ for all *N* when $\mu\neq 0$, there is still a pronounced even-odd effect in the DOS, and we argue that this effect should be observable in quantum wires fabricated from cuprate superconductors. We speculate further that it may be of relevance to the study of disorder-induced pseudogaps in bulk *d*-wave superconductors, which have been the subject of much controversy in recent years.[4]

II. MODEL

We consider the DOS of a *d*-wave superconducting chain (DWSC) that is coupled to $N-1$ other DWSC's. The chains form a two-dimensional (2D) system and the ®rst chain is at the boundary. Similar problems were considered in previous studies of random ¯ux systems [8] and quasi-one-dimensional disordered tight-binding models.[9,10] In this paper we will ignore the effect of disorder and study the odd-even effect in a pure system of coupled DWSC's. Such a behavior is also known for a system of coupled spin chains, which has a gap (no gap) if the number of chains is even (odd).[6,7]

There are several possible geometries one can assume for this problem. The most natural, and the one we consider here, is a wire parallel to the 100 (or 010) crystal direction. In this geometry, the boundaries of the wire are aligned with both the underlying CuO_2 crystal and the gap maxima (which are tied to the crystal lattice). Other geometries, such as a 110 oriented wire, are expected to show similar even-odd effects to the ones described below, but these will be mixed with Andreev scattering resonances[11] and thus will be more dif®cult to interpret. In addition, we anticipate that the 100 oriented wire is the most accessible to current technology.

The Bogoliubov±de Gennes Hamiltonian of the 2D DWS

$$H=(-\nabla^2+\mu)\sigma_3+\Delta\sigma_1$$

is de®ned on a square lattice with

$$-\nabla^2 f(r)=-t\sum_{j=1}^{2}[f(r+e_j)+f(r-e_j)]$$

and the DWS order parameter

$$\Delta f(r)=\Delta_0\sum_{j=1}^{2}(-1)^j[f(r+e_j)+f(r-e_j)].$$

With this de®nition, the gap in familiar k-space representation is $\Delta_k = 2\Delta_0[\cos(k_x) - \cos(k_y)]$. In the following calculations we will measure energies in units of t for simplicity. Moreover, it is assumed that chains are in®nitely long and arranged parallel to the y axis of our 2D system.

III. PERIODIC BOUNDARIES

The ®nite set of chains can be closed periodically in the x direction by identifying the ®rst with the $(N+1)$th chain. While this is not particularly physical, the calculation is fairly transparent and therefore worthwile for pedagogical reasons. For this translational-invariant N-chain system the integration in y direction (i.e., along the chains) can be performed and gives the DOS at zero energy

$$\rho(E=0) = -\frac{1}{\pi N}\sum_{k_x}\int_{-\pi}^{\pi}\frac{dk_y}{2\pi}\mathrm{Im}\, G_0(\mathbf{k}, +i\epsilon)$$

$$= \lim_{\epsilon\to 0}\frac{\epsilon\rho_0}{N}\sum_{n=0}^{N-1}\frac{1}{\sqrt{\epsilon^2 + [\mu + 4t\cos(k_x)]^2}}, \qquad (1)$$

where

$$\rho_0 = \frac{2t}{\pi\sqrt{t^2+\Delta_0^2}\sqrt{16t^2-\mu^2}}.$$

Here G_0 is the Green's function for a clean 2D d-wave superconductor, $k_x = 2\pi n/N$ $(n = 0,1,\ldots,N-1)$, and we have set the lattice constant to unity. First, we consider the DOS at half-®lling $(\mu = 0)$. We ®nd that $\rho(E=0)$ is ®*nite* for N a multiple of 4 since the allowed values of k_x include $k_x = \pi/2$ and $3\pi/2$, which produce ®nite contributions to Eq. (1). For other values of N, on the other hand, expression (1) always vanishes. At $\mu = 0$, then, we have

$$\rho_N(E=0) = \begin{cases} 2\rho_0/N & \text{for } N = 4k, k = 1,2,\ldots \\ 0 & \text{otherwise.} \end{cases}$$

This periodicity in N re¯ects the conditions necessary to form a standing wave in the x direction at the Fermi energy. For $\mu = 0$, it is the four nodal points at $\mathbf{k} = (\pm\pi/2, \pm\pi/2)$ that produce the standing wave. The wave function at $E=0$ is thus exactly the same as in the normal state; it is therefore not surprising that $\rho(E=0)$ is only weakly dependent on Δ_0.

For given N, there will be a discrete set of μ, which produces a ®nite density of states at $E=0$. For generic μ, the nodal eigenstates do not contribute at $E=0$, but we expect on the basis of Eq. (1) that a qualitative width-parity effect will remain at nonzero E. As we shall see in the next section, numerical studies on realistic models ®nd a pronounced effect of this type.

IV. OPEN BOUNDARIES

Periodic boundary conditions are not realistic for typical experiments because the superconductor is a planar object. Therefore, a better choice is open boundaries if we have a situation with a ®nite number of chains. The DOS is calculated numerically for $N = 4,5,20,21$, as shown in Figs. 1±5. Since we have just shown that Δ_0 plays a minor role in the parity effect, we proceed (for simplicity) under the assumption that $\Delta_0/t = 1$ unless explicitly stated otherwise. In numerical work (e.g., Fig. 6 below), it is shown that this assumption does not change the qualitative results. From the ®gures the alternating structure of the DOS for odd and even number of chains is immediately obvious, and may be characterized by the DOS of the end chain.

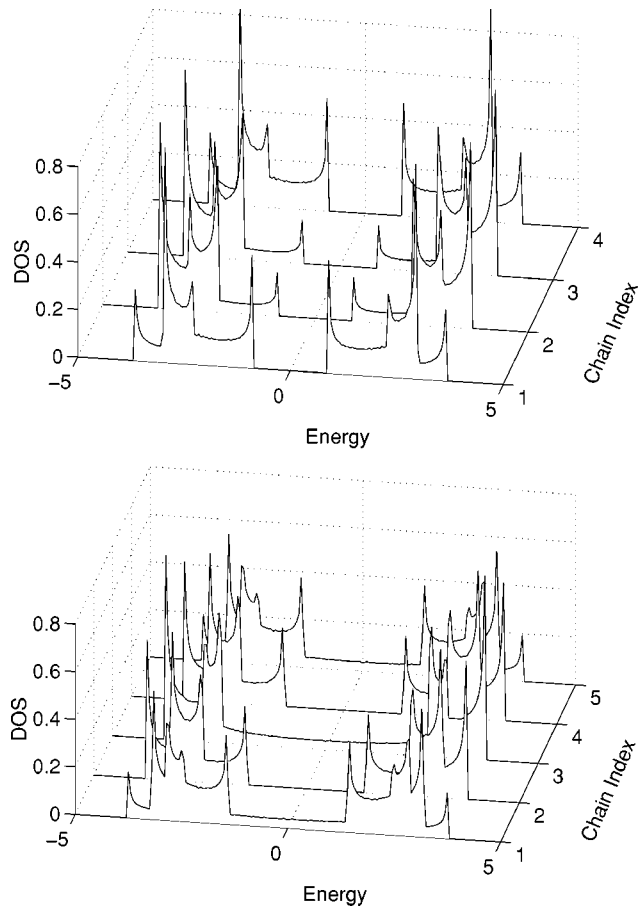

FIG. 1. Density of states for four and ®ve chains with $\Delta_0/t = 1$ and $\mu = 0$.

A. Recursive method

Some insight into the dependence of these gaps and residual DOS's on system size and other parameters may be obtained from analytical methods. First, the Hamiltonian H can be diagonalized with respect to y direction by a Fourier transformation $y \to k_y$. Then the structure with respect to the x direction can be expressed in a matrix form for $x = 1,2,\ldots,N$ as

$$\tilde{H}_N = \begin{pmatrix} H_{NN} & H_{NN-1} & 0 & \ldots & 0 \\ H_{N-1N} & H_{N-1N-1} & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & H_{22} & H_{21} \\ 0 & \ldots & 0 & H_{12} & H_{11} \end{pmatrix}.$$

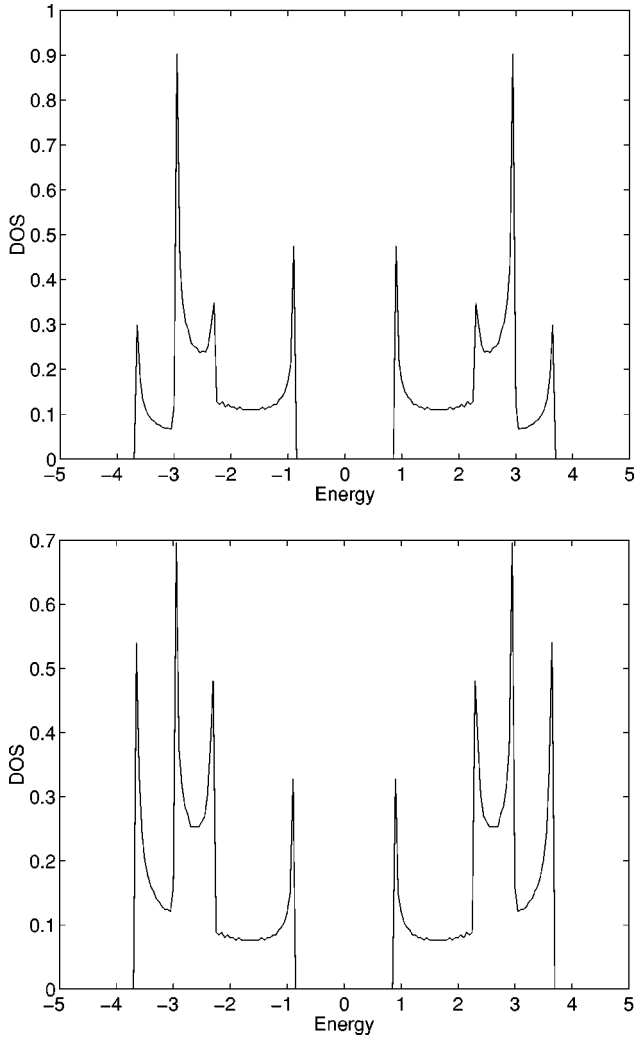

FIG. 2. Density of states for four chains: DOS of the end chain and average over all chains with $\Delta_0/t=1$ and $\mu=0$.

For a compact notation we introduce a block-matrix representation

$$\tilde{H}_N := \begin{pmatrix} H_{NN} & \tilde{H}_{NN-1} \\ \tilde{H}_{N-1N} & \tilde{H}_{N-1} \end{pmatrix}$$

with

$$\tilde{H}_{NN-1} = (H_{NN-1}, 0, \ldots, 0), \tag{2}$$

$$\tilde{H}_{N-1N} = \begin{pmatrix} H_{N-1N} \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{3}$$

The corresponding Green's function at zero energy, which is required for the evaluation of the DOS, can then be written (after a shift $H \to H + i\epsilon\sigma_0$) as

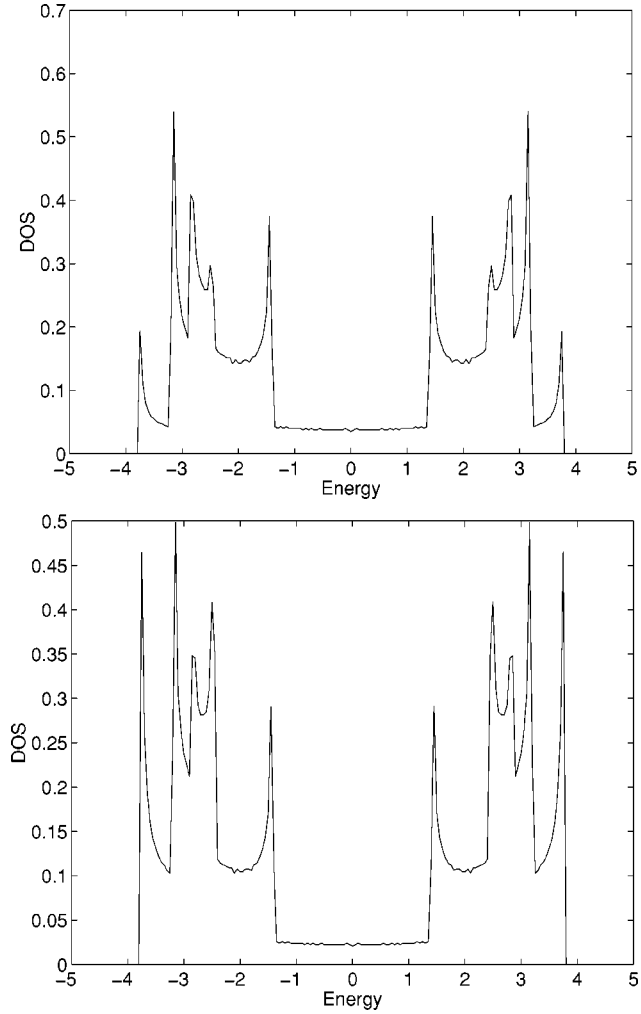

FIG. 3. Density of states for ®ve chains: DOS of the end chain and average over all chains with $\Delta_0/t=1$ and $\mu=0$.

$$[\tilde{H}_N^{-1}]_{NN} = (H_{NN} - \tilde{H}_{NN-1}\tilde{H}_{N-1}^{-1}\tilde{H}_{N-1N})^{-1}$$
$$= (H_{NN} - H_{NN-1}[\tilde{H}_{N-1}^{-1}]_{N-1N-1}H_{N-1N})^{-1}.$$

The second equation is due to the special form of the matrices given in Eqs. (2) and (3). Using $\Gamma_N = [\tilde{H}_N^{-1}]_{NN}$ the recurrence relation reads

$$\Gamma_N = (H_{NN} - H_{NN-1}\Gamma_{N-1}H_{N-1N})^{-1}. \tag{4}$$

This is a continued-fraction representation of the 2×2 matrix Γ_N, the Green's function of end chain labeled by N at a given k_y. It can be used even in the presence of random terms along the x direction because no diagonalization of the matrix is necessary.

Now we will apply the recursive method to evaluate the DOS of the end chain of N DWSC's. The calculation is simpli®ed greatly if we assume $\Delta_0 = t = 1$ (the more general case is treated in numerical calculations). In this special case we have

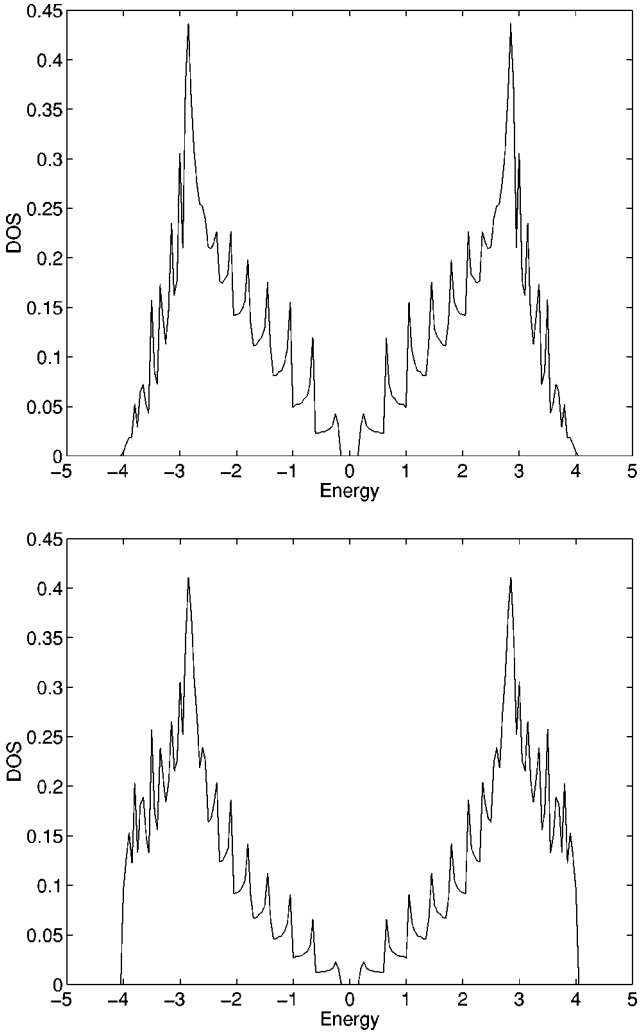

FIG. 4. Density of states for 20 chains: DOS of the end chain and average over all chains with $\Delta_0/t=1$ and $\mu=0$.

$$H_{NN}=\begin{pmatrix} \mu+2\cos k_y+i\epsilon & -2\cos k_y \\ -2\cos k_y & -\mu-2\cos k_y+i\epsilon \end{pmatrix} =(\mu+2\cos k_y)\sigma_3-2\cos k_y\sigma_1+i\epsilon\sigma_0\equiv h+i\epsilon\sigma_0 \tag{5}$$

and

$$H_{NN-1}=H_{N-1N}=\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}=\sigma_1+\sigma_3 .$$

The initial value (single chain) is

$$\Gamma_1=(H_{11})^{-1}=\frac{-i\epsilon\sigma_0+(\mu+2\cos k_y)\sigma_3-2\cos k_y\sigma_1}{\epsilon^2+(\mu+2\cos k_y)^2+4\cos^2 k_y}.$$

B. Few chains

By direct iteration of Eq. (4) we can obtain the DOS analytically for the end chain of a system of N chains, provided we restrict consideration to $\mu=0$. Using $c=2\cos k_y$, for $N=1$ we get

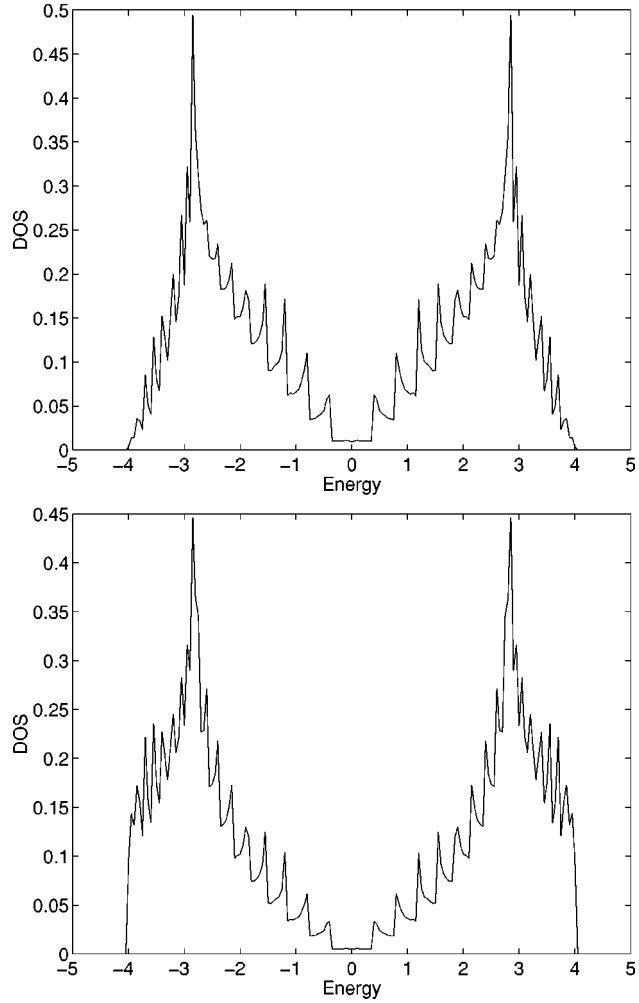

FIG. 5. Density of states for 21 chains: DOS of the end chain and average over all chains with $\Delta_0/t=1$ and $\mu=0$.

$$\rho_1(0)=\lim_{\epsilon\to 0}\frac{\epsilon}{\pi}\int_{-\pi}^{\pi}\frac{1}{\epsilon^2+2c^2}\frac{dk_y}{2\pi}=\frac{1}{\sqrt{8}\pi}$$

in agreement with the result in Sec. III. For $N=2$ we have

$$\rho_2(0)=\lim_{\epsilon\to 0}\frac{\epsilon}{\pi}\int_{-\pi}^{\pi}\frac{1}{\epsilon^2+2c^2+2}\frac{dk_y}{2\pi}.$$

From the pole structure of the integrand, we see that there is a gap $2E_g=2\sqrt{2}\approx 2.83$. In the case of $N=3$ there is again a nonzero DOS at $E=0$

$$\rho_3(0)=\lim_{\epsilon\to 0}\frac{\epsilon}{\pi}\int_{-\pi}^{\pi}\frac{\epsilon^2+2c^2+2}{(\epsilon^2+2c^2)^2+4(\epsilon^2+2c^2)}\frac{dk_y}{2\pi}=\frac{1}{2\sqrt{8}\pi}.$$

and for $N=4$

$$\rho_4(0)=\lim_{\epsilon\to 0}\frac{\epsilon}{\pi}\int_{-\pi}^{\pi}\frac{\epsilon^2+2c^2+4}{(\epsilon^2+2c^2)^2+6(\epsilon^2+2c^2)+4}\frac{dk_y}{2\pi},$$

which has a gap $2E_g=2\sqrt{3-\sqrt{5}}\approx 1.75$ (see Fig. 1). In general the energy gap observed depends on the size of the su-

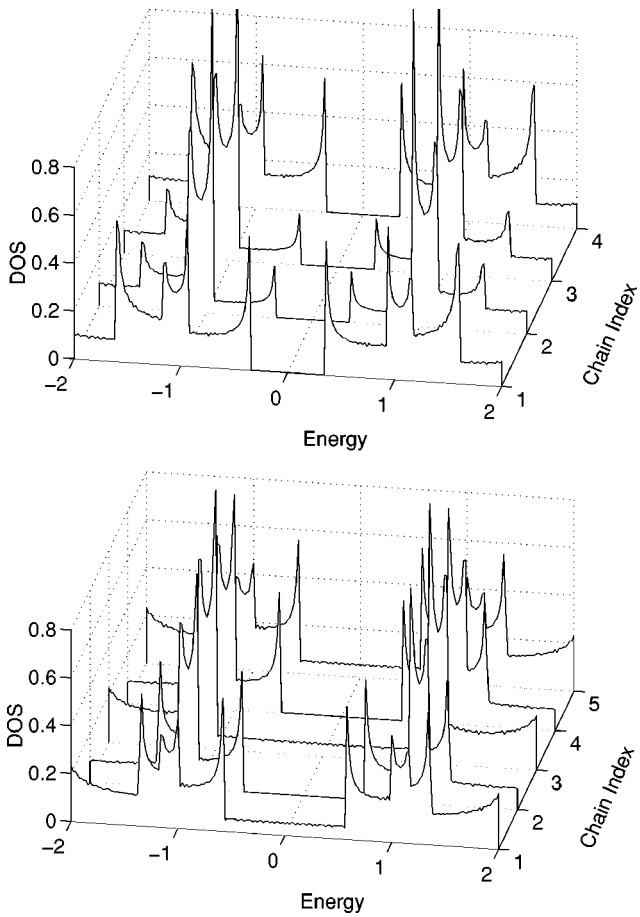

FIG. 6. Density of states for four and ®ve chains with $\Delta_0/t=0.3$ and $\mu=0$.

perconducting order-parameter maximum Δ_0 in a nonlinear way, although relatively simple expressions may be obtained for a small number of chains.

The reader will notice that the even-odd effect described here differs from the periodic-boundary case, where gapless states arise for N a multiple of 4. This is expected, since the effect we are reporting arises from self-interference of quantum wave functions in a nanoscale system. The path length for a constructively interfering closed path in the x direction is $2L=2n\pi/k_F$ for open boundary conditions, and $L=2n\pi/k_F$ for periodic boundary conditions.

C. Many chains: Stationary behavior for $N\rightarrow\infty$

While in systems mesoscopic in both directions (®nite length L quantum wires), even-odd parity effects in N are known to survive the thermodynamic limit $L\rightarrow\infty$,[10] they must disappear as $N\rightarrow\infty$ when we recover the fully $2D$ system. This is evident from the numerical evaluation of the DOS for large N (Figs. 4 and 5), and we can see this analytically by showing that as $N\rightarrow\infty$, $\rho(0)=0$ independent of N.

A single iteration of Eq. (4) yields a relation between the Green's functions of an even (or odd) number of chains, respectively,

$$\Gamma_N=(H_{NN}-H_{NN-1}[H_{N-1N-1}-H_{N-1N-2}\Gamma_{N-2}H_{N-2N-1}]^{-1}H_{N-1N})^{-1}. \tag{6}$$

For the DWSC's this reads

$$\Gamma_N=\left\{H_{NN}-\left[\frac{1}{2}(\sigma_1+\sigma_3)H_{N-1N-1}(\sigma_1+\sigma_3)-\Gamma_{N-2}\right]^{-1}\right\}^{-1}.$$

For constant $\mu=0$ we get from expression (5)

$$H_{N-1N-1}=h+i\epsilon\sigma_0$$

and

$$\frac{1}{2}(\sigma_1+\sigma_3)H_{N-1N-1}(\sigma_1+\sigma_3)=-h+i\epsilon\sigma_0$$

such that

$$\Gamma_N=(h+i\epsilon\sigma_0+[h-i\epsilon\sigma_0+\Gamma_{N-2}]^{-1})^{-1}$$

with the initial expressions

$$\Gamma_1=\frac{1}{\epsilon^2+2c^2}(h-i\epsilon\sigma_0)$$

and

$$\Gamma_2=\left(1+\frac{2}{\epsilon^2+2c^2}\right)^{-1}\Gamma_1.$$

The symmetric 2×2 matrix h can be diagonalized by an orthogonal transformation, leading to diagonal elements $\lambda_{1/2}=\pm\sqrt{2}c$. This also diagonalizes the initial expressions $\Gamma_{1,2}$ as well as the recurrence relation

$$\gamma_{N+2,j}=\cfrac{1}{\lambda_j+i\epsilon+\cfrac{1}{\lambda_j-i\epsilon+\gamma_{N,j}}} \tag{7}$$

with diagonal elements $\gamma_{N,1/2}$ of Γ_N. Then the recursion (7) has two ®xed points

$$\mathring{\gamma}_j^{\pm}=-\frac{z_j^*}{2}(1\pm\sqrt{1+4/|z_j|^2})$$

with $z_j=\lambda_j+i\epsilon=-(-1)^j\sqrt{2}c+i\epsilon$. For $\epsilon>0$ a positive imaginary part of $\gamma_{N,j}^{+}$ implies a positive imaginary part of $\gamma_{N+2,j}^{+}$. Since the imaginary parts of the initial values are positive, only the ®xed point $\mathring{\gamma}_j^{+}$ can be reached in the case under consideration.

The DOS of the end chain can be calculated from the ®xed point and reads

$$\rho(0)=-\frac{1}{\pi}\lim_{\epsilon\rightarrow0}\mathrm{Im}\int_{-\pi}^{\pi}(\mathring{\gamma}_1^{+}+\mathring{\gamma}_2^{+})\frac{dk_y}{2\pi}\propto\lim_{\epsilon\rightarrow0}\epsilon\ln(1/\epsilon)=0.$$

This re¯ects the well-known result of the in®nite 2D DWSC, which has a linear pseudogap.

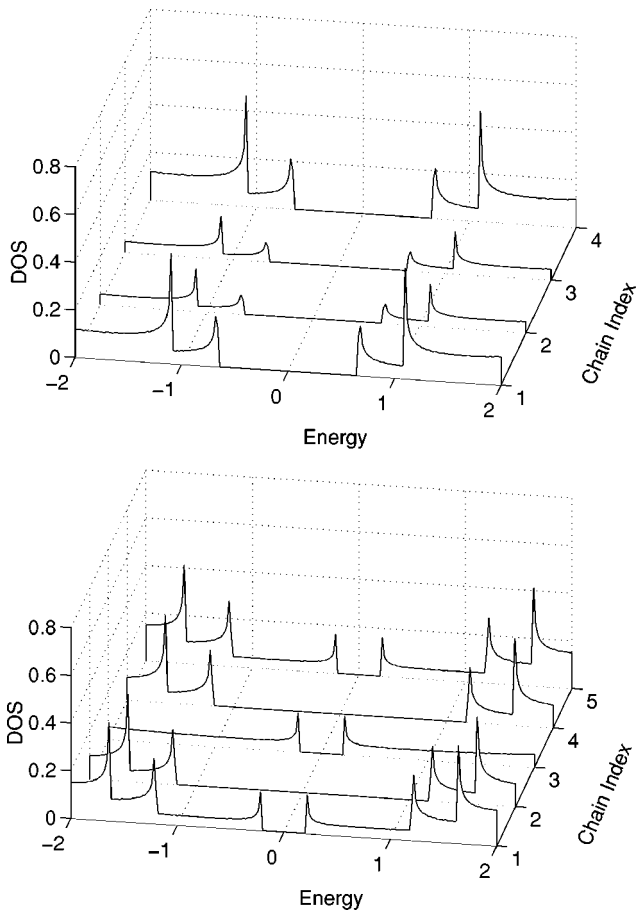

FIG. 7. Density of states for four and ®ve chains with $\Delta_0/t=1$ and $\mu/t=0.3$.

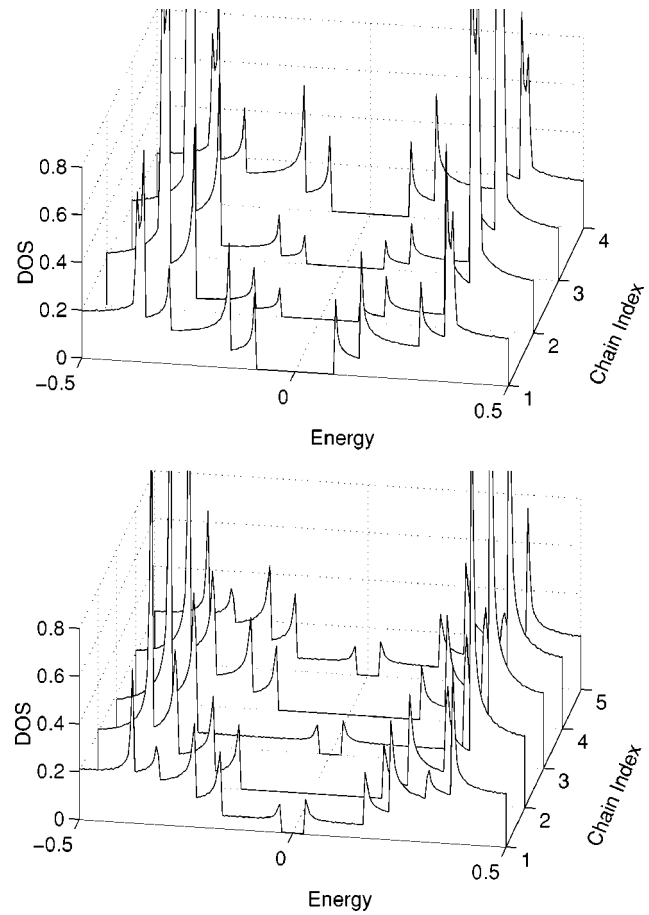

FIG. 8. Density of states for four and ®ve chains with $\Delta_0/t=0.1$ and $\mu/t=0.3$.

D. Realistic models

The preceding discussion has assumed a half-®lled tight-binding band and $\Delta_0/t=1$; both conditions correspond to special symmetries of the Hamiltonian that might be expected to in¯uence the form of the spectrum. The assumption $\Delta_0/t=1$ was in fact made simply in order to obtain the analytical results discussed in Secs. IV A±IV C, and it may easily be checked numerically (Fig. 6) that for small values of Δ_0/t and $\mu=0$, the qualitative even-odd effect in the chain width parity is still obtained. This is consistent with the qualitative results in the case of periodic boundaries.

More signi®cant changes occur when $\mu\neq 0$. In Fig. 7 we see that for an even number of chains, the full gap in all chains is preserved, while for an odd number, those chains that at half-®lling had a ®nite density of states have now acquired a small gap. Analytic results for this case are complicated and not particularly enlightening, but it is clear that for $\mu\ll\Delta_0$, the small gap on the $x=$odd chains in the odd-N case is of the order of μ itself. This is also evident by analogy to Eq. (1), where the pole in the denominator of the integral is shifted by the chemical potential.

A more realistic parameter choice for the optimally doped cuprates would correspond to a doping of 15%, or about $\mu\simeq 0.3t$ for the simple tight-binding spectrum on a square lattice, and a much smaller gap magnitude, of order $\Delta_0=0.1t$. In this case the large gap is set by $2\Delta_0$, but in the odd-chain systems there is a much smaller gap on alternating chains, see Fig. 8. Thus the density of states still generally exhibits a pronounced odd-even width-parity effect.

V. CONCLUSIONS

We have exhibited, using both analytical and numerical means, a number-parity effect in the width N of a mesoscopic d-wave superconducting quantum wire, wherein a ®nite DOS is found at the Fermi level for odd N and zero DOS (with energy gap) is found for even N. The result should be of some practical interest in the not-so-distant future for nanoscale d-wave wire structures. Superconductivity in single layers of the cuprates has already been demonstrated and it seems plausible that a sample of controlled width might be fabricated, and that a scanning-tunnel microscope experiment on such a sample would be able to observe the effects we predict.

It is interesting to note some unusual features of the system we treat here, to our knowledge for the ®rst time, in the presence of impurities. First of all, although the superconducting order parameter has d-wave symmetry, the system may (for N even) have a full gap in the excitation spectrum. In such a situation, one may ask what is the effect of isolated impurities added to the system, and at least naively would

obtain single-impurity *d*-wave-like bound states in this gap without broadening arising from coupling to the quasiparticle continuum. Since the density of states in the odd-*N* systems has an oscillatory behavior across the sample width, the existence and lifetime of these states is expected to depend sensitively on their location in the wire as well.

In addition, the observation we make here may be of interest to the study of the in¯uence of disorder on the DOS of fully 2D *d*-wave superconductors, a subject that has received intense attention recently.[4] The result appears to be that the DOS is generically zero in a 2D *d*-wave superconductor at zero energy, but can be constant or divergent in cases manifesting special symmetries. At the same time, Brouwer *et al.*[10] have shown in disordered quasi-1D systems with chiral symmetry that $\rho(0)$ is zero or divergent according to the number parity of the wire width. It appears that the states in odd- or even-chain systems are modi®ed in different ways by the combined effects of level repulsion and symmetry. Understanding the differences in the odd or even approach to the thermodynamic limit in the presence of disorder may give insight into the physics of localization and DOS supression in the 2D *d*-wave case, which is still poorly understood. We will address these questions in a subsequent work.

ACKNOWLEDGMENTS

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