Bound states in d-density-wave phases

2001 J. Phys.: Condens. Matter 13 11669

(http://iopscience.iop.org/0953-8984/13/50/326)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **13** (2001) 11669–11678 PII: S0953-8984(01)27692-9

Bound states in d-density-wave phases

Carsten Honerkamp and Manfred Sigrist

Theoretische Physik, ETH-Hönggerberg, CH-8093 Zürich, Switzerland

Received 7 August 2001
Published 30 November 2001
Online at stacks.iop.org/JPhysCM/13/11669

Abstract

We investigate the quasiparticle spectrum near surfaces in a two-dimensional system with d-density-wave order within a mean-field theory. For Fermi surfaces with perfect nesting for the ordering wavevector (π, π) of the d-density wave, a zero-energy bound state occurs at 110 surfaces, in close analogy with the known effect in d-wave superconducting states or graphite. When the shape of the Fermi surface is changed by doping, the bound-state energy moves away from the Fermi level. Furthermore, away from half-filling we find inhomogeneous phases with domain walls of the d-density-wave order parameter. The domain walls also support low-energy bound states. These phenomena might provide an experimental test for hidden d-density-wave order in the high-T_c cuprates.

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

1. Introduction

In the search for an explanation of the so-called pseudogap regime of the underdoped high-T_c cuprates, Chakravarty *et al* [1] recently proposed a novel type of order, known as d-density-wave order. This state was discussed earlier by Schulz [2] and in more detail by Nayak [3]. It breaks translational and time-reversal symmetry and is related to flux phases known from t–J and Hubbard models at infinite or large onsite repulsion [4, 5]. Its order parameter, written with the electrons' creation and annihilation operators and ordering wavevector $\vec{Q} = (\pi, \pi)$

$$\Phi_{\mathrm{ddw}} = \sum_{\vec{k},s} f(\vec{k}) \left\langle c^{\dagger}_{\vec{k},s} c_{\vec{k}+\vec{Q},s} \right\rangle \tag{1}$$

is purely imaginary due to the sign change of the $d_{x^2-y^2}$-wave form factor

$$f(\vec{k}) \sim \cos k_x - \cos k_y \tag{2}$$

under $\vec{k} \to \vec{k} + \vec{Q}$. In real space it gives rise to circulating in-plane currents around elementary plaquettes. The orientation of the current flow, i.e. the sign of the flux penetrating the plaquettes, is alternating from plaquette to plaquette.

Since the staggered flux order parameter is of Ising type the d-density-wave can order in two spatial dimensions at non-zero temperatures. In one spatial dimension it can still lead to long range order in the ground state, as recently shown for the two-leg ladder by Fjaerestad and Marston [6].

Apart from the implications of the proposed type of order on observable bulk quantities like specific heat, spin susceptibilities and conductivities [1, 7, 8], the d-wave structure of the order parameter opens another field of phenomena. These are surface effects, which have already played a significant role in the experimental attempts to identify the *superconducting* pairing symmetries in the high-T_c cuprates and other unconventional superconductors [9, 10]. Explicitly we mention the possibility of Andreev bound states at surfaces of unconventional superconductors [11–17] with suitable orientation (and quality in experimental studies) at low or zero energies. The theoretically appealing feature of these surface bound states is that they are a consequence of the symmetry of the order parameter and depend less on the details of the (most of the time drastically simplified) models used to calculate them. Since the d-density-wave order described above also occurs with a non-trivial symmetry, it appears to be interesting to search for surface effects in a d-density wave ordered state. Related to latter phenomena are of course local deformations of the bulk state at impurities. In the context with d-density-wave states, these were recently studied theoretically by Zhu *et al* [18], Wang [19], and Morr [20], which all found low-energy states in the vicinity of non-magnetic impurities.

In this paper we analyse the possibility of surface bound states for electrons on a two-dimensional square lattice with nearest neighbour hopping in the presence of d-density-wave order. After a simplified analytical treatment showing the existence of surface bound states at [110] surfaces, we solve the mean-field equations for the d-density-wave amplitude self-consistently on a square lattice strip with finite width. The d-density-wave order is generated by a repulsive nearest-neighbour density–density interaction. We find low-energy surface states at the [110] surface of the lattice and study their dependence on the band filling. Further we analyse the d-density-wave state away from perfect (π, π)-nesting at half-filling and find indications for domain walls of the order parameter forming between locally half-filled d-density-wave domains. These domain walls themselves can again host bound states with subgap energies.

Of course a realistic description of the high-T_c cuprates may require a more sophisticated theory, so that our simplified mean-field treatment might neglect a substantial part of the physics. Nevertheless we emphasize that the occurrence of surface bound states relies mainly on the symmetry of the order parameter. Thus our findings should be a robust feature remaining true in more detailed studies. Moreover the theoretical analysis of a large number of experiments in the framework of d-density-wave order by Chakravarty *et al* [1] was performed on a comparable level of approximations.

2. Analytical treatment

In order to understand the main features at the surface, let us consider electrons on a two-dimensional square lattice with hopping between nearest neighbours at half-filling. Then the free Fermi surface is the perfectly nested square. We assume that the system has d-density-wave order, giving rise to a term in the Hamiltonian

$$H_{\mathrm{ddw}} = \sum_{\vec{k}} \mathrm{i} W_0 \, (\cos k_x - \cos k_y) \left[c^{\dagger}_{\vec{k}} c_{\vec{k}+\vec{Q}} - c^{\dagger}_{\vec{k}+\vec{Q}} c_{\vec{k}} \right] \tag{3}$$

after mean-field decoupling, with real W_0 and $\vec{Q} = (\pi, \pi)$ (in units of the inverse lattice constant a^{-1}). In real space this term also couples nearest-neighbour sites, analogous to the

ordinary hopping term, so that the total Hamiltonian has a bipartite structure. In the following we will use this property and rewrite the Hamiltonian by doubling the unit cell and separating the wavefunction into components belonging to the A- and B-sublattice, $\Psi_A(\vec{r})$ and $\Psi_B(\vec{r})$

$$\begin{bmatrix} 0 & \varepsilon_{\vec{k}} + \mathrm{i}\gamma_{\vec{k}} \\ \varepsilon_{\vec{k}} - \mathrm{i}\gamma_{\vec{k}} & 0 \end{bmatrix} \begin{pmatrix} \Psi_A(\vec{r}) \\ \Psi_B(\vec{r}) \end{pmatrix} = E \begin{pmatrix} \Psi_A(\vec{r}) \\ \Psi_B(\vec{r}) \end{pmatrix} \tag{4}$$

where $\varepsilon_{\vec{k}} = -2t(\cos k_x + \cos k_y)$ and $\gamma_{\vec{k}} = W_0(\cos k_x - \cos k_y)$ and $\vec{k} = -\mathrm{i}\vec{\nabla}$. Obviously this formulation leads to the proper excitation spectrum in the uniform case which has two Fermi points on the boundary of the reduced Brillouin zone at $\vec{k} = \vec{K} = (\frac{\pi}{2}, \frac{\pi}{2})$ and $\vec{K}' = (\frac{\pi}{2}, -\frac{\pi}{2})$. Close to these points the spectrum has the approximate form of a Weyl spectrum for a chiral particle with opposite chirality at $\vec{K}$ and $\vec{K}'$. In this respect the spectrum of the d-density-wave state has obvious similarity with the spectrum of a graphite sheet [21].

Now we consider the problem of a surface with normal vector parallel to the [110]-direction which defines the coordinate $x' = (x + y)/\sqrt{2}$ ($x' > 0$ and the surface is located at $x' = 0$). Here we will not attempt a self-consistent solution of the mean-field problem, but keep the d-density-wave order parameter W_0 constant for $x' > 0$. This is sufficient to show that this surface possesses surface bound states at zero energy. The translation symmetry along the direction parallel to the surface ($y' = (x - y)/\sqrt{2}$) is maintained so that the momentum $k'_y = (k_x - k_y)/\sqrt{2}$ is conserved. Let us consider electronic states in the vicinity of the non-interacting Fermi line $k'_x = (k_x + k_y)/\sqrt{2} = \pi$ (in units of inverse of the lattice constant $a^* = \sqrt{2}a$ of the doubled unit cell) at the boundary of the reduced Brillouin zone. We extract the fast oscillating and y-dependent parts from the wavefunctions by writing

$$\Psi_{A(B)}(\vec{r}) = f_{A(B),k'_y}(x')\, \mathrm{e}^{\mathrm{i}\pi x'} \mathrm{e}^{\mathrm{i}k'_y y'}. \tag{5}$$

Next we linearize the kinetic energy $\varepsilon_{\vec{k}}$ around the line $k'_x = \pi$ and introduce $p'_x = k'_x - \pi$. Then, for $f_{A(B),k'_y}$ the Hamiltonian has the form

$$\begin{bmatrix} 0 & \epsilon_{\vec{k}} \\ \epsilon^*_{\vec{k}} & 0 \end{bmatrix} \begin{pmatrix} f_{A,k'_y}(x') \\ f_{B,k'_y}(x') \end{pmatrix} = E \begin{pmatrix} f_{A,k'_y}(x') \\ f_{B,k'_y}(x') \end{pmatrix} \tag{6}$$

where

$$\epsilon_{\vec{k}} = v_{F,x'}(k'_y)\, p'_x + 2\mathrm{i}W_0 \sin\left(\frac{k'_y}{2}\right).$$

Here we replace $p'_x = -\mathrm{i}\partial_{x'}$. For the [110]-surface the outer-most sites belong to one sublattice, say A. Then we assume that the wavefunction takes non-zero values only on this sublattice and vanishes on the other. This behaviour of the bound-state wavefunction is confirmed by the self-consistent solution described next. Thus, we impose the condition $f_{B,k'_y}(x') = 0$ and $E = 0$ and analyse the conditions to obtain a zero-energy bound state from the Hamiltonian above [22]. The resulting equation is

$$-\mathrm{i}\partial_{x'} f_{A,k'_y}(x') = 2\mathrm{i}\,\frac{W_0}{v_{F,x}}\,\sin\left(\frac{k'_y}{2}\right)\, f_{A,k'_y}(x') \tag{7}$$

which has an exponentially decaying bound-state solution $f_{A,k'_y}(x') = C\mathrm{e}^{-\kappa x'}$. The existence condition is $k'_y > 0$ with $\kappa = 2W_0 \sin(k'_y/2)/v_{F,x}$ and $W_0 > 0$. As k'_y approaches 0 the bound state extends deeper and deeper into the bulk. Zero-energy bound states only exist for one sign of the momentum parallel to the surface, an indication of broken time-reversal symmetry of the bulk phase. Furthermore, the bound state has non-bonding character as it occupies only one sublattice. Applying the time-reversal operation or interchanging A- and B-sublattices reverses k'_y. A related situation occurs at so-called zigzag edges of graphite

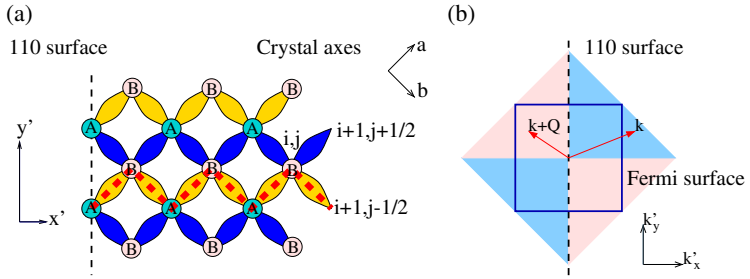

Figure 1. The [110] surface of the two-dimensional square lattice. (a) Real space picture. The circles denote the lattice sites of the A- and B-sublattice, and the differently shaded bonds between them indicate the sign structure of the $d_{x^2-y^2}$-density-wave amplitude $\langle c^\dagger_{i,j} c_{i+1,j\pm1/2}\rangle$. (b) $\vec{k}$-space view.

where the bound-state spectrum has similar properties, but does not violate time-reversal symmetry [22][1] and [23].

We may also include a small shift of the chemical potential μ ($\ll t$). Within our approximative scheme this merely leads to a shift of the bound-state energy E to $-\mu$. A similar shift of the spectrum was also obtained by Zhu *et al* [18] and Wang [19] for the impurity case. Below, we will find the same effect in the self-consistent treatment.

Concluding this analysis we observe that the [110]-surface of a d-density-wave ordered state on a two-dimensional square lattice should support low-lying surface states. We note that at [100] surfaces no bound state can form according to a Bogoliubov–deGennes analysis. In the next section we confirm our qualitative results for the [110] surface with a self-consistent mean-field calculation using tight binding model, which also takes into account the suppression on the d-density-wave order parameter at the odd parity surface.

3. Model and self-consistent mean-field scheme

As a model for the [110] surface, we consider a strip of a rotated square lattice with infinite extension along the surface (see figure 1). For simplicity we neglect the effects of the d-density-wave order on the spin degrees of freedom. Then for each spin orientation the kinetic energy through hopping between neighbouring sites gives rise to a term

$$H_t = -t \sum_{(i,j)} \left[c^\dagger_{i,j} c_{i+1,j+1/2} + c^\dagger_{i,j} c_{i+1,j-1/2} + \text{c.c.} \right]. \tag{8}$$

The index i labels the lattice sites along a zigzag chain in x-direction, while the indices $i+1$, $j \pm 1/2$ label the right upper or lower neighbours of the site i, j. Next we introduce a repulsive nearest-neighbour interaction

$$H_V = V \sum_{i,j} \left[c^\dagger_{i,j} c_{i,j} c^\dagger_{i+1,j+1/2} c_{i+1,j+1/2} + c^\dagger_{i,j} c_{i,j} c^\dagger_{i+1,j-1/2} c_{i+1,j-1/2} \right]. \tag{9}$$

We have already left out the interaction between densities of spin-up and spin-down electrons on neighbouring sites, as this does not contribute to the d-density-wave decoupling. In real space, the static d-density-wave amplitude between nearest neighbours $\vec{x}$ and $\vec{y}$ has the following form [3]:

$$W(\vec{x},\vec{y}) = \langle c^\dagger_{\vec{x},s} c_{\vec{y},s'} \rangle = \frac{\mathrm{i}}{2} W_0 \, \delta_{s,s'} \, \mathrm{e}^{\mathrm{i}\vec{Q}\vec{x}} \left(\delta_{\vec{y},\vec{x}-\hat{a}} + \delta_{\vec{y},\vec{x}+\hat{a}} - \delta_{\vec{y},\vec{x}-\hat{b}} - \delta_{\vec{y},\vec{x}+\hat{b}} \right) \tag{10}$$

[1] A similar approach to graphite edge states has been discussed by Igami [22].

where $\hat{a}$ and $\hat{b}$ denote vectors along the crystal axes with length of the lattice constant a. In our rotated system (see figure 1), the mean-field decoupling is performed by introducing the j- or y-independent imaginary mean field

$$W_{i,i+1} = \frac{V}{2}\left[\langle c^{\dagger}_{i,j} c_{i+1,j+1/2}\rangle - \langle c^{\dagger}_{i,j} c_{i+1,j-1/2}\rangle\right] \tag{11}$$

into the interaction term (9). The minus sign between the two expectation values takes care of the sign change of the $d_{x^2-y^2}$-symmetric order parameter under $\pi/2$-rotation of the lattice. Furthermore for the $d_{x^2-y^2}$-density-wave state (10) we expect $W_{i,i+1}$ to alternate $\propto (-1)^i$, but we do not enforce this behaviour in the numerical mean-field treatment. Using this notation, the maximal gap magnitude in the homogeneous bulk state is $2|W_{i,i+1}|$.

Next we exploit the translational invariance along the y-direction by introducing the partial Fourier transform

$$c_{i,j} = \frac{1}{\sqrt{N_y}} \sum_k c_{i,k}\, \mathrm{e}^{\mathrm{i}ky_j}.$$

N_y denotes the number of lattice sites in the y-direction, which we choose to be large enough for the numerical calculation. Since the distance in the y-direction between the zigzag chains along the x-direction is $a^* = \sqrt{2}a$, $k = k'_y$ has to range from $-\pi/a^*$ to π/a^*. In the following we set $a^* = 1$. With this the Hamiltonian becomes

$$H = -2t \sum_{i,k} \left[c^{\dagger}_{i,k} c_{i+1,k} + c^{\dagger}_{i+1,k} c_{i,k}\right] \cos\frac{k}{2} - \mu \sum_{i,k} c^{\dagger}_{i,k} c_{i,k}$$
$$-\mathrm{i} \sum_{i,k} W_{i,i+1}\left[c^{\dagger}_{i,k} c_{i+1,k} + c^{\dagger}_{i+1,k} c_{i,k}\right] \sin\frac{k}{2}. \tag{12}$$

This Hamiltonian can be easily diagonalized for each k on the finite strip. The self-consistent scheme is complemented with the gap equation

$$W_{i,i+1} = -\frac{\mathrm{i}}{N} \sum_k \langle c^{\dagger}_{ik} c_{i+1,k}\rangle \sin\frac{k}{2}. \tag{13}$$

From this equation and the eigenfunctions of (12) we can calculate the local d-density-wave amplitude $W_{i,i+1}$. Inserting this back into (12) we can repeat the process until self-consistency is reached.

4. Numerical results

4.1. Results for perfect nesting: zero-energy states

Let us first discuss the results at half-filling. We choose $\mu = 0$ and $V = 2t$. In figure 2(a) we show the spatial variation of the d-density amplitude at the surface. One clearly observes the staggered real space structure of the mean field $W_{i,i+1}$, in agreement with (10). At the surface the amplitude is slightly suppressed on the length scale of a few lattice constants, similar to the suppression of the d-wave superconducting gap function in analogous superconducting cases [11, 24]. In figure 2(b) we show the local density of states at the surface and in the bulk of the system. The bulk density of states exhibits a well formed gap edge at $2|W^{\mathrm{bulk}}_{i,i+1}|$ with some low-energy states due to the nodes of the d-density-wave gap. The surface density of states shows a pronounced zero-energy peak. Studying the wavefunctions corresponding to these low-energy eigenvalues, we find that the peak indeed arises due to bound states (see figure 2(d)), confirming expectations from the analysis of section 2. The bound-state wavefunctions take non-zero values only on one sublattice and their decay length depends on

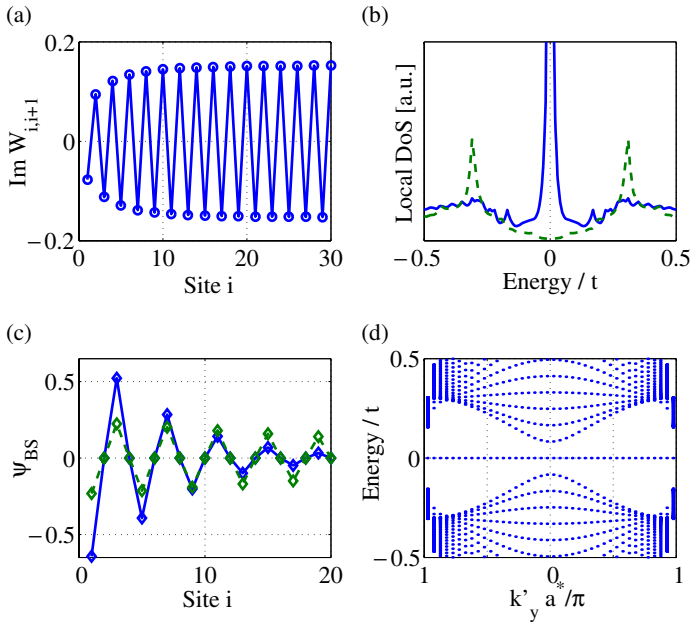

Figure 2. (a) Spatial variation of the (purely imaginary) d-density-wave amplitude $W_{i,i+1}$. (b) Surface (on the first lattice site, solid curve) and bulk (dashed curve) density of states versus energy. (c) Wavefunctions of two zero-energy bound states corresponding to the transverse wavevectors $k'_y \approx -3\pi/4$ (solid curve) and $-\pi/4$ (dashed curve). The data shown are calculated for a system with 300 sites in the x-direction, $V = 2t$, $\mu = 0$ and $T = 0.01t$. (d) Spectrum as a function of the transverse wavevector k'_y. The zero-energy states for positive and negative k'_y are localized on opposite surfaces of the strip. All states at non-zero energy extend over the whole system.

the size of the d-density-wave bulk gap: for small k'_y close to the nodes of the bulk d-density-wave gap the bound-state wavefunction extends far into the system, while for larger values of k'_y, corresponding to a larger bulk gap, the decay length is shorter. Furthermore we find surface bound states either for positive or negative k'_y values, depending on the sign of the d-density-wave amplitude at the surface. A detailed analysis shows that a sizable part of the weight in the zero-energy peak is taken from relatively high energies $\approx 3t$–$4t$. This appears to be comprehensible in view of the small extension of the bound state.

4.2. Surface bound states, domain walls and domain-wall bound states away from half-filling

Next we change the band filling away from half-filling by varying the chemical potential μ. Then the first striking observation is that beyond a certain critical μ away from $\mu = 0$ the self-consistent scheme converges to non-homogeneous solutions where the d-density-wave pattern exhibits domain walls with phase jumps of π, as shown in figure 3 for $\mu = -0.1t$ corresponding to an average occupation number of ≈ 0.98 particles per site. Analysing the charge distribution $\langle n_i \rangle$ (the dashed curves in figure 3 show the local deviation from half-filling), we find that the system chooses to form locally half-filled regions with intact d-density-wave order. The holes are concentrated in the domain walls. On increasing the temperature, the correlation length of the d-density-wave order gets longer and the domain walls evaporate so that the bulk state becomes homogeneous again. If we move further away from half-filling, the domain-wall density increases and finally, at another critical chemical potential (determined by the strength

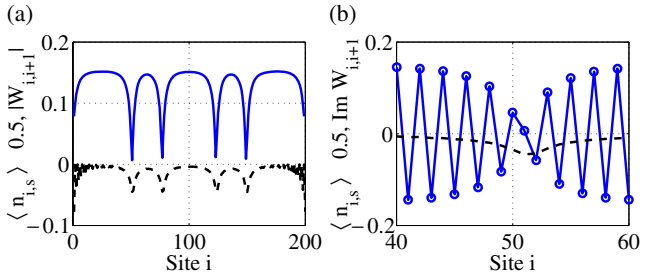

Figure 3. (a) Spatial variation of the modulus of the d-density-wave amplitude $W_{i,i+1}$ (solid curve) and the local charge $\langle n_{i,s}\rangle$ (dashed curve) per spin with respect to half-filling. (b) Detailed structure of the domain wall showing the phase shift by π. The data are calculated on a system with 200 sites in the x-direction, $V = 2t$, $\mu = -0.1t$ and $T = 0.01t$.

of the nearest-neighbour interaction V, for $V = 2t$ at $\mu \approx -0.12t$), the local d-density-wave order disappears completely.

No attempt was undertaken to investigate the role of the boundary conditions for the domain-wall formation or to show that these inhomogeneous solutions indeed correspond to global minima of the total free energy. Furthermore, if this was the case, the model should be extended to also include possible inhomogeneities in the direction along the surface. Here we do not want to take this difficult route, or explore the mean-field phase diagram of this model in detail. Instead we will now assume that the domain walls along the [110] direction are stable or can be stabilized by some additional interactions, and continue to analyse the local excitation spectrum at the surface and in the domain wall.

According to the analytic calculation in section 2 we expect the zero-energy bound state to move to finite energies. This is also the result of the self-consistent calculation, as shown in figure 4 for $\mu = -0.08t$. For this chemical potential the bulk state is still homogeneous. Apart from the bound-state energy, the whole spectrum has moved and is now centred around a finite energy $\approx -\mu$, as also found by Zhu *et al* [18] and Wang [19] for the impurity case. For the bulk system this shift is equivalent to the assumption of Chakravarty *et al* [1] that upon hole-doping away from half-filling the d-density-wave dispersion stays rigid as in a semiconductor and that the doped holes form Fermi surface pockets around the nodal points of the half-filled state.

We now include a finite next-nearest-neighbour hopping t'. This has the effect of destroying the (π, π) nesting in the homogeneous state even at half-filling. Nevertheless, we find stable d-density-wave solutions, in particular near the so-called van Hove filling for $\mu = 4t'$ where the bulk Fermi surface touches the van Hove singularities in the density of states at $(\pi, 0)$ and $(0, \pi)$. For $V = 2t$ and $t' = -0.2t$, stable solutions exist between $\mu \approx -0.61t$ ($\langle n\rangle \approx 0.92$ per site) and $\mu \approx -0.85t$ ($\langle n\rangle \approx 0.82$ per site). For band fillings smaller or larger than these critical values the mean-field solutions for the d-density-wave state collapse rapidly with very narrow doping regions close to these critical dopings where inhomogeneous solutions occur. This suggests that the non-zero next-nearest-neighbour hopping t' inhibits the formation of well shaped domain walls with regions of intact d-density wave order and charge accumulations in between. In figure 4(b) we plot the surface and bulk density of states for the homogeneous case $t' = -0.2t$ and $\mu = -0.7t$. Both curves have a large asymmetry with respect to zero energy and the peak in the surface density of states is centred at comparably high excitation energies.

Now let us turn back to the domain walls for $t' = 0$ at sufficient doping away from half-filling. As shown in figure 5, the local density of states at the domain wall exhibits a low-energy

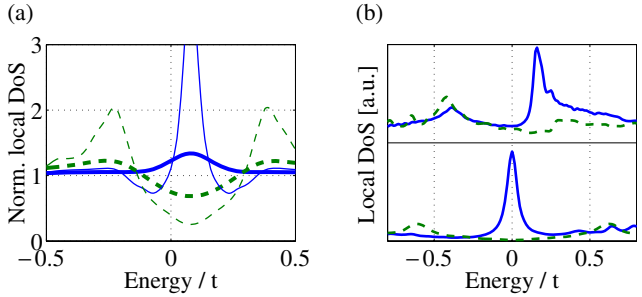

Figure 4. (a) Local density of states at the surface (solid curves) and in the bulk density of states (dashed curves) versus energy, for $V = 2t$, $\mu = -0.08t$ and $T = 0.01t$ (thin curves) and $T = 0.08t$ (thick curves), normalized with respect to the values above the d-density-wave transition at $T_c^{ddw} \approx 0.125t$. The local density of states was smeared out by Lorentzians with width $2T$. (b) Upper curves: surface (solid curve) and bulk (dashed curve) density of states in the d-density-wave state for $t' = -0.2t$ and $\mu = -0.7t$ at $T = 0.02t$; lower curves: surface (solid curve) and bulk (dashed curve) density of states for the homogeneous d-wave superconducting order coexisting with the d-density-wave order (non-self-consistent) of comparable amplitude.

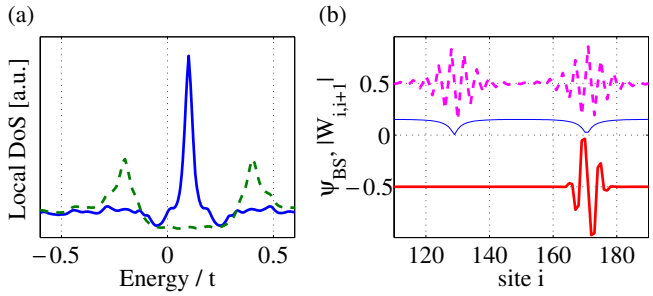

Figure 5. (a) Local density of states at a domain wall (solid curve) and bulk density of states (dashed curve) versus energy. The data are calculated on a system with 300 sites in the x-direction, $V = 2t$, $\mu = -0.1t$ and $T = 0.001t$. The local density of states was smeared out through Lorentzians with width $0.01t$. (b) The upper ($k'_y a^* = -2.5$) and lower ($k'_y a^* = -3$) curves (shifted by ± 0.5) show wavefunctions of states with the different transverse wavevector k contributing to the low-energy peak at a domain wall. The thin line in the middle shows the absolute magnitude of the d-density-wave amplitude $W_{i,i+1}$.

peak similar to the one at the surface. For a given transverse wavevector we can analyse the wavefunctions contributing to this peak. Two of these wavefunctions for different transverse wavevectors k'_y are shown in figure 5(b): the lower curve belongs to a wavefunction with $k'_y a^* = -3$, while the upper curve is for $k'_y a^* = -2.5$. The latter wavefunction has visible amplitude in two domain walls. The difference between the two wavefunctions can be easily understood: the wavefunction with larger transverse momentum belongs to a larger bulk gap (in our coordinate system, the bulk gap is maximal for $k'_y a^* = \pi$). Therefore the wavefunction decays rapidly away from the domain wall. The wavefunction for the smaller k'_y has a larger decay length and thus can effectively hybridize with solutions localized at the neighbouring domain wall. For even smaller values of the transverse wavevector, the wavefunctions corresponding to the subgap energy states distribute their weight over several domain walls.

5. Conclusions

We have calculated the local density of states in the presence of d-density-wave order on the two-dimensional square lattice. At [110] surfaces we find zero energy (for perfect (π, π) nesting of the Fermi surface at half-filling) or low-energy (away from perfect nesting) surface states, which give rise to peaks in the calculated surface density of states, in good qualitative agreement with recent results for the local density of states around impurities [18–20]. The surface density of states is measurable in in-plane tunnelling experiments, as demonstrated for the high-T_c cuprates in the superconducting state [12–15]. Similar to the proposals by Zhu *et al* [18], Wang [19] and Morr [20], this provides another experimental test for possible d-density-wave long-range order in the pseudogap phase of the underdoped cuprates, as proposed by Chakravarty *et al* [1]. Since surface effects crucially depend on the quality of the surface, it could still be that the bound-state features are wiped out by surface imperfections, even if d-density-wave order is present. Moreover the temperature smearing reduces the low-bias peaks considerably. Therefore we propose to perform experiments on strongly underdoped samples with large pseudogap and low superconducting transition temperatures which have [110] surfaces that exhibit a zero-bias peak in the superconducting state. The effect of surface imperfections on the latter feature should be comparable to that on the d-density bound states. Thus, if the superconducting state does exhibit an Andreev bound state one may also expect a d-density surface state in the pseudogap phase. We note that so far the experimental results do not point towards d-density wave order: published conductance measurements on underdoped $YBa_2Cu_3O_{7-x}$ films and $La_{2-x}Sr_xCuO_4$ single crystals [14] and tunnelling data on 001 tilt grain boundaries in underdoped YBCO [13] show zero-energy peaks below the superconducting T_c and no feature above T_c.

For finite next-nearest-neighbour hopping, the peak in the calculated local density of states due to the surface states moves to rather large excitation energies, such that one might wonder if this peak could still be distinguished from a gap edge similar to the one in the bulk density of states. We think that the distinction is still possible, because the peak due to the surface states has to move to zero energy when the system enters the d-wave superconducting state. In contrast with that the gap-edge feature due to the extended bulk states should move to higher excitation energies in the superconducting state (see lower curves in figure 4(b)), if the latter is indeed formed on top of the d-density-wave order, as suggested by Chakravarty *et al* [1]. One may even try to observe a shift of the bound-state feature—if existent above the superconducting T_c—from non-zero energies due to the imperfect nesting to zero energy when one goes from the d-density-wave phase into the d-wave superconducting state. Another interesting experimental question might be the search for domain walls of the d-density-wave order parameter along the [110] direction which again should give rise to low-energy peaks in the local c-axis tunnelling density of states. We note however that our calculation is not a stringent proof of the existence of domain walls for reasons explained above.

Acknowledgments

It is a pleasure to thank Chetan Nayak, Ying Liu, Masatsura Igami, Manfred Salmhofer and Katsunori Wakabayashi for helpful discussions. This work was financially supported by the Swiss National Science Foundation.

References

[1] Chakravarty S, Laughlin R B, Morr D K and Nayak C *Phys. Rev.* B **63** 094503
(Chakravarty S, Hae-Young Kee and Nayak C 2001 *Preprint* cond-mat/0101204)
[2] Schulz H J 1989 *Phys. Rev.* B **39** 2940
[3] Nayak C 2000 *Phys. Rev.* B **62** 4880
[4] Affleck I and Marston J B 1988 *Phys. Rev.* B **37** 3774
Affleck I, Zou Z, Hsu T and Anderson P W 1988 *Phys. Rev.* B **38** 745
[5] Wen X G and Lee P A 1996 *Phys. Rev. Lett.* **76** 503
Kishine J, Lee P A and Wen X G 2001 *Phys. Rev. Lett.* **86** 5365
[6] Fjaerestad J O and Marston J B 2001 *Preprint* cond-mat/0107094
[7] Qiang-Hua Wang, Jung Hoon Han and Dung-Hai Lee 2000 *Preprint* cond-mat/0011398
[8] Wonkee Kim, Jian-Xin Zhu, Carbotte J P and Ting C S 2001 *Preprint* cond-mat/0106594
[9] van Harlingen D J 1995 *Rev. Mod. Phys.* **67** 515
Tsuei C C and Kirtley J R 2000 *Rev. Mod. Phys.* **72** 969
[10] Sigrist M 1998 *Prog. Theor. Phys.* **99** 899
[11] For a review, see Kashiwaya S and Tanaka Y 2000 *Rep. Prog. Phys.* **63** 1641
[12] Covington M, Aprili M, Paraonu E, Greene L H, Xu F, Zhu J and Mirkin C A 1997 *Phys. Rev. Lett.* **79** 277
[13] Alff L, Kleefisch S, Schoop U, Zittartz M, Kemen T, Bauch T, Marx A and Gross R 1998 *Eur. Phys. J.* B **5** 423
[14] Dagan Y, Kohen A, Revcolevschi A and Deutscher G 2000 *Phys. Rev.* B **61** 7012
[15] Yeh N C, Wei J Y T, Chen C T, Si W D and Xi X X 2000 *Physica* C **341** 1639
[16] Wälti C, Ott H R, Fisk Z and Smith J L 2000 *Phys. Rev. Lett.* **85** 5258
[17] Laube F, Goll G, Löhneysen H v, Fogelström M and Lichtenberg F 2000 *Phys. Rev. Lett.* **84** 1595
[18] Jian-Xin Zhu, Wonkee Kim, Ting C S and Carbotte J P 2001 *Preprint* cond-mat/0105580
[19] Qiang-Hua Wang 2001 *Preprint* cond-mat/0106327
[20] Morr D K 2001 *Preprint* cond-mat/0106285
[21] See for example Dresselhaus M S and Dresselhaus G 1981 *Adv. Phys.* **30** 139
[22] Igami M unpublished
[23] Fujita M, Wakabayashi K, Nakada K and Kusakabe K 1996 *J. Phys. Soc. Japan* **65** 1920
[24] Honerkamp C, Wakabayashi K and Sigrist M 2000 *Eur. Phys. Lett.* **50** 368