Bound states in $d$-density-wave phases

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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 wave vector $(\pi, \pi)$ 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.

I. INTRODUCTION

In the search for an explanation of the so-called pseudogap regime of the underdoped high-$T_c$ cuprates, Chakravarty, Laughlin, Morr, and Nayak recently proposed a novel type of order, known as $d$-density-wave order. This state was discussed earlier by Schulz and in more detail by Nayak. 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. Its order parameter, written with the electrons’ creation and annihilation operators and ordering wavevector $\vec{Q} = (\pi, \pi)$,

$$\Phi_{d\text{dw}} = \sum_{\vec{k},s} f(\vec{k}) \langle c_{\vec{k},s}^\dagger c_{\vec{k}+\vec{Q},s}\rangle$$

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

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

under $\vec{k} \rightarrow \vec{k} + \vec{Q}$. 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 nonzero 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.

Apart from the implications of the proposed type of order on observable bulk quantities like specific heat, spin susceptibilities and conductivities, 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. Explicitly we mention the possibility of Andreev bound states at surfaces of unconventional superconductors 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., Wang, and Morii, which all found low energy states in the vicinity of non-magnetic impurities.

In this paper we analyze the possibility of surface bound states for electrons on a two-dimensional square lattice with nearest neighbor 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 neighbor 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 analyze the $d$-density-wave state away from perfect $(\pi, \pi)$-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 sub-gap 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. was performed on a comparable level of approximations.

II. 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 neighbors 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, 

\[ H_{dw} = \sum_{\vec{k}} iW_0 (\cos k_x - \cos k_y) \left[ c^\dagger_{k} c_{k+\vec{Q}} - c^\dagger_{k+\vec{Q}} c_{\vec{k}} \right]. \]  

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

\[
\begin{pmatrix}
0 \\
\varepsilon_{\vec{k}} - i\gamma_{\vec{k}} \\
0
\end{pmatrix}
\begin{pmatrix}
\Psi_A(\vec{r}) \\
\Psi_B(\vec{r}) \\
\psi(\vec{r})
\end{pmatrix}
= E
\begin{pmatrix}
\Psi_A(\vec{r}) \\
\Psi_B(\vec{r}) \\
\psi(\vec{r})
\end{pmatrix},
\]

(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 \( \vec{k} = -i\vec{\gamma} \). 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 \( \vec{k} = \vec{K} = (\frac{\pi}{a}, \frac{\pi}{a}) \) and \( \vec{k}' = (\frac{\pi}{a}, -\frac{\pi}{a}) \). 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 [14].

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 wave functions by writing

\[ \Psi_{A,B}(\vec{r}) = f_{A,B}(k'_y)(x') e^{i\pi x'} e^{ik'_y y'} \]

(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

\[
\begin{pmatrix}
0 \\
\varepsilon_{\vec{k}} - W_0 \\
0
\end{pmatrix}
\begin{pmatrix}
\langle x' \rangle \\
\langle y' \rangle \\
0
\end{pmatrix}
= E
\begin{pmatrix}
\langle x' \rangle \\
\langle y' \rangle \\
0
\end{pmatrix},
\]

(6)

where

\[ \varepsilon_{\vec{k}} = v_{F,x}(k'_y)p'_x + 2iW_0 \sin \left( \frac{k'_y}{2} \right). \]

Here we replace \( p'_x = -i\partial_{x'} \). For the [110]-surface the outer most sites belong to one sublattice, say \( A \). Then we assume that the wave function takes nonzero values only on this sublattice and vanishes on the other. This behavior of the bound state wave function is confirmed by the self-consistent solution described below. Thus, we impose the condition \( f_{B,k'_y}(x') = 0 \) and \( E = 0 \) and analyze the conditions to obtain a zero energy bound state from the Hamiltonian above [1]. The resulting equation is

\[-i\partial_{x'} f_{A,k'_y}(x') = 2iW_0 \sin \left( \frac{k'_y}{2} \right) f_{A,k'_y}(x')\]

(7)

which has an exponentially decaying bound state solution \( f_{A,k'_y}(x') = Ce^{-\kappa x'} \). 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 where the bound state spectrum has similar properties, but does not violate time reversal symmetry [2].
We may also include a small shift of the chemical potential \( \mu (\ll t) \). 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.\cite{12} and Wang\cite{13} 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.

III. 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 Fig. 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 neighboring sites gives rise to a term

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

\( (8) \)

The index \(i\) labels the lattice sites along a zig-zag chain in \(x\)-direction, while the indices \(i + 1, j \pm 1/2\) label the right upper or lower neighbors of the site \(i,j\). Next we introduce a repulsive nearest neighbor interaction

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

\( (9) \)

We have already left out the interaction between densities of spin-up and spin-down electrons on neighboring sites, as this does not contribute to the \(d\)-density-wave decoupling. In real space, the static \(d\)-density-wave amplitude between nearest neighbors \(\hat{x}\) and \(\hat{y}\) has the following form

\[
W(\vec{x},\vec{y}) = \langle \vec{c}_{\vec{x}\hat{x}}^\dagger \vec{c}_{\vec{y}\hat{y}}^\dagger \rangle = \frac{i}{2} W_0 \delta_{\vec{k},\vec{\alpha}} e^{i\vec{k}\cdot\vec{y}}
\]

\[
\left( \delta_{\vec{y},\vec{x}-\vec{a}} + \delta_{\vec{y},\vec{x}+\vec{a}} - \delta_{\vec{y},\vec{x}+\vec{b}} - \delta_{\vec{y},\vec{x}-\vec{b}} \right)
\]

\( (10) \)

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

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

\( (11) \)

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 \((-1)^j\), but we do not enforce this behavior 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 \(y\)-direction by introducing the partial Fourier transform

\[
c_{i,j} = \frac{1}{\sqrt{N_y}} \sum_k c_{i,k} e^{iky_j}.
\]

\( (12) \)

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

\[
H = -2t \sum_{i,k} \left[ c_{i,k}^\dagger c_{i+1,k} + c_{i+1,k}^\dagger c_{i,k} \right] \cos \frac{k}{2}
\]

\[-\mu \sum_{i,k} c_{i,k}^\dagger c_{i,k}
\]

\[-i \sum_{i,k} W_{i,i+1} \left[ c_{i,k}^\dagger c_{i+1,k} + c_{i+1,k}^\dagger c_{i,k} \right] \sin \frac{k}{2}. \]

\( (12) \)

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

\[
W_{i,i+1} = -\frac{i}{N} \sum_k \langle c_{ik}^\dagger c_{i+1,k} \rangle \sin \frac{k}{2}.
\]

\( (13) \)

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.

IV. NUMERICAL RESULTS

A. Results for perfect nesting: zero energy states

Let us first discuss the results at half-filling. We choose \(\mu = 0\) and \(V = 2t\). In the left plot Fig. 3 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 \( (11) \). 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. In the right plot 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 $2|W_{i,i+1}^{\text{bulk}}|$ 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 wave functions corresponding to these low energy eigenvalues, we find that the peak indeed arises due to bound states (see lower plot of Fig. 3), confirming the expectations from the analysis of Sec. II. The bound state wave functions take nonzero values only on one sublattice and their decay length depends on 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 wave function 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 $k_y'$, 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.

B. 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 $\mu$. Then the first striking observation is that beyond a certain critical $\mu$ 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 $\pi$, as shown in Fig. 3 for $\mu = -0.1t$ corresponding to an average occupation number of $\approx 0.98$ particles per site. Analyzing the charge distribution $\langle n_i \rangle$ (the dashed lines in Fig. 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. With increasing temperature, the correlation length of the $d$-density-wave order gets longer and the domain walls evaporate such 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 of the nearest neighbor 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. Further, if this was the case, the model should be extended to include possible inhomogeneities in the direction along the surface as well. 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 analyze the local excitation spectrum at the surface and in the domain wall.

According to the analytic calculation in Sec. II we expect the zero energy bound state to move to finite en-
energies. This is also the result of the self-consistent calculation, as shown in Fig. 3 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 centered around a finite energy $\approx -\mu$, as also found by Zhu et al. [14] and Wang [12] for the impurity case. For the bulk system this shift is equivalent to the assumption of Chakravarty et al. [15] that upon hole-doping away from half-filling the $d$-density-wave dispersion stays rigid like 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 neighbor hopping $t'$. This has the effect of destroying the $(\pi, \pi)$ 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 nonzero next nearest neighbor hopping $t'$ inhibits the formation of well shaped domain walls with regions of intact $d$-density wave order and charge accumulations in between. In the right plot of Fig. 4 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 centered 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 Fig. 3, the local density of states at the domain wall exhibits a low energy peak similar to the one at the surface. For a given transverse wavevector we can analyze the wave functions contributing to this peak. Two of these wave functions for different transverse wavevectors $k'_y$ are shown in the right plot of Fig. 3, the lower curve belongs to a wave function with $k'_ya^* = -3$, while the upper curve is for $k'_ya^* = -2.5$. The latter wave function has visible amplitude in two domain walls. The difference between the two wave functions can be easily understood: the wave function with larger transverse momentum belongs to a larger bulk gap (in our coordinate system, the bulk gap is maximal for $k'_ya^* = \pi$). Therefore the wave function decays rapidly away from the domain wall. The wave function for the smaller $k'_y$ has a larger decay length and thus can effectively hybridize with solutions localized at the neighboring domain wall. For even smaller values of the transverse wavevector, the wave functions corresponding to the sub-gap energy states distribute their weight over several domain walls.

![FIG. 4. Left plot: Local density of states at the surface (solid lines) and in the bulk density of states (dashed lines) versus energy, for $V = 2t$, $\mu = -0.08t$ and $T = 0.01t$ (thin lines) and $T = 0.08t$ (thick lines), normalized with respect to the values above the $d$-density wave transition at $T^d_{crit} \approx 0.125t$. The local density of states was smeared out through Lorentzians with width 0.01t. Right plot: upper curve: surface (solid line) and bulk (dashed line) density of states in the $d$-density-wave state for $t' = -0.2t$ and $\mu = -0.7t$ at $T = 0.02t$. Right plot, lower curves: surface (solid line) and bulk (dashed line) density of states for homogeneous $d$-wave superconducting order coexisting with $d$-density-wave order (non-self-consistent) of comparable amplitude.](image)

V. 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 $(\pi, \pi)$ 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 [16]. The surface density of states is measurable in in-plane tunneling experiments, as demonstrated for the high-$T_c$ cuprates in the superconduct-
imperfections, even if the bound state features are wiped out by surface imperfections, it could still be that the bound state features are comparable to that 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 expect a \( d \)-density surface state in the pseudogap phase as well. We note that so far the experimental results do not point towards \( d \)-density wave order: published conductance measurements on underdoped YBCO films and LSCO single crystals and tunneling data on 001 tilt grain boundaries in underdoped YBCO show zero energy peaks below the superconducting \( T_c \) and no feature above \( T_c \).

For finite next-nearest neighbor 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 the right plot of Fig. [4]), if the latter is indeed formed on top of the \( d \)-density-wave order, as suggested by Chakravarty et al. [4]. One may even try to observe a shift of the bound state feature – if existent above the superconducting \( T_c \) – from nonzero 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 tunneling density of states. We note however that our calculation is not a stringent proof of the existence of domain walls for the reasons explained above.

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