Staggered Local Density of States around the Vortex in Underdoped Cuprates
The elucidation of the ground state properties of the high
$T_c$ cuprates has been one of the major challenges in con-
densed matter physics. Recent STMs experiments on vor-
tices [1,2] have indicated the existence of a normal core
with a gap structure characteristic of the normal state pseu-
dogap above $T_c$. The theoretical description of the normal
core, however, remains unresolved [3–5]. Based on the
SU(2) slave-boson theory of the high $T_c$ superconductors
[6,7], Lee and Wen [8] proposed a model of the vortex with
a staggered flux (SF) core, characterized by a pseudogap
and staggered orbital current. The signature of the SF order
in zero field was found in the Gutzwiller-projected $d$-wave
superconducting state by a variational Monte Carlo method
[9] and exact diagonalization of the $t$-$J$ model [10]. By
using a Gutzwiller-projected U(1) slave-boson mean-field
wave function, Han and co-workers recently found evi-
dence of the SF order near the vortex core [11,12]. The
natural question arises as to whether the SF core has ob-
servable consequences for the tunneling spectra using
atomic resolution STM. This is the question addressed by
this Letter.

We first summarize some of the salient feature of the
SU(2) vortex structure. In the SU(2) slave-boson theory [6],
the physical electron is represented by a spin-1/2 fermion operator $f_{i \sigma}$ and a charge-1 boson operator
$h_i^T = (b_{1i}, b_{2i})$: $c_{i \sigma} = \frac{1}{\sqrt{2}} h_i^\dagger \psi_{i \sigma}$, where $h_i$
and $\psi_{i \sigma}^\dagger = (f_{i \sigma}, \epsilon_{\sigma \delta} f_{j \delta}^\dagger)$ are SU(2) doubles.
The slave-boson mean-field state is characterized by $2 \times 2$
matrices $U_{ij} = (e^{\Delta_{ij} i \chi_i}, \Delta_{ij})$ on the links and boson con-
densation $h_i$ on the sites. The $U_{ij}$ describe the hopping of the fermions and bosons. The mean-field solu-
tion is obtained by integrating out the fermions and mini-
mizing the mean-field energy $E(U_{ij}, h_i)$, which
leads to $\chi_{ij} = \langle f_i^{\dagger \sigma} f_i^{\dagger \sigma} \rangle$ and $\Delta_{ij} = \langle \epsilon_{\sigma \delta} f_i^{\dagger \delta} f_j \rangle$. The
SU(2) gauge invariance is realized through the relation
$E(U_{ij}, h_i) = E(W_i U_{ij} W_j^\dagger, W_i h_i)$, for any
$W_i \in SU(2)$. In the underdoped region, the mean-field solution has the following form (in the SF gauge):
$U_{ij}^{SF} = -\frac{\Delta}{\chi} \exp[i(-1)^{i+j} \Phi_0 \tau^z]$, with $\Delta = \sqrt{\chi^2 + \Delta^2}$
and $\Phi_0 = \tan^{-1}(\Delta/\chi)$. This describes fermions hopping
with flux $\pm 4\Phi_0$ on alternating plaquettes [13]. The
advantage of the SF gauge is that it is apparent that the
SU(2) symmetry has been broken down to the residual
SU(1), since $U_{ij}^{SF}$ contains only $\tau^3$. As a result, the low
lying fluctuations have a simple form in the SF gauge:
$U^{SF}_{ij} = -\frac{\Delta}{\chi} \exp[i(-1)^{i+j} \Phi_0 \tau^z] \exp[-ia^3_0 \tau^3]$.

These fluctuations are described by the lattice gauge field $\hat{a}^{ij}_{\ell}$. In the presence of a magnetic field, the mean-field solution contains vortices. Since the bosons are lo-

cally condensed to the bottom of the band, they can be
parametrized by $(\hat{h}_{i}^{SF})^3 = 1 - i(-1)^{i+j} z_{i,j}$, where
$z_{i,j}$ slowly vary in space and time. The vortex is now described by the twisted $z_i$ field and $U_{ij}$ in Eq. (1). To write down the vortex structure explicitly, let us introduce $z_{i,j} = e^{i\phi_i / 2}$ and $z_{i,j} = e^{i\phi_i / 2}$, where $\phi_i = \alpha_i - \phi_i / 2$; and $\phi_j = \alpha_i + \phi_i / 2$. The phase angles $\alpha_i$ and $\phi_i$ are associated with the electromagnetic (EM) U(1) and the $a^3$ U(1) gauge structures, respectively. The internal degrees of freedom $\phi$ and $\theta$ can be visualized by the vector $I_i = \hat{z}_i^{\dagger} z_i = (\sin \theta_i, \sin \phi_i, \cos \phi_i, \cos \theta_i)$, which has
the meaning of the quantization axis for the $z_i$ fields.

In the vortex structure proposed by Lee and Wen [8],
both $\alpha_i$ and $\phi_i$/2 wind by $\pi$ and consequently give an
appropriate $hc/2e$ vortex for the EM gauge field $A(r)$, i.e., $\nabla \phi = \nabla \phi / 2 = \hat{e}_\phi / 1$ which leads to $\nabla \phi = \hat{e}_\phi / 2$ and $\nabla \phi = \hat{e}_\phi / 2$, where $\hat{e}_\phi$ denotes the azimuthal unit vector in the physical space. That is to say, only
$\phi_i$ changes its phase $\phi_i$ by $2\pi$ as we go around the
vortex, while $\phi_i$ does not. Outside the vortex core, $I_i = (\sin \phi_i, -\cos \phi_i, 0)$ [see Fig. 1(a)], which describes
a $d$-wave superconducting state. As we approach the core,
the $b_2$ changes its phase $\phi_2$ by $2\pi$ as we go around the $\phi$.

The vortex center is represented by $I_i = (0, 0, 1)$, which is just the metallic SF state. The $I_i$
vector tilts smoothly from the equator to the north pole
of the vortex, and its hyperboloidal structure extends
to the $\ell_e$. At the same time, the gauge flux $h = \nabla \times a^3$ is distributed over a distance scale of $\lambda_o$, and it is expected
that $\lambda_o \sim x^{-1} \geq \ell_e$. Inside $\lambda_o$, the gauge invariant
combination
visualized by making a local gauge transformation $g_i$ transforms this configuration to (b) in the $d$-wave gauge, where the internal phases of the Bose condensate are gauged away.

$$\mathcal{V}_{ij} = \frac{\phi_i - \phi_j}{2} - a_{ij}^3$$

and its continuum limit, $\mathcal{V}(r) = \frac{1}{2} \nabla \phi(r) - a^3(r)$, is finite. This is the analog of the superfluid velocity inside the London penetration depth $\lambda_L$ in conventional vortices, except that here $\lambda_a \ll \lambda_L$ and the effect of the EM field $A$ is negligible.

The physics of the local electronic state is better visualized by making a local gauge transformation $\eta_{ij} \rightarrow g_i \eta_{ij}, \quad U_{ij}^{SF} \rightarrow g_i U_{ij}^{SF} g_j$, and $(\tilde{h}_i^{SF})^t \rightarrow (g_i \tilde{h}_i^{SF})^t = e^{i\phi_i} \sqrt{c_i}, 0$, i.e., the local boson isospin vector points toward the north pole, as shown in Fig. 1(b). The explicit $g_i$ is given by $g_i = \exp[i(-1)^{\eta_i + \phi_i/2} \tau_1^{1}] \exp[i \phi_i/2]$. The advantage of this gauge is that the physical electron operator $c_\sigma \approx f_\sigma$. The new $U_{ij}$ has a physical meaning as governing the hopping and pairing of electrons. We shall refer to this as the $d$-wave gauge. Indeed, locally there is a single boson component and the problem reduces to the more familiar $U(1)$ mean-field theory, but with $\chi_{ij}$ and $\Delta_{ij}$ which vary in space. This is precisely the problem treated by Han and co-workers [11,12] and it is gratifying that they found numerically the staggered current around the vortex core, as proposed in Ref. [8].

Now we are ready to ask the question: Is any signature of the unit cell doubling directly measurable by STM tunneling? It turns out that there is no effect in the SF phase in the center of the core, because the period doubling of the current does not show up in the local density of states (LDOS). This leads us to look outside the immediate core and examine the effect of the phase winding, i.e., the effect of $\mathcal{V}_{ij}$. After a local gauge transformation to the $d$-wave gauge, we find that Eq. (1) becomes

$$\bar{U}_{ij}^d = \chi_{ij} \left( r^3 \cos \frac{\theta_i - \theta_j}{2} + r^2 \sin \frac{\theta_i - \theta_j}{2} \right)$$

$$- \Delta_{ij} \left[ i(-1)^{\eta_i + \phi_i/2} \cos \frac{\theta_i + \theta_j}{2} \right] - (-1)^{\eta_i + \phi_i/2} \tau_1 \sin \frac{\theta_i + \theta_j}{2} \right],$$

where

$$\chi_{ij} = A \cos \Phi_{ij}, \quad \Delta_{ij} = A \sin \Phi_{ij},$$

and

$$\Phi_{ij} = \Phi_0 + (-1)^{\eta_i + \phi_i/2} \mathcal{V}_{ij}.$$
As we approach the core from the outside, the $I_i$ vector in the SF gauge representation gradually rises from the equatorial plane [see Fig. 1(a)]. This gives rise to a crossover region characterized by the coexistence of the amplitude and phase modulations, where the $\theta$ dependence of $U_{ij}^d$ becomes significant. However, to study the effects of a $\theta$-dependent $U_{ij}^d$ is beyond the scope of this paper. From now on, we shall compute the LDOS by setting $\theta_i = \theta = \pi/2$. We expect our results to be qualitatively valid for $r \approx \ell$, as long as we avoid the exact core center.

The presence of staggered modulation of $\chi_{ij}$ and $\Delta_{ij}$ in this region suggests that this may be the best place to look for unit cell doubling effects. To model the tunneling current, we assume that the electrons tunnel from the tip, located at $r$, to a linear combination of Wannier orbitals centered at lattice sites $i$, i.e., \[ \sum_i \alpha_i(r)\phi(r_i - r). \]

Then the LDOS in the $d$-wave gauge is written as
\[
N(r, \omega) = -\frac{2\pi}{\pi} \text{Im} \sum_{i,j} \alpha_i(r)\alpha_j(r) [G_{ij}^d(i\omega)]_{11} \mid_{\omega=\omega+i\delta}.
\]

The subscript 11 means the 11 component of the lattice fermion propagator in a $2 \times 2$ matrix form, \[ G_{ij}^F(i\omega) = -\int_0^\beta d\tau e^{i\omega\tau} T\bar{\psi}_i(\tau)\psi_j(\tau). \]

Here we demonstrate that the LDOS exhibits a conspicuous staggered pattern only when measured on the bonds. For example, we pick up the sites 1, 2, . . . , 6 indicated in Fig. 2 and consider the midpoints on the bonds, $B_{1,2}$. The LDOS at $B_1$ and $B_2$ are almost equivalent, except for a small in-equivalence coming from the nonuniformity of the slowly-varying $\mathbf{V}(\mathbf{r})$ field. Similarly, $G_{12}^{F} \sim G_{56}^{F}$ since the bonds 12 and 56 are almost equivalent, except for a small in-equivalence coming from the nonuniformity of the slowly-varying $\mathbf{V}(\mathbf{r})$ field. Therefore, $N_{(C_1, \omega)} \sim N_{(C_2, \omega)}$. Similarly, the LDOS at the lattice sites is almost uniform. On the other hand, the LDOS at $B_1$ and $B_2$ comes from $\sum_{i,j=1,2} G_{ij}^{d}$, and \[ G_{12}^{d} \text{ and } G_{56}^{d} \text{ are clearly inequivalent because they connect bonds with alternating hopping-pairing amplitudes. Furthermore, it is seen that the staggered modulation of the LDOS becomes most conspicuous when scanned along the $a$ or $b$ axis [see the inset of Fig. 3(a)], because on these bonds the circulating $\mathbf{V}(\mathbf{r})$ field becomes parallel to the bond directions. From now on, we shall concentrate on the LDOS at the point $r = (0, i_y + 1/2)$ with lattice unit. To evaluate $G_{ij}^{d} (i\omega)$, we shall use the following two approaches which may be complementary to each other: (I) gradient expansion, and (II) uniform $\mathbf{V}$ approximation.

(I) Gradient expansion.—First, we expand Eq. (4) with respect to $\mathbf{V}(\mathbf{r})$ up to first order, which gives \[ \delta U_{ij} = U_{ij}^d + \delta U_{ij}^d \text{ with } \delta U_{ij} = \frac{(-1)^{i_y+1} \delta \mathbf{V}(\mathbf{r})}{\mathbf{V}(\mathbf{r})} \mathbf{V}(\mathbf{r}). \]

Second, we treat the effect of $\delta U_{ij}$ within the Born approximation. In this case, we can take into account the circulating configuration of the $\mathbf{V}(\mathbf{r})$ field.

The LDOS on the bonds is written as \[ N(\mathbf{r}, \omega/x\omega^2) = \tilde{N}_0(\omega) + \delta \tilde{N}(\mathbf{r}, \omega) \]. The uniform counterpart is given by \[ \tilde{N}_0(\omega) = \frac{-1}{\pi} \sum_k \cos k \text{ Im} \left[ G_k^{F}(k, i\omega) \right]_{11} \mid_{\omega=\omega+i\delta}, \]

where \[ G_k^{F}(k, i\omega) = U_k/(i\omega - E_k) + V_k/(i\omega + E_k), \]

\[ U_k = \frac{1}{2} \left[ 1 + \gamma \cos \theta + \eta \sin \theta \right]/E_k, \quad V_k = \frac{1}{2} \left[ 1 - \gamma \cos \theta + \eta \sin \theta \right]/E_k, \]

and $\gamma = -J\cos k_1 + i\theta\cos k_2 + i\theta\cos k_3$ and $\eta = J\cos k_1 - i\theta\cos k_2 - i\theta\cos k_3$. We took account of the second and third nearest neighbor hopping of the fermions $t_2 = -0.550$ and $t_3 = 0.087$ to reproduce the real band structure of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ as measured by angle-resolved photoemission spectroscopy [14].

The staggered counterpart is given by
\[
\delta \tilde{N}(\mathbf{r}, \omega) \sim \frac{(-1)^{i_y}}{4} \mathbf{V}(\mathbf{r}) \sum_{k \in \mathbf{R}} \sin^2 k_x \times \left[ L_k^\dagger \delta(\omega; E_k, E_k + q) + L_k^\dagger \delta(\omega; -E_k, -E_k + q) + N_k^+ \delta(\omega; E_k, -E_k + q) + N_k^- \delta(\omega; -E_k, E_k + q) \right],
\]

where \[ \mathbf{r} = (0, i_y + 1/2) \].

It is remarkable that, inside the overall V-shaped profile with the sharp peaks at $\tilde{\omega} = \omega/\mathbf{v}_f = \pm 0.323$ associated with the $d$-wave superconducting gap, there appears additional staggered structure around $\tilde{\omega} = \pm 0.179$ and $\tilde{\omega} = 0.226$. This structure comes from resonant scattering between the fermions with $k$ and $k + \mathbf{Q}$. As $\omega$ increases from zero, the energy contours $E_k = \omega$ and $E_k + q = \omega$ first touch on the reduced zone boundary at $\tilde{\omega} = \pm 0.179$, as indicated in Fig. 3(b), and resonance occurs. Then, at $\tilde{\omega} = \pm 0.226$, they touch again at $(\pi/2, \pi/2)$ and the second resonance occurs. The second resonance comes up.
FIG. 3. (a) LDOS profile at the points A, B, C, and D indicated in the inset. The LDOS at B and C are just \( \hat{N}_0(\omega) \). The energy contours \( E_k = \omega \) and \( E_{k+Q} = \omega \) touch at \( \omega = 0.179 \) and \( \omega = 0.226 \), as indicated in (b) and (c), respectively. The sharp peaks at \( \omega = \pm 0.323 \) are associated with the superconducting gap. The small wiggles outside the V-shaped profile come from numerical fluctuations. (d) Profile of \( \hat{N}_0(\omega) = \hat{N}_{\pm}(\omega) \) for \( \omega = 0.2 \). The energy contours of the split bands \( E_k^{\pm} \) along the path \( \Gamma(0,0) \rightarrow M(\pi/2, \pi/2) \rightarrow Y(0, \pi) \rightarrow \Gamma \). Fine band splittings on the reduced zone boundary are magnified in the inset. (e) Fine structure of \( \hat{N}_0(\omega) \) around \( \omega \approx 0.2 \), detected with higher numerical resolution.

only in the electron (\( \omega > 0 \)) side due to the matrix element effect [\( L_k^\dagger \) vanishes at \( (\pi/2, \pi/2) \)]. It is naturally expected that this resonant scattering may open a gap in the fermion excitation spectrum if we go beyond the perturbative scheme. This point can be confirmed through the exact treatment under the uniform \( \mathbf{V} \) approximation shown below.

(II) Uniform approximation.—Next we consider the case of uniform \( \mathbf{V} = (V_x, V_y) \) which may locally capture the effects of the circulating \( \mathbf{V}(r) \). In this case, we exactly diagonalize the fermion Hamiltonian. The LDOS on the bonds is written in a form \( N(\omega)/x \alpha^2 = \hat{N}_0(\omega) + \delta \hat{N}(\omega) \), where \( \pm \) signs alternate from bond to bond. As was inferred from the perturbative analysis, the unit cell doubling splits the one-particle spectrum into two branches [see Fig. 3(e)], \( \pm E_k^\pm \) and \( \pm E_k^\mp \).

In Fig. 3(d), we show the profile of \( \hat{N}_0(\omega) \) and \( \hat{N}_0(\omega) = \delta \hat{N}(\omega) \) for \( \mathbf{V} = (0.1, 0) \), the direction and strength of which correspond to \( \mathbf{V}(r) \) around the points B, D, and A, C in Fig. 3(a), respectively. We used the same parameter set as in the case of Fig. 3(a). We see that the staggered modulation profile, \( \hat{N}_0(\omega) + \delta \hat{N}(\omega) \), is in remarkable agreement with that obtained by the perturbative analysis. The structures correspond to van Hove singularities associated with the gap opening on the reduced zone boundary, as shown in Fig. 3(e). However, a striking difference is that the dip structure around \( \tilde{\omega} = 0.2 \) appears even in the uniform counterpart \( \tilde{N}_0(\omega) \). This suggests that in reality the dip structure may be detected not only on the bonds but also at sites. In Fig. 3(d), due to numerical resolution [\( 320 \times 320 \) mesh of the Brillouin zone] we resolve structures around \( \tilde{\omega} = \pm 0.2 \) and \( \tilde{\omega} = 0.26 \). As indicated in Fig. 3(e), there are fine band splittings on the reduced zone boundary leading to van Hove singularities at \( \tilde{\omega} = 0.186, 0.216, 0.229, \) and \( 0.265 \). The corresponding fine structure in \( \tilde{N}_0(\omega) \) could be detected with much higher numerical resolution [\( 720 \times 720 \) mesh of the Brillouin zone], as shown in Fig. 3(f).

We note that, in both approximations, the modulated structure in the LDOS is predominant on the particle side (\( \omega > 0 \)). We can understand this asymmetry by first turning off the superconductivity and considering the effect of unit cell doubling. Since we are doping with holes, the gaps being opened by the unit cell doubling are on the empty side of the Fermi surface. Matrix element effects preserve this particle-hole asymmetry even after we turn on the superconductivity.

Combining the results obtained through the gradient expansion and the uniform \( \mathbf{V} \) approximation, we may reasonably say that the signature of the unit cell doubling may be most prominently detected through the characteristic dip structure inside the V-shaped profile. The structure predicted here is very specific and its observation will be a strong confirmation of the SU(2) vortex model.

J. K. is supported by a Monbusho Grant for overseas research. P. A. L. and X. G. W. acknowledge support by NSF under the MRSEl Program DMR 98-08491. X. G. W. also acknowledges support by NSF Grant No. DMR 97-14198.

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