Quantum oscillations in $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$ from period-8 d -density wave order

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We consider quantum oscillation experiments in $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$ from the perspective of Fermi surface reconstruction using an exact transfer matrix method and the Pichard–Landauer formula for the conductivity. The specific density wave order responsible for reconstruction is a period-8 d -density wave in which the current density is unidirectionally modulated, which is also naturally accompanied by a period-4 charge order, consistent with recent nuclear magnetic resonance experiments. This scenario leads to a natural explanation as to why only oscillations from a single electron pocket of a frequency of about 500 T is observed, and a hole pocket of roughly twice the frequency as dictated by the twofold commensurate order and the Luttinger sum rule is not observed. In contrast period-8 d -density wave leads to a hole pocket of roughly half the frequency of the electron pocket. The observation of this slower frequency will require higher, but not unrealistic, magnetic fields than those commonly employed. There is already some suggestion of the slower frequency in a measurement in fields as high as 85 T.

superconductivity | magnetism | electron correlation

The problem of pseudogap in high-temperature superconductors is one of the most challenging problems in condensed matter physics; see ref. 1 and references therein. At present there are two views: (i) it is either a form of particle-hole condensate reflecting a density wave order, or (ii) it is a remnant of the fundamental superconducting order, a particle-particle condensate, that occurs at a lower temperature. In this manuscript we are adopting the view that it corresponds to a broken symmetry corresponding to the formation of a density wave.

The discovery of quantum oscillations (2) in the Hall coefficient (R_H) of hole-doped high-temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{6+\delta}$ (YBCO) in high magnetic fields approximately between 35 and 62 T was an important event that is likely to shed light on the origin of the pseudogap (3). Although the original measurements were performed in the underdoped regime, close to 10% hole doping, later measurements have also revealed clear oscillations for $\text{YBa}_2\text{Cu}_4\text{O}_8$ (Y248), which corresponds to about 14% doping (4, 5). Fermi surface reconstruction due to a density wave order that could arise if superconductivity is effectively destroyed by high magnetic fields has been a promising focus of attention (6–11). Similar quantum oscillations in the c -axis resistivity in $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ (NCCO) (12–14) have been easier to interpret in terms of a twofold commensurate density wave order, even quantitatively, including magnetic breakdown effects (15, 16).

At this time, in YBCO, there appears to be no general agreement about the precise nature of the translational symmetry breaking. A pioneering idea invoked an order corresponding to period-8 antiphase spin stripes (6). The emphasis there was to show how, over a reasonable range of parameters, the dominant Fermi pockets are electron pockets, thus explaining the observed negative Hall coefficient. At around the same time one of us suggested a twofold commensurate d -density wave (DDW) order that could also explain the observations (7). There are several reasons for such a choice. One of them is that the presence of both hole and electron pockets with differing scattering rates leads to a natural explanation (7) of oscillations of R_H . An incom-

mensurate period-8 DDW was also considered (8). Fermi surfaces resulting from this order are very similar to those due to spin stripes. The lack of Luttinger sum rule and a multitude of possible reconstructed Fermi surfaces appeared to have little constraining power in a Hartree–Fock mean-field theory. However, since then many experiments that indicate the importance of stripe physics (17), and even possible unidirectional charge order, have led us to reconsider the period-8 DDW.

Whereas commensurate models can explain measurements in NCCO, they appear to fail to explain the measurements in YBCO. Luttinger sum rule leads to a concomitant hole pocket with an oscillation frequency roughly about twice the frequency of the electron pocket (approximately 500 T). Despite a motivated search no such frequency has been detected. In contrast, for period-8 DDW the hole pockets can be quite small for a range of parameters. To convincingly detect such oscillation, it is necessary to perform experiments in much higher fields than is currently practiced, which may have bearing on the absence of the hole pocket. However, a tantalizing evidence of a frequency (270 ± 20 T) has been reported in a recent 85 T measurement (18) but its confirmation will require further experiments. Another consequence of our work is that, depending on disorder, one may even have a situation in which the slower frequency arising from the hole pocket can be more prominent than the faster frequency from the electron pocket.

A number of further considerations suggest that singlet DDW order is a good candidate. Tilted field measurements have revealed spin zeros in quantum oscillations, which are indicative of a symmetry breaking order parameter that is a spin singlet rather than a triplet (19, 20). Also, NMR experiments in high fields indicate that there is no spin order but a period-4 charge order that develops at low temperatures (21). This fact can be easily incorporated in our theory because in Landau theory period-8 DDW order of the wave vector $\mathbf{Q}$ can result in a period-4 $2\mathbf{Q}$ charge order. It is important to note that DDW order is very effectively hidden (22, 23). As long as the CuO-plane is square-planar, the currents induced by the DDW cannot induce net magnetic moment to couple to the nuclei in an NMR measurement. Any deviation from the square planar character could give rise to an NMR signal (24). To the extent these deviations are small the effects will also be small. First, we describe our model. Second, we outline the transfer matrix calculation of the conductivity. Third, we describe our results, most importantly the quantum oscillation spectra. The final section contains a discussion and an overall outlook.

Model

Band Structure. The parameterization of the single particle band structure for YBCO from angle-resolved photoemission spectroscopy (ARPES) is not entirely straightforward because cleaving

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at any nominal doping leads to an overdoped surface. Nonetheless an interesting attempt was made to reduce the doping by a potassium overlayer (25). Further complications arise from bilayer splitting and chain bands. Nonetheless, the inferred band structure appears to be similar to other cuprates where ARPES is a more controlled probe (26). Here we shall adopt a dispersion that has become common and has its origin in a local density approximation (LDA) based calculation (27), which is as follows:

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y). \quad [1]$$

The band parameters are chosen to be $t = 0.15$ eV, $t' = 0.32$ t, and $t'' = 0.5$ t' (27). The only difference with the conventional LDA band structure is a rough renormalization of t (from 0.38 eV to 0.15 eV), which is supported by many ARPES experiments that find that LDA overestimates the bandwidth. A more recent

ARPES measurement on thin films paints a somewhat more complex picture (28).

Incommensurate DDW Without Disorder. An Ansatz for period-8 incommensurate DDW (8) involves the wave vector $\mathbf{Q} = (\frac{\pi}{a}, \frac{\pi}{a}) - \frac{\pi}{a}(2\eta, 0) = \frac{\pi}{a}(\frac{3}{4}, 1)$ for $\eta = 1/8$. With the 8-component spinor defined by

$$\chi_{\mathbf{k}}^{\dagger} = (c_{\mathbf{k},\alpha}^{\dagger}, c_{\mathbf{k}+\mathbf{Q},\alpha}^{\dagger}, c_{\mathbf{k}+2\mathbf{Q},\alpha}^{\dagger}, \dots, c_{\mathbf{k}+7\mathbf{Q},\alpha}^{\dagger}). \quad [2]$$

The Hamiltonian without disorder can be written as

$$\mathcal{H} = \sum_{\mathbf{k},\alpha} \chi_{\mathbf{k}\alpha}^{\dagger} Z_{\mathbf{k},\alpha} \chi_{\mathbf{k}\alpha}. \quad [3]$$

The up and down spin sector eigenvalues merely duplicate each other, and we can simply consider one of them:

$$Z_{\mathbf{k}} = \begin{pmatrix} \epsilon_{\mathbf{k}} - \mu & iG_{\mathbf{k}} & V_c & 0 & 0 & 0 & 0 & 0 \\ \text{c.c} & \epsilon_{\mathbf{k}+\mathbf{Q}} - \mu & iG_{\mathbf{k}+\mathbf{Q}} & V_c & 0 & 0 & 0 & 0 \\ V_c & \text{c.c} & \epsilon_{\mathbf{k}+2\mathbf{Q}} - \mu & iG_{\mathbf{k}+2\mathbf{Q}} & 0 & 0 & 0 & 0 \\ 0 & V_c & \text{c.c} & \epsilon_{\mathbf{k}+3\mathbf{Q}} - \mu & iG_{\mathbf{k}+3\mathbf{Q}} & V_c & 0 & 0 \\ 0 & 0 & V_c & \text{c.c} & \epsilon_{\mathbf{k}+4\mathbf{Q}} - \mu & iG_{\mathbf{k}+4\mathbf{Q}} & V_c & 0 \\ 0 & 0 & 0 & V_c & \text{c.c} & \epsilon_{\mathbf{k}+5\mathbf{Q}} - \mu & iG_{\mathbf{k}+5\mathbf{Q}} & V_c \\ V_c & 0 & 0 & 0 & V_c & \text{c.c} & \epsilon_{\mathbf{k}+6\mathbf{Q}} - \mu & iG_{\mathbf{k}+6\mathbf{Q}} \\ iG_{\mathbf{k}+7\mathbf{Q}} & V_c & 0 & 0 & 0 & V_c & \text{c.c} & \epsilon_{\mathbf{k}+7\mathbf{Q}} - \mu \end{pmatrix}, \quad [4]$$

where $G_{\mathbf{k}} = (W_{\mathbf{k}} - W_{\mathbf{k}+\mathbf{Q}})/2$, and the DDW gap is $W_{\mathbf{k}} = \frac{W_0}{2}(\cos k_x - \cos k_y)$. On symmetry grounds, one can quite generally expect that an incommensurate DDW with wave vector $\mathbf{Q}$ will induce a charge density wave (CDW) of wave vector $2\mathbf{Q}$ (22). This fact is taken into account by explicitly incorporating a period-4 CDW by introducing the real matrix elements V_c . The chemical potential μ and the DDW gap amplitude W_0 can be adjusted to give the desired quantum oscillation frequency of the electron pocket as well as the doping level. The Fermi surfaces corresponding to the spectra of Eq. 3 (an example is shown in Fig. 1) are not essentially different from the theory of 1/8 magnetic anti-phase stripe order (6). This higher order commensuration generically produces complicated Fermi surfaces involving open orbits, hole pockets, and electron pockets.

To picture the current modulation and to define the order parameter of period-8 DDW in the real space Hamiltonian we need to calculate $\langle c_{\mathbf{R}}^{\dagger} c_{\mathbf{R}} \rangle$ for $\mathbf{R}' \neq \mathbf{R}$. We get, correcting here a mistake in ref. 8,

$$\begin{aligned} \langle c_{\mathbf{R}}^{\dagger} c_{\mathbf{R}} \rangle &= \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}'} \langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}'} \rangle \exp[-i(\mathbf{k}' \cdot \mathbf{R}' - \mathbf{k} \cdot \mathbf{R})] \\ &= \pm \frac{iW_0}{2} (-1)^{n'+m'} \tilde{V}_{\mathbf{R}',\mathbf{R}}, \end{aligned} \quad [5]$$

where $\mathbf{R}' = (m'a, n'a)$, and $\tilde{V}_{\mathbf{R}',\mathbf{R}}$ is

$$\begin{aligned} \tilde{V}_{\mathbf{R}',\mathbf{R}} &= \left[\frac{1 + \cos 2\pi\eta}{2} (\delta_{\mathbf{R}',\mathbf{R}+a\hat{x}} + \delta_{\mathbf{R}',\mathbf{R}-a\hat{x}}) \right. \\ &\quad \left. - (\delta_{\mathbf{R}',\mathbf{R}+a\hat{y}} + \delta_{\mathbf{R}',\mathbf{R}-a\hat{y}}) \right] \cos 2m'\pi\eta \\ &\quad + \frac{\sin 2\pi\eta \sin 2m'\pi\eta}{2} (\delta_{\mathbf{R}',\mathbf{R}+a\hat{x}} - \delta_{\mathbf{R}',\mathbf{R}-a\hat{x}}). \end{aligned} \quad [6]$$

The current pattern is then

$$J_{\mathbf{R}',\mathbf{R}} = i[\langle c_{\mathbf{R}'}^{\dagger} c_{\mathbf{R}} \rangle - \langle c_{\mathbf{R}}^{\dagger} c_{\mathbf{R}'} \rangle] = -W_0 (-1)^{n'+m'} \tilde{V}_{\mathbf{R}',\mathbf{R}}, \quad [7]$$

which is drawn in Fig. 2. The incommensurate d -density wave order parameter is proportional to

$$\tilde{W}_{\mathbf{R}',\mathbf{R}} = \frac{iW_0}{2} (-1)^{n'+m'} \tilde{V}_{\mathbf{R}',\mathbf{R}}. \quad [8]$$

Fig. 1. Reconstructed Fermi surfaces with $\mathbf{Q} = \frac{\pi}{a}(\frac{3}{4}, 1)$, $W_0 = 0.65$ t, $V_c = 0.05$ t, and $\mu = -0.83$ t. There are electron pockets, hole pockets, and open orbits. The electron pocket frequency corresponds to 530 T and the hole pockets to 280 T. The doping corresponds to 12.46%. Note that the figure is shown in the extended Brillouin zone for clarity.

Fig. 2. Current pattern for $Q = (\frac{3\pi}{4a}, \frac{\pi}{a})$. The relative magnitudes of the currents are depicted by the arrows in the legend. Note the antiphase domain wall structure.

The Real Space Hamiltonian Including Disorder. In real space, the Hamiltonian in the presence of both disorder and magnetic field is

$$H = \sum_{\mathbf{R}} [V(\mathbf{R}) + 2V_c \cos(\pi m/2)] c_{\mathbf{R}}^\dagger c_{\mathbf{R}} + \sum_{\mathbf{R}', \mathbf{R}} t_{\mathbf{R}', \mathbf{R}} e^{i a_{\mathbf{R}', \mathbf{R}}} c_{\mathbf{R}'}^\dagger c_{\mathbf{R}} + \sum_{\mathbf{R}', \mathbf{R}} \tilde{W}_{\mathbf{R}', \mathbf{R}} e^{i a_{\mathbf{R}', \mathbf{R}}} c_{\mathbf{R}'}^\dagger c_{\mathbf{R}} + h.c. \quad [9]$$

Here $t_{\mathbf{R}', \mathbf{R}}$ defines the band structure. The nearest neighbor, the next nearest neighbor, and the third nearest neighbor hopping terms: t , t' , t'' . And $2V_c \cos(\frac{\pi}{2}m)$ is responsible for the period-4 charge stripe order, where m is $\mathbf{R} \cdot \hat{x}/a$ and a is lattice spacing. We include correlated disorder in the form (29)

$$V(\mathbf{R}) = \frac{g_V}{2\pi l_D^2} \int d\mathbf{x} e^{-\frac{|\mathbf{R}-\mathbf{x}|^2}{2l_D^2}} u(\mathbf{x}), \quad [10]$$

where l_D is the disorder correlation length and the disorder averages are $\langle u(\mathbf{x}) \rangle = 0$ and $\langle u(\mathbf{x})u(\mathbf{y}) \rangle = \delta(\mathbf{x} - \mathbf{y})$; the disorder intensity is set by g_V .

Whereas white noise disorder seems to be more appropriate for NCCO with intrinsic disorder, correlated disorder may be more relevant to relatively cleaner YBCO samples in the range of well-ordered chain compositions. Thus, here we shall focus on correlated disorder. A constant perpendicular magnetic field B is included via the Peierls phase factor $a_{\mathbf{R}', \mathbf{R}} = \frac{e}{\hbar c} \int_{\mathbf{R}}^{\mathbf{R}'} \mathbf{A} \cdot d\mathbf{l}$, where $\mathbf{A} = (0, -Bx, 0)$ is the vector potential in the Landau gauge; the lattice vector $\mathbf{R}' = (m'a, n'a)$ is defined by an arbitrary set of integers.

Transfer Matrix. The transfer matrix technique is a powerful method to compute conductance oscillations. It requires neither quasiclassical approximation nor ad hoc broadening of the Landau level to incorporate the effect of disorder. Various models of disorder, both long- and short-ranged, can be studied ab initio. The mean-field Hamiltonian, being a quadratic noninteracting Hamiltonian, leads to a Schrödinger equation for the site amplitudes, which is then recast in the form of a transfer matrix; the derivation has been discussed in detail previously (15, 29). The conductance is then calculated by a formula that is well-known in the area of mesoscopic physics, the Pichard–Landauer formula (30, 31), which yields Shubnikov–de Haas oscillations of the ab -plane resistivity, ρ_{ab} .

We consider a quasi one-dimensional system, $N \gg M$, with a periodic boundary condition along y -direction. Here Na is the length in the x -direction and Ma is the length in the y -direction. Let $\Psi_n = (\psi_{n,1}, \psi_{n,2}, \dots, \psi_{n,M})^T$, $n = 1, \dots, N$, be the amplitudes on the slice n for an eigenstate with a given energy. Then the

amplitudes between the successive slices depending on the Hamiltonian must form a transfer matrix, $\mathbb{T}$.

The complete set of Lyapunov exponents, γ_i , of $\lim_{N \rightarrow \infty} (\mathcal{T}_N \mathcal{T}_N^\dagger)^{1/N}$, where $\mathcal{T}_N = \prod_{j=1}^N \mathbb{T}_j$ determine the conductance, $\sigma_{ab}(B)$ from the Pichard–Landauer formula:

$$\sigma_{ab}(B) = \frac{e^2}{h} \text{Tr} \sum_{j=1}^{2M} \frac{2}{(\mathcal{T}_N \mathcal{T}_N^\dagger) + (\mathcal{T}_N \mathcal{T}_N^\dagger)^{-1} + 2}. \quad [11]$$

In this work we have chosen $M = 30$ and N of the order of 10^5 , which guaranteed 4% accuracy of the smallest Lyapunov exponent. Note that at each step we have to invert a $4M \times 4M$ matrix and numerical errors prohibit much larger values of M .

Results

Specific Heat Without Disorder. The coefficient of the linear-specific heat is

$$\gamma = \frac{\pi^2}{3} k_B^2 \rho(0). \quad [12]$$

The density of states $\rho(\omega)$ measured with respect to the Fermi energy can be easily computed by taking into account all eight bands in the irreducible part of the full Brillouin zone and a factor of 2 for spin. A Lorentzian broadening of the δ -functions was used in computing the density of states. Although Lorentzian broadening is useful for numerical computation, the smoothing is a rough way of incorporating the effect of disorder on the density of states.

For a single CuO-layer we get,

$$\gamma \approx 5.4 \frac{\text{mJ}}{\text{mole} \cdot \text{K}^2}, \quad [13]$$

where we have used the density of states at the Fermi energy from numerical calculation to be approximately 2.3 states/eV, as shown in Fig. 3. Including both layers $\gamma = 2 \times 5.4 = 10.8 \frac{\text{mJ}}{\text{mole} \cdot \text{K}^2}$, approximately a factor of 2 larger than the observed $5 \frac{\text{mJ}}{\text{mole} \cdot \text{K}^2}$ at 45 T (32).

Charge Modulation Without Disorder. Before we carry out an explicit calculation it is useful to make a qualitative estimate. For $V_c = 0.05 t$, the total charge gap is to $4V_c = 0.2 t$. To convert to modulation of the charge-order parameter, we have to divide by a suitable coupling constant. In high-temperature superconductors, all important coupling constants are of the order bandwidth, which is $8 t = 1.2 \text{ eV}$. Therefore, as a rough estimate, we

Fig. 3. Total density of states, $t = 0.15$, including eight bands in the reduced Brillouin zone per layer. The horizontal axis is in terms of electron volts and the vertical axis is a pure number, that is, the number of states. The rounding at the tails is due to the Lorentzian broadening of the δ -functions by $\Gamma = 0.1 t$. The remaining parameters are the same as in Fig. 1. Further smoothing will reduce the density of states at the Fermi energy and lower the value of γ .

deduce that the charge modulation is $0.025 e$, expressed in terms of electronic charge.

To explicitly calculate charge modulation at a site, we diagonalize the 8×8 Hamiltonian matrix $Z(k_x, k_y)$ for each $\mathbf{k}$ in the reduced Brillouin zone (RBZ). We get eight eigenvalues and the corresponding eigenvectors: E_{n,k_x,k_y} and ψ_{n,k_x,k_y} for $n = 1, 2, \dots, 8$. The eigenvector ψ_{n,k_x,k_y} has eight components of the following form:

$$\psi_{n,k_x,k_y} = [\alpha_{n,k_x,k_y}(1), \alpha_{n,k_x,k_y}(2), \dots, \alpha_{n,k_x,k_y}(8)]. \quad [14]$$

Then the wave function in the real space for each state $\{n, k_x, k_y\}$ is

$$\psi_{n,k_x,k_y}(\mathbf{R}) = \sum_{j=1}^8 \alpha_{n,k_x,k_y}(j) \frac{1}{\sqrt{N}} \exp i[\mathbf{k} + (j-1)\mathbf{Q}] \cdot \mathbf{R}. \quad [15]$$

So, by definition, the local number density is

$$n(\mathbf{R}) = 2 \sum'_{n,k_x,k_y} |\psi_{n,k_x,k_y}(\mathbf{R})|^2. \quad [16]$$

Here the prime in the sum means that all occupied states with energy below the chemical potential are considered. The factor of 2 is for spin and the summation over k_x, k_y is performed in the RBZ. For different parameter sets the numerical results are, as follows:

- Parameter set 1
 $W_0 = 0.71 t$, $V_c = 0.05 t$, $\mu = -0.78 t$, $x = 11.73\%$
Averaged number density of electrons is $n = 0.882$ per site, whereas the estimated deviation is about $\delta n = 0.029$ per site. So $\delta n/n = 3.2\%$. The cyclotron effective masses calculated are 0.567 for the hole pocket and 1.98 for the electron pocket in units of the free electron mass.
- Parameter set 2
 $W_0 = 0.65 t$, $V_c = 0.05 t$, $\mu = -0.83 t$, $x = 12.46\%$
Averaged number density of electrons is $n = 0.877$ per site, whereas the estimated deviation is about $\delta n = 0.031$ per site. So $\delta n/n = 3.58\%$. The cyclotron effective masses calculated are 0.652 for the hole pocket and 2.04 for the electron pocket in units of the free electron mass.

Of course, for both cases, the period of the CDW modulation is $4a$, where a is the lattice spacing. It is also interesting to calculate the ratio of the modulation of the local density of states to the average density of states at the Fermi energy; we find $\delta\rho(\mu)/\rho(\mu) \approx 13\text{--}15\%$ depending on the parameters. As pointed out in ref. 11, the modulation of the density of states leads to an estimate of the corresponding variation of the Knight shift.

Oscillation Spectra in the Presence of Correlated Disorder. Previously it was found from the consideration of $1/8$ magnetic antiphase stripe order that there is a remarkable variety of possible Fermi surface reconstructions depending on the choice of parameters (6), which is also true for the incommensurate period-8 DDW. In contrast, twofold commensurate DDW order leads to much less variety. Whereas twofold commensuration is more satisfying, period-4 charge modulation observed in NMR measurements (21) and the nonexistence of the larger hole pocket commensurate with the Luttinger sum rule have forced us to seriously consider the period-8 DDW.

Although we cannot constrain the parameters uniquely, we have used a number of guiding principles. First, disorder was chosen to be correlated with a length scale ℓ_D smaller than the transverse width of the strip, Ma . Because the YBCO samples studied appear to have a lesser degree of disorder than the intrinsic dis-

order of NCCO, the white noise disorder did not appear sensible. Because the experimentally measured charge modulation in NMR is $0.03 \pm 0.01e$, it is necessary to keep V_c small enough to be consistent with experiments. A value of V_c in the neighborhood of $0.05 t$ seemed reasonable. Of course, the charge potential could be adjusted to agree precisely with experiments, but the resulting agreement would not have been very meaningful.

The band structure parameter t was chosen to be $0.15 eV$ as opposed to LDA value of $0.38 eV$. Although reliable ARPES measurements are not available for YBCO, measurements in other cuprates have indicated that the bandwidth is renormalized by at least a factor of 2. Had we chosen $t = 0.38 eV$, the agreement with specific heat measurements would have been essentially perfect, but we could not see any justification for adopting the bare band structure parameter. The parameters t'/t and t''/t' are the same as the commonly used LDA values, as the shape of the Fermi surface in most cases appear to be given correctly by LDA. We searched the remaining parameters, μ , g_V , and W_0 extensively. There are a number of issues worth noting. Oscillation spectra hardly ever show any substantial evidence of harmonics, which should be used as a constraining factor. Moreover, as we believe that it is the electron pocket that is dominant in producing negative R_H , it is necessary that we not employ parameters that wipe out the electron pocket altogether. The coexistence of electron and hole pockets give a simple explanation of the oscillations of R_H as a function of the magnetic field. We generically found hole pocket frequencies in the range $150\text{--}300 T$, which is one of our crucial observations. It implies that to resolve clearly such a slow frequency, one must go to much higher fields than are currently possible. We argue that the absence of observations at higher magnetic fields may be a plausible reason why the hole pocket has not been observed except for one experiment which goes up to $85 T$; in this experiment some evidence of a $250 T$ frequency is observed (18).

The DDW gap and the disorder level are consistent with the observed data. Overall we find satisfactory consistency with doping levels between $11\text{--}12.5\%$ within our calculational scheme. Lower doping levels produce less satisfactory agreement, but can be made better with further adjustment of parameters, but we have avoided fine-tuning as much as possible. The broad brush picture can already be seen in the oscillation spectra in Figs. 4–7. Two general trends are that electron pockets dominate at higher doping levels within the range we have checked, and an increase in disorder intensity reduces the intensity of the Fourier spectra of the electron pockets. A few harmonics are still present. Interestingly, depending on disorder one may have a situation in which the faster oscillations from the electron pocket can disappear leaving the slower frequency from the hole pocket intact; see, for example, Figs. 5 and 7.

Fig. 4. Fourier transform of the oscillation spectra after a background subtraction with a cubic polynomial. $W_0 = 0.71 t$, $V_c = 0.05 t$, $\mu = -0.78 t$, $M = 30 a$, $N = 10^5 a$, $\ell_D = 8 a$, $g_V = 0.1 t$. Doping is 11.73% .

Fig. 5. Fourier transform of the oscillation spectra after a background subtraction with a cubic polynomial. $W_0 = 0.71$ t, $V_c = 0.05$ t, $\mu = -0.78$ t, $M = 30$ a, $N = 10^5$ a, $\ell_D = 8$ a, $g_V = 0.3$ t. Doping is 11.73%.

Discussion

The complex material physics of high-temperature superconductors lead to a fairly large number of dimensionless parameters. Thus, it is not possible to frame a unique theory. Tuning these parameters can indeed lead to many different phases. However, there may be a general framework that could determine the overall picture. To be more specific, let us consider the quantum oscillation measurements that we have been discussing here.

- Are the applied magnetic fields sufficiently large to essentially destroy all traces of superconductivity and thereby reveal the underlying normal state from which superconductivity develops? Whereas for NCCO H_{c2} is less than 10 T and the quantum oscillation measurements are carried out between 30–65 T, far above H_{c2} , for YBCO lingering doubts remain. However, one may argue that the high-field measurements are such that one may be in a vortex liquid state where the slower vortex degrees of freedom may simply act as quenched disorder to the nimble electrons, which is the picture we have adopted here.
- The emergent picture of Fermi pockets are seemingly at odds with ARPES, unless only half the pocket is visible in ARPES, as was previously argued (33). On the other hand, reliable ARPES in YBCO is not available. For electron-doped NCCO the signatures of pockets are quite strong (34).
- Quantum oscillations of R_H are easier to explain if there are at least two closed pockets in the Boltzmann picture (7). Thus associated with the electron pocket there must be a hole pocket or vice versa. In NCCO, we have shown how magnetic breakdown (15), and a greater degree of intrinsic disorder, provides

Fig. 6. Fourier transform of the oscillation spectra after a background subtraction with a cubic polynomial. $W_0 = 0.65$ t, $V_c = 0.05$ t, $\mu = -0.83$ t, $M = 30$ a, $N = 10^5$ a, $\ell_D = 8$ a, $g_V = 0.1$ t. Doping is 12.46%.

Fig. 7. Fourier transform of the oscillation spectra after a background subtraction with a cubic polynomial. $W_0 = 0.65$ t, $V_c = 0.05$ t, $\mu = -0.83$ t, $M = 30$ a, $N = 10^5$ a, $\ell_D = 8$ a, $g_V = 0.2$ t. Doping is 12.46%.

a simple resolution as to why only one pocket, in this case a small but prominent hole pocket, is seen. In any case, oscillations of R_H in NCCO are yet to be measured. With respect to YBCO the apparent lack of two closed pockets becomes a serious problem. Any commensurate picture would lead to a hole pocket frequency about twice that of the electron pocket frequency if the Luttinger sum rule is to be satisfied. Despite a motivated effort, no evidence in this regard has emerged. An escape from the dilemma discussed here is that the relevant electron pocket is accompanied by a much smaller hole pocket and some open orbits. To convincingly observe such small hole pockets, one would require extending these measurements to higher fields; see ref. 18.

- All oscillation measurements to date have been convincingly interpreted in terms of the Lifshitz–Kosevich theory for which the validity of Fermi liquid theory and the associated Landau levels seem to be obligatory.
- The contrast between electron and hole-doped cuprates is interesting. In NCCO the crystal structure consists of a single CuO plane per unit cell, and, in contrast to YBCO, there are no complicating chains, bilayers, ortho-II potential, stripes, etc. (34). Thus, it would appear to be ideal for gleaning the mechanism of quantum oscillations. On the other hand, disorder in NCCO is significant. It is believed that well-ordered chain materials of YBCO contain much less disorder by comparison.
- In YBCO studies involving tilted field seem to rule out triplet order parameter, hence spin density wave (SDW) (19, 20). Moreover, from NMR measurements at high-fields, there appears to be no evidence of a static spin density wave order in YBCO (21). Similarly there is no evidence of SDW order in fields as high as 23.2 T in $\text{YBa}_2\text{Cu}_4\text{O}_8$ (35), whereas quantum oscillations are clearly observed in this material, although above 45 T (4, 5). Also no such evidence of SDW is found up to 44 T in $\text{Bi}_2\text{Sr}_{2-x}\text{La}_x\text{CuO}_{6+\delta}$ (36). Energetically a perturbation even as large as 45 T field is weak on the scale of relevant electronic energies (37).
- As to singlet order, relevant to quantum oscillations (38–40), CDW is a possibility which has recently found some support in the high-field NMR measurements in YBCO (21). But because the mechanism is helped by the oxygen chains, it is unlikely that the corresponding NMR measurements in NCCO will find such a charge order. Moreover, the observed charge order in YBCO sets in at a much lower temperature (20–50 K) compared to the pseudogap. Thus the charge order may be a secondary phenomenon because its scale is significantly different from the pseudogap scale, especially in the under doped regime. As to singlet DDW, there are two neutron scattering measurements that seem to provide evidence for it (41, 42).

However, these measurements have not been confirmed by further independent experiments. However, DDW order should be considerably hidden in NMR involving nuclei at high symmetry points because the orbital currents should cancel.

As mentioned above, a mysterious feature of quantum oscillations in YBCO is the fact that only one type of Fermi pockets is observed. If twofold commensurate density wave is the mechanism, the Luttinger sum rule (7, 43–45) will be violated. We had previously provided an explanation of this phenomenon in terms of disorder arising from both defects and vortex scattering in the vortex liquid phase (29); however, the arguments are not unassailable. In contrast, for NCCO, the experimental results are quite consistent with a simple theory presented previously (15, 16). The

present work, based on incommensurate DDW, may provide another, if not a more plausible alternative in YBCO.

The basic question as to why Fermi liquid concepts should apply remains an important unsolved mystery (46). It is possible that if the state revealed by applying a high magnetic field has a broken symmetry with an order parameter (hence a gap), the low energy excitations will be quasiparticle-like, not a spectra with a branch cut, as in variously proposed strange metal phases.

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