Quantum oscillations in electron doped high temperature superconductors

Jonghyoun Eun, Xun Jia, and Sudip Chakravarty
Department of Physics and Astronomy, University of California Los Angeles, Los Angeles, California 90095-1547, USA
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Quantum oscillations in hole doped high temperature superconductors are difficult to understand within the prevailing views. An emerging idea is that of a putative normal ground state, which appears to be a Fermi liquid with a reconstructed Fermi surface. The oscillations are due to formation of Landau levels. Recently the same oscillations were found in the electron doped cuprate, \( \text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4 \), in the optimal to overdoped regime. Although these electron doped non-stoichiometric materials are naturally more disordered, they strikingly complement the hole doped cuprates. Here we provide an explanation of these observations from the perspective of density waves using a powerful transfer matrix method to compute the conductance as a function of the magnetic field.

I. INTRODUCTION

Periodically new experiments tend to disturb the status quo of the prevailing views in the area of high temperature cuprate superconductors. Recent quantum oscillation (QO) experiments fall into this category. The first set of experiments were carried out in underdoped high quality crystals of well-ordered \( \text{YBa}_2\text{Cu}_3\text{O}_6 + \delta \) (YBCO), stoichiometric \( \text{YBa}_2\text{Cu}_3\text{O}_8 \) (Y124) and the overdoped single layer \( \text{Tl}_2\text{Ba}_2\text{CuO}_4 \). More recently oscillations are also observed in electron doped \( \text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4 \) (NCCO). The measurements in NCCO for 15\%, 16\%, and 17\% doping are spectacular. The salient features are: (1) The experiments are performed in the range 30 \(-\) 64T, far above the upper critical field, which is about 10T or less; (2) the material involves single CuO plane, and therefore complications involving chains, bilayers, Ortho-II potential, etc. are absent; (3) stripes may not be germane in this case. However, that neither spin density wave (SDW) nor \( d \)-density wave (DDW) are yet directly observed in NCCO in the relevant doping range, but QOs seem to require their existence, at least the wave (SDW) nor

II. MEAN FIELD HAMILTONIAN

We suggest that the experiments in NCCO can be understood from a suitable normal state because the applied magnetic fields between 30-65 T are so far above the upper critical field, which is less than 10 T, that vortex physics and the superconducting gap are not important. Our assumption is that a broken translational symmetry state with an ordering vector \( \mathbf{Q} = (\pi/\alpha, \pi/\alpha) \) (\( \alpha \) being the lattice spacing) can reconstruct the Fermi surface resulting in two hole pockets and one electron pocket within the reduced Brillouin zone, bonded by the constraints on the wave vectors \( k_x \pm k_y = \pm \pi/\alpha \). One challenge here is to understand why the large electron pockets corresponding to 15 and 16\% doping resulting from the band structure parameters for NCCO defined below are not observed, but the much smaller hole pockets are. Another challenge is to understand why the large Fermi surface at 17\% doping is not observed until the applied field reaches about 60

[...]

expressing the area of an extremal orbit, \( A \), as \( A = \pi k_F^2 \). By setting \( m^* \omega_F = h k_F \) the explicit dependence on the parameters \( m^* \) and \( \omega_F \) was eliminated. Assuming that the mean free paths for the hole and the electron pockets are more or less the same, not an unreasonable assumption, the larger pockets, with larger \( k_F \), will be strongly suppressed for the same value of the magnetic field because of the exponential sensitivity of \( D \) to the pocket size. This argument is consistent with our exact transfer matrix calculation using the Landauer formula for the conductance presented below.

Here we show that the oscillation experiments in NCCO reflect a broken translational symmetry\(^{15}\) that reconstructs the Fermi surface in terms of electron and hole pockets. The emphasis is not the transfer matrix method itself, but its use in explaining a major experiment in some detail. We study both SDW and singlet DDW orders with the corresponding mean field Hamiltonians. A more refined calculation, beyond the scope of the present paper, will be necessary to see the subtle distinction between the two order parameters.

In Sec. II we introduce our mean field Hamiltonians and in Sec. III we discuss the transfer matrix method for the computation of quantum oscillations of the conductance. Sec. IV contains the results of our numerical computations and Sec. V our conclusions.
T. The reason we believe is the existence strong cation disorder in this material. It is therefore essential to incorporate disorder in our Hamiltonian. For the Hamiltonian itself, we consider a mean field approach, and for this purpose we consider two possible symmetries, one that corresponds to a singlet in the spin space (DDW) and one that is a triplet in the spin space (SDW). Note that these are particle-hole condensates for which orbital function does not constrain the spin wave function unlike a particle-particle condensate (superconductors) because there are no exchange requirements between a particle and a hole.

We believe that it is reasonable that as long as a system is deep inside a broken symmetry state, mean field theory and its associated elementary excitations should correctly capture the physics. The fluctuation effects will be important close to quantum phase transitions. However, there are no indications in the present experiments that fluctuations are important. The microscopic basis for singlet DDW Hamiltonian is discussed in some detail in Refs. 19,20 and in references therein. So, we do not see any particular need to duplicate this discussion here. The mean field Hamiltonian for the singlet DDW in real space, in terms of the site-based fermion annihilation and creation operators of spin \( \sigma \), \( c_i,\sigma \) and \( c_i,\sigma^\dagger \), is

\[
H_{DDW} = \sum_{i,\sigma} \epsilon_i c_i,\sigma^\dagger c_i,\sigma + \sum_{i,j,\sigma} t_{i,j} e^{i\delta_{i,j}} c_i,\sigma^\dagger c_j,\sigma + h.c.,
\]

where the nearest neighbor hopping matrix elements are

\[
t_{i,i+\mathbf{x}} = -t + iW_0/4(-1)^{(i_x+i_y)},
\]

\[
t_{i,i+\mathbf{y}} = -t - iW_0/4(-1)^{(i_x+i_y)},
\]

Here \( W_0 \) is the DDW gap. We also include the next nearest neighbor hopping \( t' \), whereas the third neighbor hopping \( t'' \) is ignored to simplify computational complexity without losing the essential aspects of the problem. The parameters \( t \) and \( t' \) are chosen (see Table I) to closely approximate the more conventional band structure, as shown in Fig. 1. We have checked that the choice \( t'' = 0 \) provides reasonably consistent results for the frequencies in the absence of disorder. For example, for DDW, and 15% doping, the hole pocket frequency is 185 T, and the corresponding electron pocket frequency is 2394 T.

Similarly, the SDW mean field Hamiltonian is

\[
H_{SDW} = \sum_{i,\sigma} [\epsilon_i + \sigma V_S(-1)^{(i_x+i_y)}] c_i,\sigma^\dagger c_i,\sigma
\]

\[
+ \sum_{i,j,\sigma} t_{i,j} e^{i\delta_{i,j}} c_i,\sigma^\dagger c_j,\sigma + h.c.
\]

and the spin \( \sigma = \pm 1 \), while the magnitude of the SDW amplitude is \( V_S \). In both cases a constant perpendicular magnetic field \( B \) is included via the Peierls phase factor \( \delta_{i,j} = 2\pi a_1 \mathbf{A} \cdot d\mathbf{l} \), where \( \mathbf{A} = (0, -Bx, 0) \) is the vector potential in the Landau gauge. We note that usually a perpendicular magnetic field, even as large as 60T, has little effect on the

| Order | \( t \) (eV) | \( t' \) (eV) | \( V_S \) (T) | \( \mu \) (eV) | \( V_0 \) (T) | \( F \) (T) |
|-------|-------------|-------------|-------------|-------------|-------------|-----------|
| DDW 15% | 0.45t | 0.47t | * | -0.39t | 0.8t | 195 |
| DDW 16% | 0.45t | 0.47t | * | -0.365t | 0.8t | 165 |
| SDW 15% | 0.45t | 0.47t | * | -0.403t | 0.8t | 195 |
| SDW 16% | 0.45t | 0.47t | * | -0.366t | 0.8t | 173 |

FIG. 1: (Color online) The solid curve represents the \( t - t' - t'' \) band structure \( (t = 0.38\text{eV}, t' = 0.32t, t'' = 0.5t') \), and the dashed curve corresponds to \( t - t' \) band structure, (see Table I). The quasiparticle energy is plotted in the Brillouin zone along the triangle \( (0, 0) \rightarrow (\pi, 0) \rightarrow (\pi, \pi) \rightarrow (0, 0) \). In the inset the chemical potential, \( \mu \), was adjusted to obtain approximately 15% doping.

We have seen previously\(^{19}\) that the effect of long-ranged correlated disorder is qualitatively similar to white noise insofar as the QOs are concerned. The effect of the nature of disorder on the spectral function of angle resolved photoemission spectroscopy (ARPES) was found to be far more important. The reason is that the coherence factors of the ARPES spectral function are sensitive to the nature of the disorder because they play a role similar to Wannier functions. In contrast, the QOs are damped by the Dingle factor, which is parametrized by a single lifetime and disorder enters in an averaged sense.

Thus, it is sufficient to consider on-site disorder. The on-site energy is \( \delta \)-correlated white noise defined by the disorder average \( \bar{\epsilon}_i = 0 \) and \( \bar{\delta}_{i,j} = V_0^2 \delta_{i,j} \). For an explicit calculation we need to choose the band structure parameters, \( W_0, V_S \), and the disorder magnitude \( V_0 \). When considering the magnitude of disorder one should keep in mind that the full band width is \( 8t \). The magnetic field ranges roughly between \( 30T \) and
64T, representative of the experiments in NCCO. The magnetic length is \( l_B = \sqrt{\hbar/eB} \), which for \( B = 30T \) is approximately 12\( \alpha \), where the lattice constant \( \alpha \) is equal to 3.95\( \AA \).

The effect of potential scattering that modulates charge density is indirect on two-fold commensurate SDW or DDW order parameter\(^\text{22} \) mainly because SDW is modulation of spin and DDW that of charge current. Thus, the robustness of these order parameters with respect to disorder protects the corresponding quasiparticle excitations insofar as quantum oscillations are concerned, as seen below in our exact numerical calculations. Thus we did not find it important to study this problem self consistently.

### III. TRANSFER MATRIX METHOD

The transfer matrix method and the calculation of the Lyapunov sketched elsewhere\(^\text{23} \) is fully described here for the case of singlet DDW; for SDW the generalization is straightforward, where the diagonal term must be modified because of \( V_S \), and the term \( W_0 \) will be absent. Consider a quasi-1D system, \( L \gg M \), with a periodic boundary condition along y-direction. Let \( \Psi_n = (\psi_{n,1}, \psi_{n,2}, \ldots, \psi_{n,M})^T \) be the amplitudes on the slice \( n \) for an eigenstate with a given energy, then the amplitudes on three successive slices satisfy the relation

\[
\begin{bmatrix}
\Psi_{n+1} \\
\Psi_n
\end{bmatrix} = \begin{bmatrix} T_n^{-1} A_n & -T_n^{-1} B_n \\
1 & 0
\end{bmatrix} \begin{bmatrix}
\Psi_n \\
\Psi_{n-1}
\end{bmatrix}
\]

where \( T_n, A_n, B_n \) are \( M \times M \) matrices. The non-zero matrix elements of the matrix \( A_n \) are

\[
(A_n)_{m,m} = c_{n,m} - \mu, \\
(A_n)_{m,m+1} = -t + \frac{iW_0}{4} (-1)^{m+n}, \\
(A_n)_{m,m-1} = -t - \frac{iW_0}{4} (-1)^{m+n},
\]

where \( \phi = 2\pi Ba^2e/\hbar \) is a constant. For the matrix \( B_n \):

\[
(B_n)_{m,m} = -\left[t - \frac{iW_0}{4}(-1)^{m+n}\right], \\
(B_n)_{m,m+1} = -t e^{i(n+\phi)}, \\
(B_n)_{m,m-1} = -t e^{i(n-\phi)}.
\]

For the matrix \( T_n \), we note that \( T_n = D_n^{1/2} \).

The 2\( M \) Lyapunov exponents, \( \gamma_i \), of \( \lim_{N \to \infty} \left( T_N T_N^\dagger \right)^{1/2N} \), are defined by the corresponding eigenvalues \( \lambda_i = e^{\gamma_i} \). All Lyapunov exponents \( \gamma_1 > \gamma_2 > \ldots > \gamma_{2M} \) are computed by a procedure given in Ref.\(^\text{23} \). The modification here is that this matrix is not symplectic. Therefore all 2\( M \) eigenvalues have to be computed. The remarkable fact, however, is that except for a small fraction, consisting of larger eigenvalues, the rest do come in pairs \( (\lambda, 1/\lambda) \), as for the symplectic case, within numerical accuracy. We have no analytical proof of this curious fact. Clearly, larger eigenvalues contribute insignificantly to the more general formula for the conductance\(^\text{24} \).

\[
\sigma(B) = \frac{e^2}{h} \text{Tr} \sum_{j=1}^{2M} \left( T_N T_N^\dagger \right)^{-1} + 2.
\]

When the eigenvalues do come in pairs, the conductance formula simplifies to the more common Landauer formula\(^\text{25} \).

\[
\sigma_{xx}(B) = \frac{e^2}{h} \sum_{i=1}^{M} \frac{1}{\cosh^2(M \gamma_i)}.
\]

The transfer matrix method is a very powerful method and the results obtained are rigorous compared to ad hoc broadening of the Landau levels, which also require more adjustable parameters to explain the experiments. Once the distribution of disorder is specified there are no further approximations. We note that the values of \( M \) were chosen to be much larger than our previous work\(^\text{22} \) at least 128 (that is 128 \( a \) in physical units) and sometimes as large as 512. The length of the strip \( L \) is varied between \( 10^5 \) and \( 10^6 \). This easily led to an accuracy better than 5% for the smallest Lyapunov exponent, \( \gamma_1 \), in all cases.

We have calculated the \( ab \)-plane conductance, but the measured \( c \)-axis resistance, \( R_c \), is precisely related to it, at least as far as the oscillatory part is concerned. This can be seen from the arguments in Ref.\(^\text{24} \). Although the details can be improved, the crux of the argument is that the planar density of states enters \( R_c \): the quasiparticle scatters many times in the plane while performing cyclotron motion before hopping from plane to plane (measured \( ab \)-plane resistivity is of the order \( 10^{-4}\Omega\text{-cm} \) as compared \( \Omega\text{-cm} \) for the \( c \)-axis resistivity even at optimum doping\(^\text{10} \)). It is worth noting that oscillations of \( R_c \) also precisely follows the oscillations of the magnetization in overdoped \( Tl_2Ba_2CuO_{6+\delta} \).

### IV. RESULTS

There are clues in the experiments\(^\text{11} \) that disorder is very important. For 15 and 16% doping the slow oscillations in experiments, of frequency 290–280T, are not observed until the field reaches above 30T, which is much greater than \( H_{c2} < 10T \). For 17% doping the onset of fast oscillations at a frequency of 10, 700T are strikingly not observable until the field reaches 60T. The estimated scattering time from the Dingle factor at even optimal doping and at \( 4K \) is quite short.

For 17% doping corresponding to \( \mu = -0.322t \) and the band structure given in Table I a slight change in disorder from \( V_0 = 0.7t \) to \( V_0 = 0.8t \) makes the difference between a clear observation of a peak to simply noise within the field sweep between 60–62T, as shown in Fig.2 and Fig.3. Since in this case \( W_0 = V_S = 0 \), there is little else to blame for the disappearance of the oscillations for fields roughly below 60T. The results are essentially identical for small values of \( W_0 \), such as 0.025t.
FIG. 2: (Color online) The main plot shows the Fourier transform of the field sweep shown in the inset. The peak is at $10.695 T$. The inset is a smooth background subtracted Shubnikov-de Haas oscillations, as calculated from the Landauer formula for 17% doping as a function of $1/B$. The disorder parameter is $V_0 = 0.7t$. The band structure parameters are given in Table I.

FIG. 3: (Color online) The same parameters as in Fig. 2 but $V_0 = 0.8t$. The background subtracted conductance is simply noise to an excellent approximation.

For 15% and 16% dopings we chose $V_0$ to simulate the fact that oscillations seem to disappear below $30T$. The field sweep was between $30 - 60T$. The results for DDW order are shown in Fig. 4 and Fig. 5. The most remarkable feature of these figures is that disorder has completely wiped out the large electron pocket leaving the small hole pocket visible. To emphasize this point we also plot the results for 15% doping but with much smaller disorder $V_0 = 0.2t$; see Fig. 6. Now we can see the fragmented remnants of the electron pocket. With further lowering of disorder, the full electron pocket becomes visible. It is clear that disorder has a significantly stronger effect on the electron pockets than on the hole pockets. This, as we noted earlier, is largely due to higher density of states around the antinodal points, which significantly accentuates the effect of disorder. We have done parallel calculations with SDW order as well. The results are essentially identi-
FIG. 8: (Color online) The same plot as in Fig. 7 except for 16% doping but using SDW order. The main peak is at 1957T. The rest of the parameters are given in Table II.

FIG. 7: (Color online) The same plot as in Fig. 4 for 15% doping and using SDW order. The main peak is at 173T. The rest of the parameters are given in Table II.

V. CONCLUSIONS

In the absence of disorder or thermal broadening, the oscillation waveforms are never sinusoidal in two dimensions and contain many Fourier harmonics. At zero temperature moderate disorder converts the oscillations to sinusoidal waveform with rapidly decreasing amplitudes of the harmonics. Further increase of disorder ultimately destroys the amplitudes altogether. Many experiments exhibit roughly sinusoidal waveform at even ultra low temperatures, implying that disorder is important. The remarkably small electronic dispersion in the direction perpendicular to the CuO-planes cannot alone account for the waveform.

For NCCO it is no longer a mystery as to why the frequency corresponding to the larger electron pocket is not observed. As we have shown, disorder is the culprit. Neither is the comparison with ARPES controversial as in the case of YBCO, since there is good evidence of Fermi surface crossing in the direction (π, 0) → (π, π), which is a signature of the electron pocket. The crossing along (π, π) → (0, 0) can be easily construed as an evidence of a small hole pocket for which half of it is made invisible both from the coherence factors and disorder effects. For electron doped materials, such as NCCO and PCCO, it is known that the Hall coefficient changes sign around 17% doping and therefore the picture of reconnection of the Fermi pockets is entirely plausible, with some likely magnetic breakdown effects. The real question is what is the evidence of SDW or DDW in the relevant doping range between 15% and 17%. From neutron measurements we know that there is no long range SDW order for doping above 13.4%. We cannot rule out field induced SDW at about 30T. For DDW, there are no corresponding neutron measurements to observe its existence. Given that DDW is considerably more hidden from common experiments, it is more challenging to establish it directly. NMR experiments in high fields for suitable nuclei can shed light on this question. The unavoidable logical conclusion from the QO measurements is that a density wave that breaks translational symmetry must be present. We suggest that motivated future experiments will be necessary to reach a definitive conclusion. Finally, at the level of mean field theory we have been unable to decide between SDW and singlet DDW. At the moment the best recourse is to experimentally look for spin zeros in the amplitude of quantum oscillations in a tilted magnetic field. A theoretical discussion of this phenomenon that can potentially shed light between a triplet order parameter (SDW) and a singlet order parameter, the singlet DDW discussed here, was provided recently. So far experiments are in conflict with each other in YBCO: one group suggests a triplet order parameter and the other a singlet order parameter.

It is unquestionable that the QO experiments are likely to change the widespread views in the field of high tempera-
nature superconductivity. Although the measurements in YBCO are not fully explained, the measurements in NCCO appear to have a clear and simple explanation, as shown here. However, given the similarity of the phenomenon in both hole and electron doped cuprates, it is likely that the quantum oscillations have the same origin.

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