Quantum oscillations in a biaxial pair density wave state

M. R. Norman*1, and J. C. Séamus Davis$2$–$4$–$1$

*Physical Sciences and Engineering Directorate, Argonne National Laboratory, Argonne, IL 60439; $2$Laboratory of Atomic and Solid State Physics, Department of Physics, Cornell University, Ithaca, NY 14853; and $4$Condensed Matter Physics Department, Brookhaven National Laboratory, Upton, NY 11973

Contributed by J. C. Séamus Davis, April 3, 2018 (sent for review February 20, 2018; reviewed by Allan H. MacDonald and Suchitra E. Sebastian)

The discovery of charge density wave correlations in cuprates by neutron and X-ray scattering, scanning tunneling microscopy (STM), and NMR has had a profound influence on the field of high-temperature superconductivity, but a number of observations indicate that the cuprate pseudogap phase involves more than just charge ordering (1). The pseudogap itself is characterized by a large suppression of spectral weight existing over a wide energy range around the Fermi energy (2–4), which seems incompatible with the weak short-range charge order observed by X-ray scattering. Given that the pseudogap is largest in the same region of momentum space that the d-wave superconducting gap is largest has led to numerous speculations that it is connected with pairing. Evidence for pairing correlations in the pseudogap phase has been suggested from a number of experiments, such as from the temperature dependence of the susceptibility [which has been interpreted as offering evidence for diamagnetism (5)], but alternate explanations for such data also exist. This is complicated by other experimental evidence indicating the presence of time-reversal symmetry breaking (6).

In an attempt to make sense of various conflicting interpretations of the pseudogap phase, it was speculated that a pair density wave (PDW) state, evident in numerical studies of the $t–J$ and Hubbard models (7, 8), could be the primary phase (with the charge modulations as a secondary effect) and also gives a natural explanation for the momentum dependence of angle-resolved photoemission data (9). More direct evidence has emerged from STM using a superconducting tip, where it was shown that the pairing order parameter was indeed modulated in space (10). This has been further bolstered by recent scanning tunneling data in a magnetic field (11). There, direct evidence was found for biaxial order in a halo surrounding the vortex cores at a wave vector that was one-half that of the charge density wave correlations, exactly as expected based on PDW phenomenology (12). This last observation leads to an obvious conjecture. One can estimate the field at which these vortex halos overlap (13), and this field is the same at which a long-range ordered charge density wave state has been seen by NMR and X-ray scattering (14). Interestingly, this is virtually the same field at which quantum oscillations also become evident (15). This implies that the small electron pockets inferred from these data are due to the state contained in these vortex halos.

The most successful model for describing quantum oscillation data is that of Harrison and Sebastien (16). By assuming a biaxial charge density wave state, they are able to form nodal pockets by folding of the Fermi arcs observed by photoemission to obtain an electron diamond-shaped pocket centered on the $Γ$-point side of the Fermi arc observed by angle-resolved photoemission (17). In their scenario, as this pocket grows, eventually a Lifshitz transition occurs, leading to a hole pocket centered around the $Γ$ point itself. A central question is whether an alternate model could have a similar phenomenology.

To explore this issue, we consider a biaxial PDW state with a wave vector of magnitude $Q = π/A_0$ as observed in the recent STM data (11). The secular matrix for such a state is of the form

\[
\begin{pmatrix}
\epsilon_{\vec{k}} & \Delta_{\vec{k}+\vec{Q}/2} & \Delta_{\vec{k}-\vec{Q}/2} & \Delta_{\vec{k}+\vec{Q}/2} & \Delta_{\vec{k}-\vec{Q}/2} \\
\Delta_{\vec{k}+\vec{Q}/2} & -\epsilon_{\vec{k}+\vec{Q}/2} & 0 & 0 & 0 \\
\Delta_{\vec{k}-\vec{Q}/2} & 0 & -\epsilon_{\vec{k}-\vec{Q}/2} & 0 & 0 \\
\Delta_{\vec{k}+\vec{Q}/2} & 0 & 0 & -\epsilon_{\vec{k}+\vec{Q}/2} & 0 \\
\Delta_{\vec{k}-\vec{Q}/2} & 0 & 0 & 0 & -\epsilon_{\vec{k}-\vec{Q}/2}
\end{pmatrix}.
\]

Here, we assume a $d$-wave form for the PDW order parameter, $\Delta_{\vec{q}} = \frac{\Delta_0}{\bar{Q}} (\cos q_x a - \cos q_y a)$, with its argument, $\bar{q} = \vec{k} + \frac{\bar{Q}}{2}$.

Significance

At higher temperatures, and in high magnetic fields at low temperatures, an extraordinary and unidentified electronic phase, dubbed the “pseudogap,” appears in lightly holodoped cuprates. At high fields and low temperatures, the pseudogap phase supports quantum oscillations that have resisted quantitative theoretical explanation since their discovery, and it also exhibits an unidentified density wave state. Although the latter has typically been referred to as a “charge” density wave because of the observed charge density modulations, theory indicates that it could actually be an electron-pair density wave (PDW) state. Here we demonstrate theoretically that a biaxial PDW state with $8a$ periodicity may provide a compelling quantitative explanation for much of the observed quantum oscillation data.
being the Fourier transform of the relative coordinate of the pair (the center of mass Fourier transform being \( \vec{Q} \)). We also ignore all of the other off-diagonal components, which arise from the secondary charge order, as they lead only to quantitative corrections to the results presented here. For \( \epsilon_F \) we assumed the tight-binding dispersion of He et al. (18) for Bi2201. We do this for two reasons. First, this was the dispersion considered in previous work on PDWs (9). Second, there are no complications in this dispersion associated with bilayer splitting.

A few remarks are in order here. First, the above truncated matrix considers only leading-order terms that connect the electron state \( \vec{k} \) to the hole states determined by the four biaxial PDW wave vectors. The leading terms ignored in this approximation would be those that connect these hole states to other electron states besides \( \vec{k} \). By examining these other states, we find that they should lead only to quantitative corrections, just like the neglected charge density wave (CDW) terms mentioned above (the full secular matrix for the commensurate wave vector \( Q = \pi/a \) would be of dimension 128). Second, the difference between this matrix and its CDW variant would simply involve taking away the negative signs along the diagonal (i.e., replace the four hole states by particle states instead). Of course, this difference has a profound impact on the results, as we discuss below.

To proceed, we need to define the spectral function, \( A \), as measured by angle-resolved photoemission:

\[
A(\omega, \vec{k}) = \frac{1}{\pi} \frac{c_i(\vec{k})^2}{(\omega - E_i(\vec{k}))^2 + \Gamma^2}.
\]

Here, \( E_i \) is the \( i \)th eigenvalue of the secular matrix, \( c_i \) the \( \vec{k} \) component of the corresponding eigenvector (the analogue of the particle-like Bogoliubov component), and \( \Gamma \) a phenomenological broadening parameter.

In Fig. 1, we show the spectral weight and eigenvalue contours at \( \omega = 0 \) for four values of \( \Delta_0 \) (the maximum energy gap of the PDW state). Deep in the pseudogap phase (large \( \Delta_0 \)), a small pocket centered along the diagonal \((0, 0) - (\pi, \pi)\) is observed whose flat edge follows the spectral weight. As such, this pocket should dominate the deHaas-vanAlphen (dHvA) amplitude, unlike the other pockets which exhibit little or no spectral weight.\(^4\) Note that the spectral weight, although small on the back side of this pocket \([c_i(\vec{k})^2] = 0.0032\) along the zone diagonal for Fig. 1C, is still nonzero along its entire contour. Moreover, despite the strong particle–hole mixing, this pocket is an electron-like pocket (its area increases as the chemical potential increases). This oval-shaped pocket is quite different from the electron pocket predicted in the CDW model, which is diamond-like in shape. As the hole doping increases (smaller \( \Delta_0 \)), this pocket undergoes a Lifshitz transition, resulting in a larger hole-like pocket also centered along the diagonal that resembles that obtained in the phenomenological Yang-Rice-Zhang (YRZ) model for the cuprates (22, 23). Although the CDW model also has a Lifshitz transition, the resulting hole pocket is quite different (a diamond-shaped pocket centered instead at the \( \Gamma \) point of the zone). Once the PDW gap collapses, then we recover the much larger hole pocket centered at \((\pi/a, \pi/a)\) that is characteristic of the overdoped state (24). We remark that the biaxial nature of the PDW order is critical in forming these smaller pockets, although hints of them can be found in earlier work that assumed a uniaxial PDW instead (25–28) (the last two of these papers addressing the dHvA data).

We quantify this by plotting the area of the pocket (in the dHvA units of tesla) along with the cyclotron mass as a function of the normal-state dispersion is given by He et al. (18). Here, the modulus of the PDW ordering vector, \( Q \), is \( \pi/a \), as observed in recent STM experiments (11). For the spectral weight, a phenomenological broadening parameter, \( \Gamma \), of 25 meV is assumed. Note the reduction of antinodal spectral weight as \( \Delta_0 \) increases, which is completely suppressed at \( \Delta_0 = 200 \) meV.

\(^1\)It could be questioned whether these semiclassical orbits exist, since one side of the contour is particle-like and the other hole-like (19). The part of the thermodynamic potential from which the oscillations arise, though, involves only the particle-like content of the states (20). Therefore, as long as \( c_i(\vec{k}) \) is nonzero along the entire contour, we argue that Landau levels associated with this contour exist. For the same reason, all other contours can be ignored when considering quantum oscillations (except for possible breakdown orbits) since their amplitudes will be suppressed due to their small \( c_i(\vec{k}) \). A similar argument applies to the overall magnitude of the specific heat. A proper treatment would require a full quantum mechanical solution of the secular matrix in the presence of a magnetic field. For a vortex lattice in a type-II superconductor (where the wave vector of its Brillouin zone plays the same role as the PDW \( Q \)), the magnetization oscillations from such a calculation are closely related to those of the lowest-lying quasiparticle band, at least for the fundamental harmonic (21).
of $\Delta_0$ in Fig. 2. We see a modest dependence of the pocket area on $\Delta_0$ except for the pronounced jump at the Lifshitz transition, along with the associated mass divergence at the Lifshitz transition. These dependencies are in good accord with the measured dHvA data as a function of hole doping (29), including the mass divergence, noting that quantitative details are influenced by the dispersion and chemical potential (that is, the conversion of the $x$ axis of Fig. 2 to doping is influenced not only by the doping dependence of $\Delta_0$, but also by the doping dependence of the band structure and chemical potential). Moreover, the results presented here offer a prediction. That is, beyond the mass divergence (as $\Delta_0$ decreases), there should be a small doping range where a large hole pocket of roughly twice the size of the electron pocket occurs before the very large hole pocket in the overdoped regime forms when the gap collapses. This prediction is consistent with Hall effect data that show a region of the phase diagram between $p = 0.16$ and $p = 0.19$ where the Hall constant rapidly changes (30), with $p = 0.16$ being where the mass divergence referred to above occurs and $p = 0.19$ where the large Fermi surface is recovered (here, $p$ is the doping).

We feel that the biaxial PDW scenario offered here is an attractive alternate to models based on a CDW. It is not only consistent with recent STS data in the vortex halos (11), but also consistent with magneto-transport data that indicate the presence of pairing correlations for magnetic fields not only up to but well beyond the resistive $H_{c2}$. This is in line as well with previous theoretical work on quantum oscillations in a d-wave vortex liquid (31). Certainly, we hope that the model offered here will lead to additional studies of high magnetic fields to definitively determine whether a PDW state really exists and, if so, what its characteristics and consequences are.

In summary, the work presented here bolsters the case that the enigmatic pseudogap phase in the cuprates is a PDW state.

ACKNOWLEDGMENTS. We thank Stephen Edkins, Mohammad Hamidian, and Andrew Mackenzie for access to their vortex halo STM data in advance of publication. We also acknowledge Neil Harrison, Peter Johnson, Marc-Henri Julien, Catherine Kallin, Steve Kivelson, Patrick Lee, Brad Ramshaw, Subir Sachdev, Suchitra Sebastian, Todadri Senthil, Louis Taillefer, and Zhiqiang Wang for discussions. This work was supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, under Award DE-AC0298CH1088.

1. Fradkin E, Kivelson SA, Tranquada JM (2015) Theory of intertwined orders in high temperature superconductors. Rev Mod Phys 87:457–482.
2. Timusk T, Statt B (1999) The pseudogap in high-temperature superconductors: An experimental survey. Rep Prog Phys 62:61–122.
3. Norman MR, Pines D, Kallin C (2005) The pseudogap: Friend or foe of high Tc? Adv Phys 54:715–733.
4. Lee PA, Nagaosa N, Wen X-G (2000) Doping a Mott insulator: Physics of high-temperature superconductivity. Rev Mod Phys 78:17–85.
5. Li L, et al. (2010) Diamagnetism and Cooper pairing above $T_c$ in cuprates. Phys Rev B 81:054510.
6. Fauque B, et al. (2006) Magnetic order in the pseudogap phase of high-Tc superconductors. Phys Rev Lett 96:197001.
7. Corboz P, White SR, Vidal G, Troyer M (2011) Stripes in the two-dimensional t-J model with infinite projected entangled pair states. Phys Rev B 84:041108.
8. Zheng B-X, et al. (2017) Stripe order in the underdoped region of the two-dimensional Hubbard model. Science 358:1155–1160.
9. Lee PA (2014) Aepplian pairing and the pseudogap phase of cuprate superconductors. Phys Rev X 4:031017.
10. Hamidian MH, et al. (2016) Detection of a Cooper-pair density wave in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$. Nature 532:343–347.
11. Edkins SD, et al. (2018) Magnetic-field induced pair density wave state in the cuprate vortex halo. arXiv:1802.04673.
12. Agterberg DF, Garaud J (2009) Striped superconductors: How spin, charge and superconducting orders intertwine in the cuprates. New J Phys 11:115005.
13. Wu T, et al. (2013) Emergence of charge order from the vortex state of a high-temperature superconductor. Nat Commun 4:2113.
14. Gerber S, et al. (2015) Three-dimensional charge density wave order in YBa$_2$Cu$_3$O$_{6.7}$ at high magnetic fields. Science 350:949–952.
15. Maharaj AV, Zhang Y, Ramshaw BJ, Kivelson SA (2016) Quantum oscillations in a bilayer with broken mirror symmetry: A minimal model for YBa$_2$Cu$_3$O$_{6.5}$. Phys Rev B 93:094503.
16. Harrison N, Sebastian SE (2011) Protected nodal electron pocket from multiple-Q ordering in underdoped high temperature superconductors. Phys Rev Lett 106:226402.
17. Norman MR, et al. (1998) Destruction of the Fermi surface in underdoped high-Tc superconductors. Nature 392:157–160.
18. He R-H, et al. (2011) From a single-band metal to a high-temperature superconductor via two thermal phase transitions. Science 331:1579–1583.
19. Dai Z, Zhang Y-H, Senthil T, Lee P (2018) Pair density wave, charge density wave and vortex in high Tc cuprates. arXiv:1802.03009.
20. Miller P, Gyorffy BL (1995) Theoretical investigations of the vortex lattice and de Haas-van Alphen oscillations in the superconducting state. J Phys Condens Matter 7:5579–5606.
21. Norman MR, MacDonald AH (1996) Absence of persistent magnetic oscillations in type-II superconductors. Phys Rev B 54:4239–4245.
22. Yang X-Y, Rice TM, Zhang F-C (2006) Phenomenological theory of the pseudogap state. Phys Rev B 73:174501.
23. Yang H-B, et al. (2011) Reconstructed Fermi surface of underdoped Bi$_2$Sr$_2$CaCu$_2$O$_{6+\delta}$ cuprate superconductors. Phys Rev Lett 107:047003.
24. Vignolle B, et al. (2008) Quantum oscillations in an overdoped high-Tc superconductor. Nature 455:952–955.
25. Berg E, Fradkin E, Kivelson SA, Tranquada JM (2009) Striped superconductors: How spin, charge and superconducting orders intertwine in the cuprates. New J Phys 11:115006.
26. Loder F, Kampf AP, Kopp T (2010) Superconducting state with a finite-momentum pairing mechanism in zero external magnetic field. Phys Rev B 81:020511.
27. Zell M, Kallin C, Berlinsky AJ (2011) Mixed state of a $\sigma$-striped superconductor. Phys Rev B 84:174525.
28. Zell M, Kallin C, Berlinsky AJ (2012) Quantum oscillations in a $\sigma$-striped superconductor. Phys Rev B 86:104507.
29. Ramshaw BJ, et al. (2015) Quasiparticle mass enhancement approaching optimal doping in a high-T_c superconductor. Science 348:317–320.
30. Badoux S, et al. (2016) Change of carrier density at the pseudogap critical point of a cuprate superconductor. Nature 531:210–214.
31. Banerjee S, Zhang S, Randeraa M (2013) Theory of quantum oscillations in the vortex-liquid state of high-Tc superconductors. Nat Commun 4:1700.