Quantum Oscillations from Nodal Bilayer Magnetic Breakdown in the Underdoped High Temperature Superconductor YBa\(_2\)Cu\(_3\)O\(_{6+x}\)

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Quantum oscillations from nodal bilayer magnetic breakdown in the underdoped high temperature superconductor YBa$_2$Cu$_3$O$_{6+x}$

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We report quantum oscillations in underdoped YBa$_2$Cu$_3$O$_{6.56}$ in magnetic fields over a significantly large range in magnetic field extending from $\approx 24$ to $94$ T, enabling three well-separated low frequencies at $\approx 440$ T, $532$ T, and $620$ T to be clearly resolved. We show that a small nodal bilayer coupling that splits a nodal pocket into bonding and antibonding orbits yields a sequence of frequencies, $F_0 - \Delta F$, $F_0$ and $F_0 + \Delta F$ and accompanying beat pattern similar to that observed experimentally on invoking magnetic breakdown tunneling at the nodes. The relative amplitudes of the multiple frequencies observed experimentally in quantum oscillation measurements are shown to be reproduced using a value of nodal bilayer gap quantitatively consistent with that measured in photoemission experiments in the underdoped regime.

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Discerning the electronic structure of underdoped YBa$_2$Cu$_3$O$_{6+x}$ in the normal state is a crucial step to understanding the origin of unconventional superconductivity in these materials [1]. While quantum oscillation measurements in underdoped YBa$_2$Cu$_3$O$_{6+x}$ have revealed multiple frequency components [2–4], it has been challenging to distinguish an electronic structure from the numerous possibilities that can uniquely explain the observed frequencies. Recent measurements of the chemical potential oscillations [5] in underdoped YBa$_2$Cu$_3$O$_{6+x}$ in strong magnetic fields have helped narrow down these possibilities by determining the multiple frequencies to arise from a single carrier pocket — likely located at the nodal region of the Brillouin zone [6] and supported by other experiments sensitive to the density-of-states at the Fermi energy [7–9]. An intriguing question therefore arises as to how such a single pocket can give rise to the multiple observed frequencies.

In this paper, we show measurements of quantum oscillations in YBa$_2$Cu$_3$O$_{6+x}$ made using a contactless resistivity technique over an unprecedented range in magnetic field extending from $\approx 24$ T to $94$ T (see Fig. 1) [10]. The large window in inverse magnetic field ($\Delta_B^{-1} \approx 0.030$ T$^{-1}$) affords clear resolution of three well-separated low frequencies, namely $\approx 440 \pm 10$ T, $532 \pm 2$ T and $620 \pm 10$ T — the experimental limit for distinguishing closely-spaced frequencies being $1/\Delta_B^{-1} \approx 32$ T. We use the unique form of the multiple frequency quantum oscillation spectrum, in which the central frequency at $532$ T is equidistantly flanked by two frequencies $532 - 90$ T and $532 + 90$ T, as a clue to infer a possible electronic structure that describes the system. We show that an electronic structure comprising a single bilayer-split nodal pocket combined with magnetic breakdown tunneling would give rise to such a frequency spectrum, and potentially provides an explanation for the angular dependence of the observed frequencies [4, 11, 12]. Similar instances of multiple frequencies arising from magnetic breakdown, are for instance found in heavy fermion and ferromagnetic families of materials [13, 14]. A prerequisite for such an explanation in underdoped YBa$_2$Cu$_3$O$_{6+x}$ is that a reduced bilayer splitting at the nodes [15] persists deep into the underdoped regime where the chains are partially occupied and a form of order [1, 6] likely reconstructs the Fermi surface.

The unit cell in YBa$_2$Cu$_3$O$_{6+x}$ contains a pair of CuO$_2$ layers, known as a bilayer (shown Fig. 2a). Coupling within a bilayer (denoted as $t_{\perp}$) splits bonding and antibonding bands by a finite gap [16]. The general expectation, therefore, is for bilayer splitting to transform a single frequency $F_0$ of a single layer Fermi surface into two separate frequencies describing a bilayer Fermi surface, where the difference between them is proportional to the orbitally-averaged strength of the coupling $t_{\perp}$ in the relevant region of the Brillouin zone.

The presence of three related low frequencies in the experimental data (Fig. 1) comprising two smaller-amplitude side frequencies equidistantly spaced from a central dominant-amplitude frequency seems difficult to reconcile with the simple expectation of two dominant-amplitude frequencies from bilayer splitting. An alternative explanation must be sought if the experimentally observed sequence of three frequencies is to be explained by a single carrier pocket. We find that such a possibility arises uniquely at the nodes in the underdoped regime, where the value of bilayer splitting ($\lesssim 16$ meV) is greatly reduced compared to that ($\approx 150$ meV) at the antinodes [17]. The effect of this significant reduction in splitting at the nodes ($\varepsilon_g$ in Fig. 3b) in the underdoped regime, as suggested by recent doping-dependent photoe-
mission measurements [17], is to introduce the possibility of magnetic breakdown tunneling [18]. We illustrate this in Fig. 3 considering the example of an elliptical nodal hole pocket (such as would be created by an ordering vector of form \( \mathbf{Q} = (\pi, \pi) \)). Bilayer coupling splits the original

\[ \epsilon_{\mathbf{Q}} = \epsilon_{\mathbf{k}} - \frac{\beta_{\mathbf{MB}}}{2} (1 - \cos(2\mathbf{k}_x a) + \cos(2\mathbf{k}_y b))^2 \]

\[ t_\perp (\mathbf{k}) = \frac{t_{10}}{4} \left[ \cos(k_x a) - \cos(k_y b) \right]^2 \] (1)

between bilayers which anticipate the splitting between bonding and antibonding bands to vanish at the nodes \([16, 19]\) (occurring along \( |k_x| = |k_y| \) in Fig. 2b). Possible explanations for the opening of a nodal gap include a non-vanishing nodal interbilayer coupling \([19, 20]\) (\( t_c \) in Fig. 2b), mixing with the chain bands \([16]\) and certain forms of Fermi surface reconstruction \([21]\).
We next turn to the question of whether the reported warping of one of the observed Fermi surface pockets [3, 4, 11, 12] is consistent with the bilayer splitting model proposed here. The splitting of the bonding and antibonding bands ($\varepsilon_b$ and $\varepsilon_a$) is given by [19, 20]

$$\varepsilon_{a,b}(k) = \varepsilon(k) \pm \sqrt{t_z^2 + t_{z\perp}^2 + 2t_z t_{z\perp} \cos(ck_z)}$$

(3)

(where $c$ is the c-axis lattice parameter, $k_z$ is the interlayer momentum and $\varepsilon(k)$ is the single layer dispersion). For comparable values of $t_z$ and $t_{z\perp}$, equation 3 takes the form

$$\varepsilon_{a,b}(k) \approx \varepsilon(k) \pm 2t_z \cos(ck_z/2).$$

The modulation along $k_z$ of this dispersion results in an angular dependence of the bilayer-split frequencies $F_0 \pm \Delta F$ which resembles that of a warped cylinder, potentially consistent with the experimentally observed angular dependence of the measured frequencies [4]. By contrast, the $k_z$ modulation is expected to be strongly suppressed in the case of a large disparity in magnitude between $t_z$ and $t_{z\perp}$ as typically occurs at the antinodal region [16]. We also note that the origin of the three frequencies ($F_0 - \Delta F$, $F_0$, and $F_0 + \Delta F$) from magnetic breakdown of a bilayer split pocket is consistent with their similar temperature-dependence reported in ref. [4].

Finally, we note that the proposed scheme for multiple frequencies arising from a single carrier pocket by nodal bilayer coupling is generally valid for a pocket at the nodal region irrespective of its geometry or specific

| orbit | $N_m$ | $R_{MB}$ | $\eta_m$ | $\eta_{MB}$ |
|-------|-------|---------|---------|-----------|
| $F_0 \pm 2\Delta F$ | - | - | 2 | $P(1-P)^2$ |
| $F_0 \pm \Delta F$ | 2 | $P$ | 4 | $P(1-P)^2$ |
| $F_0$ | 2 | $P$ | 4 | $P(1-P)^2$ |

TABLE I: A table counting the number $N_m$ of instances each orbit $m$ of frequency $F_0 + m\Delta F$ and cumulative magnetic breakdown probability $R_{MB}$ occurs within the magnetic breakdown network. The bilayer-split elliptical (see Fig. 3b) and the diamond (see Fig. 4) pocket scenarios are considered.
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\[ H_{\text{in}} = \begin{pmatrix} \varepsilon(k) & -t_{\perp}(k) - t_{\parallel} e^{i ck_z} \\ -t_{\perp}(k) - t_{\parallel} e^{-i ck_z} & \varepsilon(k) \end{pmatrix}. \]

The resulting form of the splitting given by Equation (3) is retained for many types of order.

While the vanishing of the bilayer coupling [Equation (1)] is protected for forms of order with characteristic vectors \( Q = (0, 0) \) or \( (\pi, \pi) \), this is no longer the case for more general ordering vectors (e.g. those in refs. [22–24]). This will contribute to the opening of a nodal gap.