Slow quantum oscillations without fine-grained Fermi Surface Reconstruction in Cuprate Superconductors

P.D. Grigoriev1,2,3 and Timothy Ziman4,5

1L. D. Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia
2National University of Science and Technology “MISiS”, Moscow 119049, Russia
3P.N. Lebedev Physical Institute, RAS, 119991, Moscow, Russia
4Institut Laue-Langevin, BP 156, 41 Avenue des Martyrs, 38042 Grenoble Cedex 9, France
5LPMMC (UMR 5493), Université de Grenoble-Alpes and CNRS, Maison des Magistères, BP 166, 38042 Grenoble Cedex 9, France

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The Fourier transform of the observed magnetic quantum oscillations (MQO) in \( \text{YBa}_2\text{Cu}_3\text{O}_6\pm\delta \) high-temperature superconductors has a prominent low-frequency peak with two smaller neighbouring peaks. The separation and positions of these three peaks are almost independent of doping. This pattern has been explained previously by rather special, exquisitely detailed, Fermi-surface reconstruction. We propose that these MQO have a different origin, and their frequencies are related to the bilayer and inter-bilayer electron hopping rather than directly to the areas of tiny Fermi-surface pockets. Such so-called “slow oscillations” explain more naturally many features of the observed oscillations and allow us to estimate the inter-layer transfer integrals and in-plane Fermi momentum.

Magnetic quantum oscillations (MQO) provide a traditional and powerful tool to study the Fermi surface and other electronic structure parameters of various metals.\(^1\)\(^2\) In the last decade, following their first observation in cuprate high-temperature superconductors,\(^3\) they have been extensively used to investigate the electronic structure of cuprates, both hole-\(^5\) and electron-doped,\(^6\) as well as in Fe-based superconductors.\(^7\)\(^–\)\(^13\) Probably most surprising are the data for the under-doped,\(^6\) as well as in Fe-based superconductors.\(^7\)\(^–\)\(^13\) The Fourier transform of these quantum oscillations has a prominent peak at frequency \( F_\alpha \approx 530T \) with two smaller shoulders at \( F_\pm = F_\alpha \pm \Delta F_\alpha \), where \( \Delta F_\alpha \approx 90T \). All these frequencies are much smaller than expected from closed pockets of the Fermi surface (FS). Many different theoretical models have been proposed to explain such a set of frequencies \(^{22,23}\), reviewed in \(^5\),\(^22\),\(^24\). While these interpretations vary in detail, such as inclusion of spin-orbit or Zeeman splittings, they are all based on Fermi-surface reconstruction due to the periodic potential created by a charge density wave (CDW). A weak, probably, inhomogeneous or fluctuating CDW order has been detected in \( \text{YBa}_2\text{Cu}_3\text{O}_6\pm\delta \) compounds by X-Ray scattering \(^{30,33}\), nuclear magnetic resonance \(^{34,35}\), and sound velocity measurements \(^{36}\). High magnetic fields suppress superconductivity and lead to long-range CDW coherence.\(^33\) Static CDW order can indeed lead to Fermi surface reconstruction, seen in new MQO frequencies, but only if the CDW potential is sufficiently strong. More precisely, the CDW energy gap must be larger than the magnetic-breakdown gap \( \Delta_{MB} \sim \sqrt{\hbar \omega_c E_F} \), where \( \hbar \omega_c \) is the cyclotron energy, \( i.e. \) the separation between the Landau levels, and \( E_F \sim 1\text{eV} \) is the Fermi energy of the unreconstructed electron dispersion. The oscillations in cuprates are measured in magnetic fields \( B \) higher than 30 tesla, where \( \Delta_{MB} \gtrsim 40\text{meV} \) is rather large and a fluctuating CDW ordering may not be enough to form new frequencies with amplitudes sufficient for experimental observation. Note that a frequency pattern somewhat similar to that of \( \text{YBa}_2\text{Cu}_3\text{O}_6\pm\delta \) is observed in the closely related stoichiometric compound \( \text{YBa}_2\text{Cu}_4\text{O}_8 \),\(^{37,39}\) where there is no experimental indication of a static superstructure. Even if this CDW is sufficiently strong, it is hard to explain the observed three-peak frequency pattern of MQO in YBCO without additional frequencies of similar amplitude from the CDW wave vector seen in X-ray experiments.\(^{34,33}\) Moreover, if FS reconstruction really is the origin of the observed \( F_\alpha, F_+, \) and \( F_- \), they should depend strongly on doping.\(^10\) Such a strong dependence is, in fact, observed in the electron-doped cuprate superconductor \( \text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4 \),\(^{11,12}\) where the frequency changes by 20%, from 290 to 245 T, when the doping level changes from 0.15 to 0.17. In contrast, in \( \text{YBa}_2\text{Cu}_3\text{O}_6\pm\delta \) the observed doping dependence of the three low frequencies is much weaker. The data are somewhat controversial: frequency changes vary from very weak, less than 5% (Ref. \(^10\), Fig.4) to about 25% (Ref. \(^23\), Fig. 5b ) when the doping changes from \( p \approx 0.1 \) to 0.14. In a recent study \( F_\alpha \) changes by only 10%, from 515 T to 570 T, for \( p \) varying from 0.09 to 0.14.\(^43\) Within the CDW scenario, a model of compensated FS pockets has been proposed,\(^18\) but the doping-dependence remains problematic. To avoid the problematic FS reconstruction scenarios an unusual source of oscillations was proposed in terms of Andreev-type bound states,\(^44\) but the predicted change in oscillation frequencies with superconducting gap contradicts experiment. In this paper, we propose a simple alternative picture, which is consistent with the observed three equidistant magnetic oscillation peaks in \( \text{YBa}_2\text{Cu}_3\text{O}_6\pm\delta \) and other features of the mea-
The unreconstructed FS of YBCO consists of one large pocket, almost a square with smoothed corners, that fills about one half of the Brillouin zone and would correspond to a large frequency $\sim 10^4$ tesla. The Fermi-surface reconstruction, possibly caused by the pseudogap, AFM or CDW order, takes place for doping level $p < 10-15\%$, as suggested by ARPES [45], or by observation of negative Hall [46, 47] and Seebeck [48] coefficients which indicate electron-like FS pockets. However, the observed MQO frequency $F_q \approx 530T$ corresponds to a FS cross-section of only 2% of the Brillouin zone, which is considerably less than the size of the expected FS pockets even for a reconstructed FS. Analogous “slow oscillations” (SIO) have been observed in organic superconductors and at a reconstructed FS. The corresponding Fermi surface pocket is shown schematically in Fig. 2 for a slight tetragonal modulation of $t_{\perp} (k_{||})$, where $k_{||}$ is the inplane momentum. The resulting electron energy spectrum is given by (20) (see, e.g., Eq. (6) of Ref. 21)

$$\epsilon_{\pm} (k_{z}, k_{||}) = \epsilon_{\parallel} (k_{||}) \pm \sqrt{t_{z}^2 + t_{\perp}^2 + 2t_{z}t_{\perp} \cos [k_{z} (h + d)]},$$  

(1)

For $t_z \ll t_{\perp}$ this spectrum contains bonding and antibonding states separated by $\sim 2t_{\perp} (k_{||})$, each with weak $k_z$ dispersion:

$$\epsilon_{\pm} (k_{z}, k_{||}) \approx \epsilon_{\parallel} (k_{||}) \pm t_{\perp} (k_{||}) \pm 2t_{z} (k_{||}) \cos [k_{z} (h + d)].$$  

(2)

The corresponding Fermi surface pocket is shown schematically in Fig. 2 for a slight tetragonal modulation of $\epsilon_{\parallel} (k_{||})$ and two different symmetries of $t_{\perp} (k_{||})$. In YBCO there are thus at least two types of splitting of the original frequencies: the larger bilayer splitting $\Delta F_{\perp} = t_{\perp} B/\hbar \omega_c$, where $t_{\perp} = \langle t_{\perp} (k_{||}) \rangle \neq 0$ and the angular brackets signify an averaging over in-plane momentum $k_{||}$ on the FS, and the smaller splitting $\Delta F_{c} = 2t_{z} B/\hbar \omega_c \ll \Delta F_{\perp} \ll F_{q}$ due to the $k_z$ electron dispersion, where we also assume $t_z = \langle t_{z} (k_{||}) \rangle \neq 0$. These two splittings result in four underlying MQO frequencies $F_{\parallel} \pm \Delta F_{\perp} \pm \Delta F_{c}$ of similar amplitudes, instead of only two $F_{\parallel} \pm \Delta F_{c}$ for organic metals without bilayers [49].

The SIO of MR originate from these four frequencies in a similar way as before [49, 51] but result in a much richer set of frequencies, as we show below.

At finite temperature the metallic conductivity along $i$-th axis $\sigma_i = \sigma_{ii}$ is given by the sum of contributions

![FIG. 1: Schematic illustration of the bilayer crystal structure in YBa$_2$Cu$_3$O$_{6.5}$ and YBa$_2$Cu$_4$O$_8$ high-temperature superconductors with two interlayer transfer integrals $t_{\perp}$ and $t_{z}$.](Image 100x190 to 252x308)

![FIG. 2: A quasi-2D Fermi surface with interlayer warping due to $2t_{z}$ and double bilayer splitting, corresponding to dispersion in Eq. 2 for $t_z (k_{||}) \approx const$, and (a) $t_{\perp} (k_{||}) = t_{\perp} (1 + 0.3 \sin 4\phi)$ and (b) $t_{\perp} (k_{||}) = t_{\perp} (1 + 0.5 \sin 2\phi)$, where $\tan \phi = k_y/k_x$.](Image 330x571 to 437x740)
from all ungapped FS pockets $\beta$:

$$\sigma_i = \sum_\beta \sigma_{i,\beta} = \sum_\beta e^2 g_{F,\beta} D_{i,\beta}. \quad (3)$$

Each pocket $\beta$ contributes to the total metallic conductivity along axis $i$ at low temperature via the product of a density of electron states (DoS) $g_{F,\beta} = g_\beta (\varepsilon = E_F)$ and an electron diffusion coefficient $D_{i,\beta}$. Both contribute to oscillations, since they vary with the magnetic field $B_z$ perpendicular to the conducting $x$-$y$ layers as:

$$g_{F,\beta} / g_{0,\beta} = 1 + A_\beta \sum_{j,i=\pm 1} \cos \left( 2\pi \frac{F_\beta + j \Delta F_\perp + l \Delta F_\parallel}{B_z} \right), \quad (4)$$

with $g_{0,\beta} = m^*_\beta / \hbar^2 d$ the average DoS at the Fermi level and $m^*_\beta$ the effective mass for the pocket $\beta$, and

$$\frac{D_{i,\beta}}{D_{0i,\beta}} = 1 + B_{i,\beta} \sum_{j,i=\pm 1} \cos \left( 2\pi \frac{F_\beta + j \Delta F_\perp + l \Delta F_\parallel}{B_z} \right), \quad (5)$$

where the non-oscillating part $D_{0i,\beta}$ of the diffusion coefficient in metals is proportional to the mean-square electron velocity $v_i$ at the Fermi level. The harmonic amplitudes $A_\beta \sim B_{i,\beta}$ contain the Dingle factor $2$, $R_{D,\beta} \approx \exp (-2\pi \Gamma / \hbar \omega_c,\beta)$, where the electron level broadening $\Gamma = \Gamma (B, T)$ comes from various types of interaction of the conducting electrons.

Combining Eqs. (3)-(5) we obtain

$$\sigma_i^{(0)} / \sigma_i^{(0)} = 1 + (A_\beta + B_{i,\beta}) \sum_{j,i=\pm 1} \cos \left( 2\pi \frac{F_\beta + j \Delta F_\perp + l \Delta F_\parallel}{B_z} \right) \times$$

$$+ A_\beta B_{i,\beta} \sum_{j,i,j',l'=\pm 1} \cos \left( 2\pi \frac{F_\beta + j j' \Delta F_\perp + l l' \Delta F_\parallel}{B_z} \right) \times$$

$$\cos \left( 2\pi \frac{F_\beta + j j' \Delta F_\perp + l l' \Delta F_\parallel}{B_z} \right), \quad (6)$$

where $\sigma_i^{(0)} = e^2 g_{0,\beta} D_{0i,\beta}$ does not oscillate. The second term in Eq. (6) gives the usual MQO with amplitudes $A_\beta$ and four fundamental frequencies $F_\beta \pm \Delta F_\perp \pm \Delta F_\parallel \sim F_\beta \gg \Delta F_\perp$. The last term in Eq. (6) is of the second order in the amplitude $A_\beta$ and gives various frequencies: (i) the 4 second harmonics $2 (F_\beta \pm \Delta F_\perp \pm \Delta F_\parallel)$, which are strongly damped by temperature and disorder and can be neglected; (ii) for $j' = 1$ and $l' = -1$ the SIO with very low frequency $2 \Delta F_\parallel \ll \Delta F_\perp \ll F_\beta$; (iii) for $j' = -1$ and $l' = \pm 1$ the SIO with intermediate frequencies $2 \Delta F_\parallel$ and $2 \Delta F_\perp \pm 2 \Delta F_\parallel$. Indeed, neglecting the high frequency ($\sim 2 F_\beta$) contributions we can rewrite the last term in Eq. (6) for $j' = 1$ as

$$A_\beta B_{i,\beta} \sum_{j,i,j',l'=\pm 1} \cos \left( 2\pi \frac{2 j \Delta F_\perp + l (1 - l') \Delta F_\parallel}{B_z} \right)$$

$$= A_\beta B_{i,\beta} \left[ 2 \cos \left( \frac{4 \pi \Delta F_\perp}{B_z} \right) + \sum_{l=\pm 1} \cos \left( 4 \pi \frac{\Delta F_\parallel + l \Delta F_\parallel}{B_z} \right) \right]. \quad (7)$$

There is an important difference between the SIO with frequency $2 \Delta F_\parallel$, produced by FS warping due to $k_z$ dispersion from $t_z$, and the SIO frequency $2 \Delta F_\parallel$ from the bilayer splitting $t_\perp$. If due to $t_z$, the slow frequency has a strongly non-monotonic dependence on the tilt angle of the magnetic field $\theta$.

$$\Delta F_\parallel (\theta) = \Delta F_\parallel (\theta = 0) J_0 (k_F c^* \tan \theta) / \cos \theta, \quad (8)$$

where $c^* = 11.65 \text{ Å}$ for YBCO is the lattice constant in the interlayer $z$-direction, and $k_F$ is the Fermi momentum. This angular dependence is as for the beat frequency of MQO or as for a square root of interlayer conductivity (AMRO) in a quasi-2D metal, but differs strongly from the standard cosine dependence

$$F (\theta) = F (\theta = 0) / \cos \theta, \quad (9)$$

typical of quasi-2D metals. Eq. (3) has an obvious geometrical interpretation: the slightly warped FS has two extremal cross-sections $S_{ext}$ perpendicular to the
magnetic field $B$, which become equal, to first order in $t_z$, at some tilt angles $\theta_{Yam}$, the SIO frequency $2F_L$ due to bilayer splitting, however, has the cosine angular dependence given by Eq. (10) rather than by Eq. (8). To show this, consider a magnetic field that is not very strong, $B \ll F_o \approx 530T$, so $\hbar \omega_c \ll 4\pi t_L$ and the field does not modify the electron spectrum of one bilayer. Consider the dispersion in Eq. (2), corresponding to the FS in Fig. 2. At $t_z < t_\perp$ the FS consists of two cylinders along the $z$-axis with base areas $S_{even}$ and $S_{odd}$, differing by $\Delta S = S_{even} - S_{odd} = 4\pi t_{\perp} m^* = const$. In a tilted magnetic field the two corresponding extremal cross-section areas are $S_{even, odd} = S_{even, odd}/\cos \theta$, leading directly to Eq. (9). The two split FS cylinders are weakly warped at finite interbilayer hopping $t_z$, but if $2t_z < t_\perp$ and the split FS do not intersect, a finite $t_z$ does not change the angular dependence in Eq. (9) to leading order in $t_z/t_\perp$.

The amplitude of the central frequency $2\Delta F_L$ in Eq. (7) is twice as large as the amplitudes of the side frequencies $2\Delta F_\pm \pm 2\Delta F_c$, and in Fig. 4 the amplitudes of side peaks are additionally damped by the finite Dingle factor. This resembles closely the experimental data in YBCO.[6, 13, 22] We therefore propose an alternative interpretation of the observed oscillations in the YBCO.[6, 13, 22] oscillations at low frequency $F_o \approx 530T$ in YBa$_2$Cu$_3$O$_{6+\delta}$ (and, possibly, in YBa$_2$Cu$_3$O$_6$[37, 39]), in which three equidistant harmonics are not due to the small pockets of the FS reconstructed by CDW order.[6, 22] but originate rather from mixing, according to Eq. (7), of four frequencies $F_\perp \pm \Delta F_\pm \pm \Delta F_c$, formed by a fundamental frequency $F_\perp$ split by bilayer and interbilayer electron hopping integrals $t_\perp$ and $t_z$. In terms of Eqs. (6)–(7) and electron dispersion in Eqs. (1) or (2), the frequencies $F_o = 2\Delta F_L \approx 530T = 2t_\perp B/\hbar \omega_c$ and $\Delta F_o = 2\Delta F_c \approx 90T \approx 4t_z B/\hbar \omega_c$ allow us to extract the values of bilayer $t_\perp$ and interbilayer $t_z$ average electron transfer integrals from experiment. We summarize arguments for this new interpretation:

1. Experimentally, the multiple extra MQO frequencies predicted from FS reconstruction are missing.[6, 22] In contrast, in the SIO model the only frequency with an amplitude $A_\beta^2$ comparable to the side peaks at $F_o \pm \Delta F_o$ would be $2\Delta F_c \approx 90T$. This low frequency, however, can be detected only at low magnetic field $B_z < \Delta F_c$, where the oscillations are strongly damped by the Dingle factor. Actually such a frequency may have been seen recently.[21] The SIO scenario also predicts a much larger frequency $F_\beta$ from FS pockets, which should be more easily observed in cyclotron resonance or dHvA than in the Shubnikov-de Haas effect. Experimentally, the $F_\beta \approx 1.65kT$ frequency was indeed observed in dHvA.[14] and Tunnel Diode Oscillation cyclotron resonance measurements, whereas the $F_o$ is much clearer in magnetotransport.

2. The observed $F_o \approx 530T$ depends weakly on the degree of doping,[14, 17], more consistent with SIO than with expectations for small FS-pockets.

3. The bilayer splitting $t_\perp$ expected from bandstructure calculations[29, 60] is consistent with the observed SIO frequency $F_o$: $2\Delta F_c = 2t_\perp B/\hbar \omega_c \approx F_o \approx 530T \approx 2% \cdot S_{BZ}$, giving $t_\perp \approx \langle t_\perp \rangle$ is $\hbar F_o/2m^*_c \approx 8m_e$. Note that the maximum value $t_\perp \approx \langle t_\perp \rangle$ of bilayer transfer may considerably exceed this average value $t_\perp$. Similarly the observed $t_z$-induced splitting $\Delta F_c \approx 90T \approx 4t_z B/\hbar \omega_c$, gives a reasonable average value $2t_z \approx 1.4m_e$.

4. Long-range spatial inhomogeneities, common in cuprates, should strongly damp oscillations from FS pockets due to smearing of the Fermi level. They should affect the proposed SIO much less, similar to slow oscillations in Ref. [49].

5. The angular dependence of the observed frequencies[15] corresponds to the SIO interpretation, predicting $F_o (\theta) = F_\perp (\theta) \approx \cos \theta$ and $\Delta F_c \cos \theta \approx J_0(k_F e^* \tan \theta)$, where $e^* \approx 11.8$ is the interlayer lattice constant. The observed strong angular dependence of the split frequency $\Delta F_c (\theta)$ (see Fig. 4a of Ref. [15]) is well fit by Eq. (8), corresponding to the FS-warping origin of this splitting. The first Yamaji angle $\theta_{Yam} \approx 43^\circ$ in $\Delta F_c (\theta)$, corresponding to the first zero of the Bessel function $J_0(k_F e^* \tan \theta)$ in Eq. (8), is clearly seen in Fig. 4a of Ref. [15]. This Yamaji angle gives the Fermi momentum $k_F = 2.4/e^* \tan \theta_{Yam} = 2.2\mu m^{-1}$ and FS-pocket area of about $\pi k_F^2 \approx 15\mu m^{-2}$, corresponding to MQO frequency $F_0 \approx S_{ext} \hbar/2\pi e \approx 1.6kT$, which is far from $F_o \approx 530T$ but close to $F_{\beta} \approx 1.65kT$ observed in Ref. [14, 17]. Thus we conclude that the FS pocket responsible for the observed oscillations, has an area corresponding to $F_\beta$ rather than $F_o$, which is a slow frequency corresponding to $t_\perp$. Note that $F_\beta$ was observed only at rather low temperatures and not in all samples.[21] consistent with our model because frequencies corresponding to real FS pockets are more strongly damped by temperature than the proposed SIO and strongly damped by sample-dependent inhomogeneities.

6. An underlying CDW is not a necessary prerequisite for observation of SIO. There are no issues to be resolved as to how a weak and fluctuating CDW ordering could overcome magnetic breakdown, which should be strong for fields up to 100 tesla.

7. The relative amplitudes of the frequencies are naturally explained without additional fitting parameters (see Fig. 7).

We note possible counter-arguments:

1. The observed magnetoresistance oscillations are quite strongly damped by temperature, with effective mass $m^* \approx 1.6m_e$.[16, 18] with $m_e$ the free electron mass, in disagreement with the simple form predicted here[49, 57] but may arise from the square of the Dingle factor $R_D$ with temperature dependence enhanced by electron-photon and the very strong electron-electron interaction in cuprates.
(2) A component at \( F_s \) is also observed in the dHvA effect. This can be due to the electron-electron interaction, roughly proportional to the product of the density of states, giving a nonlinearity in the magnetization as a functional of the oscillating density of states.

(3) Oscillations with a frequency \( \approx 840T \) (but without side-frequency splitting), corresponding to 3% of the Brillouin zone, have been observed in HgBa\(_2\)CuO\(_4+\delta\), where there is no bilayer splitting, but a much larger \( t_2 \) is expected from the shorter interlayer distance. In fact this is consistent with SIO, but as the spectrum is simpler the evidence is not as compelling.

To summarize, we propose an alternative interpretation of the observed magnetic oscillations in YBa\(_2\)Cu\(_3\)O\(_{6+\delta}\) high-Tc superconductors, with frequencies \( F_s \approx 530T \) and \( F_s \pm \Delta F_s \) related to the bilayer splitting and corrugation rather than to tiny FS pockets. This is based on the new result [7], as illustrated in Fig. 3. The frequencies allow us to estimate values of bilayer splitting \( t_\perp = \hbar F_s /2m^* \) and of \( k_z \)-dispersion \( t_z = \hbar \Delta F_s /4m^* \). Angular dependence points to a true FS pocket close to \( F_\beta \approx 1.6kT \). While this can explain current observations without recourse to CDWs, neither does it rule out their potential to make new frequencies appear. Such frequencies would, however, be more sensitive to inhomogeneity as well as magnetic breakdown.

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