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Citation: Chen, Kuang-Ting , and Patrick A. Lee. "Violation of the Onsager relation for quantum oscillations in superconductors." Physical Review B 79.18 (2009): 180510. © 2009 The American Physical Society

As Published: <http://dx.doi.org/10.1103/PhysRevB.79.180510>

Publisher: American Physical Society

Persistent URL: <http://hdl.handle.net/1721.1/51880>

Version: Final published version: final published article, as it appeared in a journal, conference proceedings, or other formally published context

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Violation of the Onsager relation for quantum oscillations in superconductors

Kuang-Ting Chen and Patrick A. Lee

Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

(Received 1 April 2009; published 26 May 2009)

We numerically study the quantum oscillations in superconducting vortex-mixed states with d -wave pairing. We show that in the parameter range of an underdoped cuprate superconductor, the commonly held assumption that the period is given by the underlying Fermi-surface area using the Onsager relation becomes invalid. Using this result, we conclude that the interpretation of the recent experimental data on YBCO as a signal of an underlying Fermi surface with four hole pockets created by a (π, π) folding cannot be ruled out.

DOI: 10.1103/PhysRevB.79.180510

PACS number(s): 74.25.Jb

Recent experiments have shown quantum oscillations in underdoped YBCO samples in strong magnetic field ~ 45 T.^{1–5} This has been interpreted as a signal of the underlying Fermi surface (FS). The period of the oscillation is large and implies that the FS has been reconstructed, probably, by some translational symmetry-breaking order in the ground state.^{6–9} However, for both materials that have been studied, the simplest construction, a (π, π) folding forming four hole pockets in the original Brillouin zone (BZ), would imply a pocket too small comparing to the nominal doping by about 25%.^{1,3} This partly motivated a number of workers to interpret the data in terms of more complicated reconstruction such as incommensurate spin-density wave (SDW).^{5,7} Furthermore, the measured Hall effect is negative¹⁰ and this led LeBoeuf *et al.* to propose that the quantum oscillations originate from electron pockets. Whether the negative Hall effect is due to flux flow¹¹ is currently a subject under debate.

We believe that in these experiments, the samples are still in a vortex-mixed state. One evidence is the measured torque hysteresis,⁵ which implies that vortices exist at least up to 45 T. Furthermore, the commonly quoted core size of 20 Å [see, for example, the extrapolation based on scanning tunneling microscopy (STM) measurement¹² as well as Nernst measurements¹³] lead to an estimate of H_{c2} of 100 T. Therefore, to interpret the oscillations data, one has to understand the quantum oscillations in the mixed state.

Up to now, all discussions assume that quantum oscillations in the mixed state maintain the same frequency as in the normal state and are given by the Onsager relation, which relates the frequency to the Fermi-surface area. This is true of all experiments performed up to date where it is possible to scan the magnetic field across H_{c2} .^{14,15} However, there is no clear argument why the frequency should remain the same and previous theories predict a small shift.^{16,17} We note that all previous experiments have been done on conventional s -wave low T_c superconductors, with the possible exception of the organics which may be d -wave, and the high- T_c cuprates may be in quite a different parameter regime. For example, the coherence length ξ_0 is very short, on the order of 4 or 5 lattice constants, and is the consequence of a large energy gap Δ_0 . The number of Landau levels N is about 10 in the high- T_c experiments, as opposed to 100's or 1000's for conventional superconductors. This means that the semiclassical orbit encloses 10 flux quanta, i.e., 20 vortex cores. There are good reasons to believe that the pairing amplitude and the gap scale Δ_0 are very robust in the under-

doped cuprates. In contrast, previous work on quantum oscillations in superconductors all deals with the s -wave pairing in the conventional parameter range.^{16–19}

In this Rapid Communication, we address the question of whether the traditional picture continues to hold in a parameter regime which has not been tested experimentally. We take as our model the Bogoliubov–de Gennes (BdG) equations in real space with a variety of vortex coordinates and competing order parameters, which can take on arbitrary spatial dependence. We take the coherence length and the pair field as parameters and make no attempt to solve the problem self-consistently. Since we do not expect the BdG equations to be the correct microscopic theory for the underdoped cuprates, it makes little sense to determine these parameters self-consistently. Rather, we treat this as a phenomenological model. To the extent that the proximity to the Mott transition is not captured by this phenomenology, the application of our theory to high- T_c problems should be treated with caution. With these caveats, we write down a tight-binding Hamiltonian on a square lattice constant a , and we set $e = \hbar = a = 1$,

$$\begin{aligned}
 H = & \sum_{i,j \in NN, \sigma} [-t + (-1)^{i_x+j_y} i \Delta_{sf}(\vec{r}_{ij})] e^{iA_{ij}} c_{i\sigma}^\dagger c_{j\sigma} \\
 & + \sum_{i,j \in NNN, \sigma} (-t') e^{iA_{ij}} c_{i\sigma}^\dagger c_{j\sigma} \\
 & + \left[\sum_{i,j \in NN} (-1)^{i_x+j_y} \Delta_d(\vec{r}_{ij}) c_{i+}^\dagger c_{j-}^\dagger + \text{H.c.} \right] \\
 & + \sum_{i, \sigma} [(-1)^{i_x+i_y} \sigma V_s(\vec{r}_i) + V_c(\vec{r}_i) - \mu] c_{i\sigma}^\dagger c_{i\sigma}, \quad (1)
 \end{aligned}$$

where t and t' are the hoppings, Δ_d is the nearest neighbor (NN) pairing, Δ_{sf} is related to the staggered flux or equivalently d -density wave (SF-DDW) order,^{20,21} and V_s , V_c are the staggered spin and charge potential, respectively. The potentials are defined on sites $\vec{r}_i = (i_x, i_y)$ and the pairing is defined on bonds $\vec{r}_{ij} = (\vec{r}_i + \vec{r}_j)/2$. The k -dependent d -wave gap would be of size $2\Delta_d(\cos k_x - \cos k_y)$. As a phenomenological model, we take t to be on the order J , the antiferromagnetic coupling. In underdoped cuprates, the gap size is then $\sim 0.5t$. A_{ij} is the electromagnetic gauge field, which satisfies $\sum_{\text{plaque}} A_{ij} = B$ and $\sum_{\text{triangle}} A_{ij} = B/2$; B is the magnetic field.

The pairing amplitude near a vortex is described by the ansatz $|\Delta_d(\vec{r})| = \Delta_0 \sin \theta$ and $\cos \theta(\vec{r}) = r_0 / \sqrt{r_0^2 + d(\vec{r})^2}$, where

Δ_0 is the NN pairing amplitude deep inside the superconductor, r_0 is the core size, and $d(\vec{r})$ is the distance to the vortex center. When multiple vortices are near by, we replace d by $d_{\min} = (\sum_i d_i^{(-p)})^{-(1/p)}$, which is smaller than the distance toward the nearest vortex. The choice of $p \geq 1$ does not qualitatively affect the result. The phase ϕ of Δ_d alone is not a gauge-invariant quantity and has to be determined together with A_{ij} . One way is to assign ϕ and then determine the gauge field under the constraint mentioned above. We choose ϕ to follow the constraints: (i) $|\Delta\phi| < \pi/2$ for every link; (ii) $\sum_{\text{loop}} \Delta\phi = 2\pi n$ where n is the number of vortices enclosed; and (iii) ϕ is periodic in the y direction. We then determine A_{ij} by minimizing the free energy $\sum_{\vec{r}} \frac{1}{2} |\Delta_d(\vec{r})|^2 v_s(\vec{r})^2$ where $v_s = \phi_i - \phi_j - A_{ij}$ is the superfluid velocity. The free energy is a function quadratic in A_{ij} , so we can optimize it by solving a linear equation, using sparse matrix routines.

V_c , Δ_{sf} , and V_s describe the order in the normal state. They can be uniform, periodic, or localized around the vortices depending on the order present. There is an additional piece in V_c which balances the charge density in the mixed state. In a finite system with periodic boundary conditions, it is not always possible to fit in a periodic vortex lattice. Instead we work with a disordered array of vortices. At each B , the vortex positions are determined by a Monte Carlo annealing process for particles with Cr^{-2} repulsion. The vortices are stuck as we gradually lower the temperature. The resulting vortex configuration has short-range order but is rather disordered. It is a reasonable representation of a snapshot of a vortex liquid or a pinned vortex solid.

In order to see the quantum oscillations, the sample size has to be quite large and the Hamiltonian cannot be efficiently diagonalized. We can instead, use the iterative Green's function's method²² to get the local density of states (DOS) (LDOS), at any fixed energy. We affix our sample to two semi-infinite stripes in the $\pm x$ direction. The stripes are normal metal described by t and t' . We take periodic boundary conditions in the y direction. Now the configuration is similar to Ref. 22 and we can use the same method

$$G^L(x) = [G^0(x)^{-1} - tG^L(x-1)t^\dagger]^{-1}, \quad (2)$$

$$G(x) = [G^0(x)^{-1} - tG^L(x-1)t^\dagger - t^\dagger G^R(x+1)t]^{-1}, \quad (3)$$

where $G^0(x)$ is the Green's function for the isolated x th column, $G^L(x)$ [$G^R(x)$] is the Green's function at column x when the right (left) side of the column is deleted, t is the hopping matrix between the two consecutive columns [contains $t, t', \Delta_d(x)$, and $\Delta_{sf}(x)$], and $G(x)$ is the Green's function for the x th column in the original setting. Everything here is a $2y \times 2y$ matrix, containing the electron and hole parts. We first go from left to right and compute G^L for every x . Next we go from right to left to compute G^R and use Eq. (3) to compute $G(x)$ for all x . The imaginary part of the y th diagonal matrix element in the electron part of $G(x)$ is then related to the local density of states at (x, y) .

Using this method, we can get the LDOS everywhere in our sample. However, the LDOS varies from place to place due to its relative position to the vortices as well as the disorder of the vortex lattice. To see the quantum oscillations, it suffices to look at the averaged DOS. In this work, if

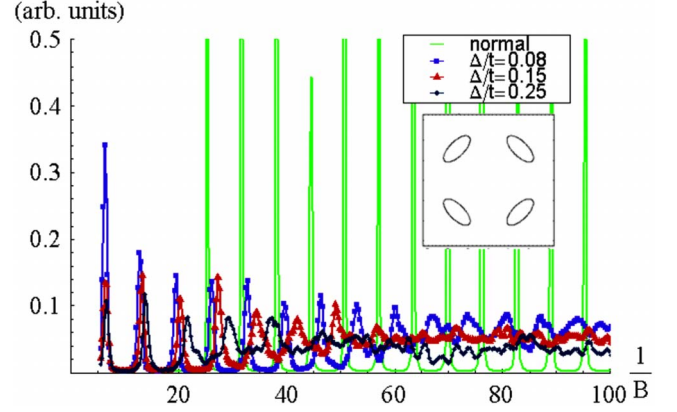


FIG. 1. (Color online) This plot shows the averaged DOS vs $1/B$ in the vortex-mixed state with (π, π) SF-DDW order. From this figure and below, if not mentioned otherwise, B is in units of $(\frac{\Phi_0}{2\pi a^2})$. If we view H_{c2} as the field strength where vortices are overlapping, it corresponds to $1/B=25$ in the plot. Different lines in the plot show states with different pairing fields. The maximum pairing gap in the antinodal direction would have size $\sim 4\Delta$. We can see that as the gap increases, the frequency decreases. The inset is a plot of the Fermi surface in the normal state. There are four hole pockets with 2.5% area each of the original BZ. This corresponds to $p=0.1$ from half filling. In this plot, $\Delta_{sf}=0.25t$.

not specified otherwise, we set $t' = -0.3t$, $r_0 = 5a$, and the lattice is of size 2000×80 . We vary the magnetic field in accord with the number of the vortices, which is from 500 to 10000.

In Fig. 1, we showed the result where we start from the state in which the Fermi surface is reconstructed by (π, π) SF-DDW order. If we define H_{c2} to be the field where vortices start overlapping and $r_0 = 5a$, this gives $(\frac{\Phi_0}{2\pi a^2}) \frac{1}{H_{c2}} = 25$, where Φ_0 here is the full flux quantum, hc/e . The experimental probe, roughly at the tenth Landau level, would be around $(\frac{\Phi_0}{2\pi a^2}) \frac{1}{H_{c2}} = 60$. We create a gap large enough to kill the electron pockets, leaving four hole pockets shown in the inset. We found that the oscillation period of the normal state matches the prediction from the Onsager relation and the Luttinger theorem. As we turn on the d -wave pairing amplitude, the period of the quantum oscillation increases. As the pairing gets large, the period of the oscillation is off from the period in the normal state by about 20%. The frequency shifts are clearly seen in the Fourier transform shown in Fig. 2. Note that in our modeling of the vortex cores, the superconducting pairing remains, albeit at reduced amplitude, even for $B > H_{c2}$. This explains why the frequency shift persists somewhat above H_{c2} , but we can ignore that region because it is not reached experimentally. Note that the oscillations survive even down to $0.5H_{c2}$. We have also done calculations for a (π, π) SDW order, and the period is shifted in a similar way [see Fig. 2(b)].

To check whether this is a generic phenomena, we ran a simpler setting with an electron pocket centered at origin. The result is showed in Fig. 3. Again, as we turned on the d -wave pairing, the frequency is reduced as the pairing is increased. It is worth noting that we shifted the chemical potential in order to maintain the total electron density as we

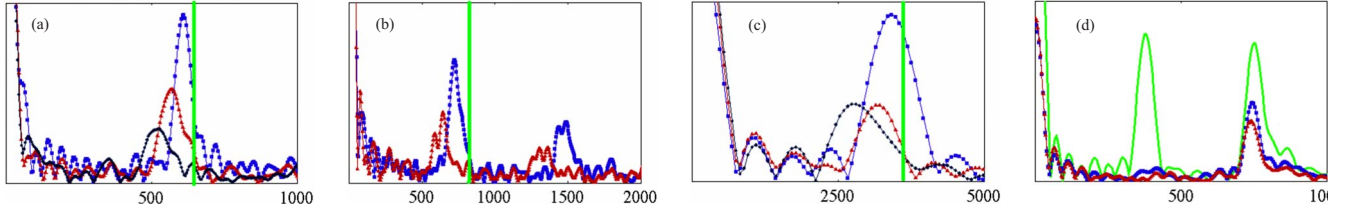


FIG. 2. (Color online) Fourier transforms of plots shown in Figs. 1, 3, and 4. We take $a=4$ Å and the frequency is then in units of tesla. The color used is the same as in the averaged DOS vs $1/B$ plots. The normal-state frequency is shown by the green line. (a) SF-DDW. (b) SDW, $p=0.125$. The peak at the right is the second harmonic. (c) Electron pocket centered at origin. (d) Two-pocket SDW; the peak at ~ 380 T is from the electron pockets and the one at ~ 750 T is from the hole pockets.

increase the pairing. We also added a charge potential to make the charge density approximately uniform inside and outside the vortex core. On the other hand, if we simply keep the chemical potential to be the same as in the normal state, the period still decreases but by about half (not shown). The effect of the chemical-potential shift is significant in the case of Fig. 3 because the pairing is strong and the electron is far from the particle-hole symmetric. It is less significant in the more realistic case of Fig. 1.

In Fig. 4, we started with a two-pocket Fermi surface reconstructed by a (π, π) SDW order and turned on a small d -wave pairing. The oscillations from the electron pockets are clearly visible in the normal state but are rapidly killed in the mixed state. Note the pair field is very small, about 10 times smaller than that in Fig. 1. One explanation is that the electron pocket originates from the antinodal region where the gap is large and is dephased by the random pairing potential due to the random vortex configurations. However, this cannot be the whole story because we find that for s -wave pairing with similar pairing gap size, the electron and hole pockets both survive. One difference we noticed is that in the s -wave case, there is a strong density-of-states peak inside the vortex core, much larger than that inside the d -wave core. At this point, we do not have a full understanding of the suppression of the electron pocket oscillations.

We have also calculated the oscillation for an “incommensurate” SDW, with period $Q=[\pi(1 \pm 2\delta), \pi]$ where $\delta=1/8$. We impose a sinusoidal $V_s(\vec{r})=V_{s0} \cos(2\pi\delta x)$ and $V_c(\vec{r})$

$=V_{c0} \cos(4\pi\delta x)$. Complicated band structures in this kind of potential were computed by Millis and Norman.⁷ It is instructive to consider the hybridization only with the primary vector Q for SDW and $2Q$ for the charge component. The upper inset in Fig. 5 shows the FS reconstruction of a pure incommensurate SDW order ($V_c=0$), and we see that after hybridization only two closed orbits are possible. One is a small hole pocket and the other is the electron pocket. The larger hole pocket becomes an open orbit. Inclusion of V_c further cuts the small hole pocket to an even smaller area.

The lower inset shows the reconstructed FS with SDW and charge-density wave (CDW) present. In the averaged DOS plot, we indeed see the oscillations from the electron pockets and the small hole pockets. The electron pocket is again heavily suppressed in the mixed state, leaving a hole frequency which is too small compared with experiment.

In conclusion, we have shown that the Onsager relation does not always apply to quantum oscillations in the vortex-mixed state. When the pairing is strong and the coherence length is short, we find a systematic decrease in the frequency. We have also checked that if the core size is increased, the shift is diminished. Thus, our result is consistent with experiments performed so far on conventional superconductors, which are in the large core size limit. The implication for the experiment on high- T_c cuprate is that the simple interpretation in terms of (π, π) folding creating four

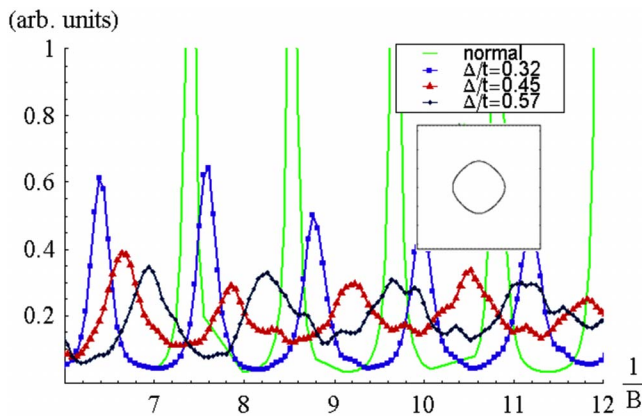


FIG. 3. (Color online) An electron pocket is centered at the origin. The pocket has an area of 14% of the original BZ. In this plot, $t'=-0.14t$. The maximum gap $\sim 1.5\Delta$.

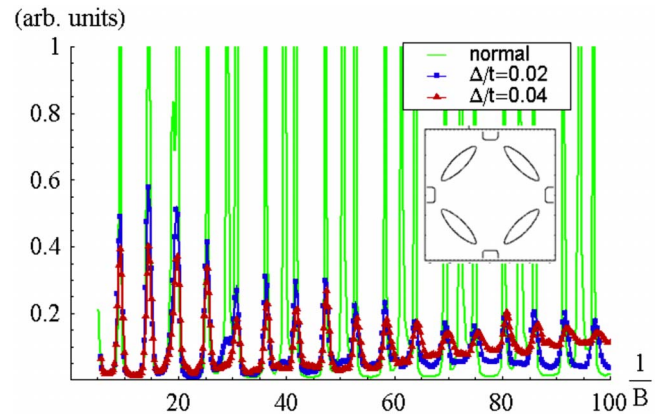


FIG. 4. (Color online) Four hole pockets and two electron pockets are present. In this plot, $A_h=2.9\%$ and $A_e=1.44\%$ of the original BZ and $p=0.086$. In the normal state, from Onsager’s relation we can determine that the peaks with period 11 are from electron pockets. The amplitude is heavily suppressed in the mixed state. In this plot, $V_s=0.2t$.

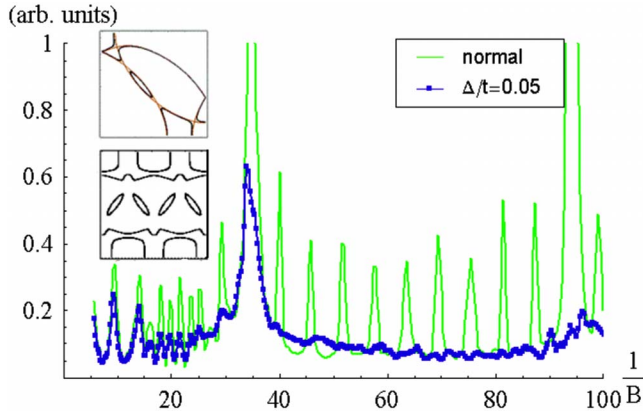


FIG. 5. (Color online) $1/8$ stripe state with $t' = -0.4t$, $V_{s0} = 0.4$, and $V_{c0} = 0.1$. The upper inset shows the hybridization of the primary band as we turn on V_s (with $V_c = 0$), and the lower inset shows the developed Fermi surface. The fast oscillations localized around $1/B \sim 20$ is a breakdown effect. At lower fields, the fast oscillation (period 6) is from the electron pockets and the very slow oscillation (only 1 period seen in the range) is from the hole pockets. As we turn on superconductivity, the oscillation from the electron pockets is diminished.

hole pockets cannot be automatically ruled out. There are two candidates for (π, π) order. One is SDW order and the second is SF-DDW order. We note that in view of the recent measurement that the g factor is much less than 2,²³ the SF-DDW scenario must be accompanied by some additional order such as an incommensurate SDW. In that case, there are possibilities for larger orbits composed of two or three hole pockets shifted by δ if magnetic breakdown is taken into account. The other interpretation is the incommensurate SDW order. In this case, the observed pocket must be identified with the electron pocket. Alternatives in terms of SF-DDW with electron pockets have also been proposed.^{6,8,9} While the electron pocket is rapidly suppressed in the mixed state in our model, it is not clear how general this conclusion is, i.e., whether it is valid beyond the BdG theory. We think that within the Fermi-liquid scenario, both are viable options at this point and further work will be needed to distinguish between them.

We thank T. Senthil for many helpful discussions. This work is supported by the NSF under Grant No. DMR-0804040.

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