Magnetic-field-induced macroscopic quantum phenomenon in a superconductor with gap nodes

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We propose the existence of a macroscopic quantum phenomenon induced by a magnetic field in unconventional superconductors. It corresponds to the *noninteger quantization of the superfluid density* in a superconductor with gap nodes due to the generation of confined field-induced density waves (CFIDW) over a portion of the Fermi surface (FS). The Landau numbers L are not sufficient to index these macroscopic quantum states and new quantum numbers ζ must be added. Distinct qualitative implications of this $|L,\zeta\rangle$ quantization are evident in a number of puzzling experiments in high-T_c cuprates including the plateaus behavior in the field profile of thermal conductivity, field-induced magnetic moments, charge textures around the vortices, and field-induced vortex-solid to cascade vortex glass transitions.

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I. INTRODUCTION

Despite almost two decades of very intense studies, high-T_c cuprates continue to throw up surprising and chalenging problems for our fundamental understanding of strongly correlated systems. Among the most fascinating challenges is the understanding of their behavior in the presence of a perpendicular to the Cu—O plane magnetic field.[1] Neutron scattering experiments reported the generation of AFM moments inside the SC state by a magnetic field applied perpendicular to the planes.[2] The moments appear suddenly above a critical field and below a critical temperature.[3] NMR measurements have confirmed the phenomenon.[4] Scanning tunneling microscopy results report in the presence of a perpendicular magnetic field a checkerboard structure that covers a region around each vortex.[5] Finally, measuring both heat capacity and magnetization on an extra clean sample of $YBa_2Cu_3O_7$, Bouquet *et al.*[6] not only confirm the presence of an unexplained first-order transition from a vortex lattice to a so-called vortex glass state, but at higher fields they observe a surprising transition from the vortex glass state to a new vortex glass state which has not found any theoretical explanation so far.

A series of seemingly unrelated but equally puzzling phenomene were reported a bit earlier. In a remarkable thermal transport experiment, Krishana *et al.*[7] have reported that, when a magnetic field is applied perpendicular to the CuO_2 planes, the thermal conductivity shows sharp first-order transitions from a field-dependent regime characteristic of gap nodes[8] to a field-independent regime indicating the elimination of the nodes. The results of Ref. 7 stimulated a controversial experimental and theoretical debate which was in fact never closed. Thermal transport measurements by other groups[9–11] have in essence confirmed the surprising findings of Krishana *et al.*[7] Unfortunately, a major group has initially reported that the phenomenon is not present in the "*majority*" of samples,[11] casting doubt on its physical reality. However, recently the same experimental group has finally admitted that the phenomenon is indeed intrinsic,[12] reporting now that the visibility of the plateaus depends on the direction of thermal transport. Very high quality samples are apparently necessary.[13] Controversy has also emerged by the strong hysteretic behavior that was reported in Ref. 9 in disagreement with Refs. 7 and 10. Our theory provides a simple explanation of all controversies and the sample dependence of the occurence of the phenomenon is a major argument for the relevance of our picture.

On the theoretical side, the phase transition point of view has been immediately adopted by Laughlin who suggested that this is a transition from $d_{x^2-y^2}$ superconductivity (SC) to $d_{x^2-y^2}+id_{xy}$ SC (Ref. 14), which is nodeless. Models based on the vortex dynamics have also been proposed,[15] explaining the saturation of the field effect, but they could not account for the "kink" and the sharp character of the transition.

Indications of a field-induced transition to a nodeless state are also present in other experiments. It has been suggested that the field-induced spliting of the zero bias conductance peak in tunnel measurements may be the result of such a transition.[16] More spectacular are recent measurements by Sonier *et al.*[17] of the penetration depth in the presence of a stronger than usually magnetic field. They also confirm the elimination of the nodes by the magnetic field adding a fundamental new element: *The elimination of the nodes is accompanied by a substantial reduction of the superfluid density*.[17] Such a reduction cannot be explained by a phase transition to a new SC state like $d_{x^2-y^2}+id_{xy}$.

In this manuscript we explore an original physical picture which may simultaneously account for *all* these seemingly unrelated puzzling experiments. We reveal a new magnetic field-induced phase transition from a $d_{x^2-y^2}$ SC state to a state in which $d_{x^2-y^2}$ SC *coexists with confined field-induced (spin and charge) density waves (CFIDW) which develop over a portion of the Fermi surface (FS) in the gap node regions*. These new states remind the d-density wave (d-DW) states currently discussed in relation to the pseudogap phase,[18] however they appear only in the presence of a magnetic field and unlike the d-DW states they have their maximum values

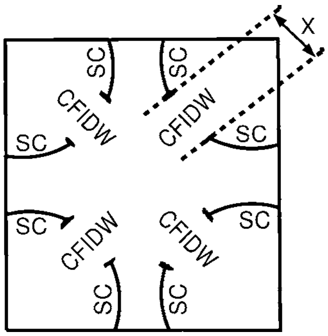

FIG. 1. Schematic view of the competition of the CFIDW with SC over the FS of a typical high-T_c superconductor. In our hybrid approach, region I is the region of the FS occupied by the SC order and region II is the region of the FS occupied by the CFIDW order.

along the nodal directions of the SC gap. We clearly demonstrate that our novel hybrid macroscopic quantum states may become energetically favorable in systems like the cuprates, and consequently they must be taken into consideration when analyzing the magnetic field behavior of superconductors with gap nodes.

Field-induced density waves have been suggested[19–23] in order to explain second order metal-insulator transitions in $(TMTSF)_2X$ (X=PF_6,ClO_4) quasi-one-dimensional synthetic compounds under pressure.[24,25]

II. HYBRID APPROACH

We consider a hybrid approach within a Fermi liquid picture which is valid in this low-temperature part of the phase diagram. Our HTSC system is built of two subsystems: subsystem I is the Fermi surface (FS) region covered by the superconducting gap and subsystem II is a virtual normal quasiparticle region created by the magnetic field and centered in the node points of the FS (cf. Fig. 1). The CFIDW will eventually develop in region II because of the orbital effect of the field in this region. The orbital effect of the field in region I induces vortices that are assumed to be irrelevant. The Zeeman effect is not considered here for simplicity, however in region II it can be shown to further stabilize our CFIDW states while in region I it is negligible. The relative momentum extension of regions I and II is unknown and fixed by the energetic competition of CFIDW with SC. The above picture has some similarity with the partially depaired Fulde-Ferrell-Larkin-Ovchinikov state[26,27] where the normal state is created by the magnetic field over a portion of the Fermi surface and competes with superconductivity.

In HTSC the gap is $d_{x^2-y^2}$ with nodes in the $(\pm\pi,\pm\pi)$ directions where region II is centered. In region II *we necessarily have open FS sheets* showing quasi-1D character at least when the extension of region II is small.[28] Therefore, we can write the dispersion of subsystem II in the form

$$\xi_{\mathbf{k}}^{II} = v_F(|k_1| - k_F) - 2t_2\cos(k_2/X) - 2t_2'\cos(2k_2/X), \quad (1)$$

where X is the unknown momentum extension of region II (see Fig. 1). k_1 is along the $(\pm\pi,\pm\pi)$ directions perpendicular to the open FS sheets of subsystem II, and k_2 is perpendicular to k_1 and therefore along the open FS sheets where we keep only two harmonics without influence on the generality of the results. With respect to the CFIDW states, k_1 is the longitudinal direction while k_2 is the transverse direction.

Our approach is *hybrid* in the sense that to a first approximation we consider the eventual development of region II (i.e., the eventual generation of CFIDW states over a finite region of the FS) as not affecting SC that covers region I. Therefore regions I and II are seen as quasi-independent systems. Such an approximation allows us to treat the otherwise unsolvable problem of the evaluation of the orbital effects in a system in which SC and SDW or CDW coexist on different regions of the same FS. Therefore, within our approach we neglect the influence of the CFIDW on the correlations responsible for the SC pairing and on the magnitude of the SC gap as well. In fact, the density of states is much higher in the antinodal areas of the FS, and to a first approximation one can consider that the SC gap magnitude is only sensitive on the density of states.

Moreover, our hybrid approach is more accurate when the scattering that mediates the superconducting pairing is dominated by the small-q processes. In fact, it has been suggested that small-q pairing may be responsible for d-wave superconductivity in the cuprates[29–31] but also in other unconventional superconductors like organics[32] and heavy fermion[33,34] systems. Phonons may be responsible for the attractive interaction that is dominated by forward scatering when strongly correlated systems are close to instabilities, while at larger wave vectors will dominate an effectively repulsive interaction (the Coulomb pseudopotential) that will in fact impose the nodes. In fact, when small-Q pairing dominates we have the phenomenon of momentum decoupling (MD)[30,32,35] which means a tendency for decorrelation of the SC behavior in the various regions of the FS that results from the reduction of the mixing scattering between different FS regions. This induces a loss of rigidity of the momentum structure of the gap and other phenomena that may account for puzzling anomalies observed in the cuprates[30] and also in organic SC.[32] In the limit of perfect MD, our hybrid hypothesis would be exact.

Within our hybrid picture, subsystem II is like a *quasi-one-dimensional* independent system having the dispersion of Eq. (1), the only difference being that *the size of its effective Brillouin zone X is an unknown variational parameter*. In these conditions, we are able to calculate explicitly the spin and charge susceptibility of subsystem II in the presence of the magnetic field exploiting methods developed for the study of $(TMTSF)_2X$ compounds[20,21] which were modeled with the same electron dispersion. Our CFIDW states in region II result from the same mechanism that generates the FISDW states in these last compounds.

In our Fermi liquid approach, a density wave in region II will develop if the zero frequency limit of the dynamic spin or charge correlation function

$$\chi(\mathbf{Q},\omega) = \frac{\chi_o(\mathbf{Q},\omega)}{1 - \lambda\chi_o(\mathbf{Q},\omega)} \quad (2)$$

will eventually diverge. In the above, as usual $\chi_o(\mathbf{Q},\omega)$ is the susceptibility of noninteracting electrons. When such an instability will occur, we will respectively have either both spin rotational and translation symmetries spontaneously broken leading to SDW or only the translational symmetry broken that leads to CDW. In this broken symmetry situation, a mean-field approach is adopted as usual with the CDW or SDW gap proportional to the off-diagonal terms of the effective propagator. Constraining the nesting in the $(\pm\pi,\pm\pi)$ directions one can show that a first-order field-induced density wave gap in region II is given by

$$\Delta_{DW}=W\exp\{-[gN(E_F)I_L^2(X)]^{-1}\}, \quad (3)$$

where

$$I_L(X)=\sum_n J_{L-2n}\left(\frac{4t_2X}{eHv_F}\right)J_n\left(\frac{2t_2'X}{eHv_F}\right). \quad (4)$$

Here $J_n(x)$ are Bessel functions of the first kind, L is the index of the Landau level configuration, e is the charge of the electron, H is the magnetic field, $N(E_F)$ is the density of states at the Fermi level (in region II), g is a scattering amplitude of Coulombic or phononic origin, W is the bandwidth in the (π,π) direction, and v_F is the Fermi velocity. Higher-order gaps are not reported here for sake of clarity.

The physical mechanism behind this field-induced density wave formation is similar to that in Bechgaard salts. If region II has a finite extension with a corresponding finite density of carriers, the corresponding Fermi surface sheets are necessarily open, exhibiting in fact a quasi-one-dimensional character. However, in the absence of a magnetic field there is no nesting of the Fermi surfaces that constitute subsystem II. When the magnetic field is applied the electronic motion is bounded and periodic in real space. This reduces the effective dimensionality of the electronic motion producing in subsystem II the nesting properties that characterize a one-dimensional electronic system. The nesting wave vector that corresponds will be the characteristic wave vector of our field-induced density modulations.

III. COMPETITION OF CFIDW WITH SUPERCONDUCTIVITY

While in our hybrid approach CFIDW may eventually develop in region II, a nonzero extension of region II over the FS and thus the presence of CFIDW in the real system will depend on the competition of the CFIDW with SC. The CFIDW states will develop over a finite portion of the FS only if the condensation free energy gain of the system due to the opening of a CFIDW gap in region II is bigger than that lost by the elimination of SC from this region. The condensation free energy when d-wave SC coexists with a SDW over the whole FS has been reported by Kato and Machida.[36] In our hybrid picture regions I and II are considered independent and therefore one has to compare the condensation free energy of SC and CFIDW in region II, bearing in mind that only the dominating order will be present in that region. We assume that the superconducting gap Δ_{SC} has d-wave symmetry and is given to a good approximation by $\Delta_{SC}=\Delta_{sc}\sin(\theta)$ where θ measures rotations in the plane around the corners of the original Brillouin zone (the $(\pm\pi,\pm\pi)$ points). We define a dimensionless parameter Z that varies from 0 to 1 and represents *the percentage of the FS that is occupied by region II (i.e., by the CFIDW)*. Indeed, Z has a direct relationship with X:

$$X\approx k_F\sin(Z\pi/2)Z \quad (5)$$

With the above assumptions the condensation free energy that may be lost by the eventual elimination of superconductivity from region II is given to a first approximation by

$$\delta F_{SC}=\frac{1}{2}\int_{-Z\pi/2}^{Z\pi/2}\Delta_{sc}^2\sin^2(\theta)d\theta=\frac{1}{4}\Delta_{sc}^2[\pi Z-\sin(\pi Z)]. \quad (6)$$

On the other hand, we assume that the CFIDW gap is θ independent over region II, and, therefore, the condensation free energy associated with the opening of the CFIDW gap in region II is to a first approximation $\delta F_{DW}=(1/2)\pi Z\Delta_{DW}^2$. Only if $\delta F_{DW}>\delta F_{SC}$ in region II the CFIDW will develop. This condition, taking into account Eqs. (3) and (4) implies the following inequality:

$$I_L^2[k_F\sin(Z\pi/2)]>\frac{2}{gN(E_F)}\left(\ln\frac{2W^2\pi Z}{\Delta_{sc}^2[\pi Z-\sin(\pi Z)]}\right)^{-1}. \quad (7)$$

Moreover, the CFIDW state must be *confined in momentum space* with a DW gap smaller or equal to the absolute superconducting gap in the borders of region II. We therefore have

$$I_L^2[k_F\sin(Z\pi/2)]\leqslant\left(gN(E_F)\ln\frac{W}{\Delta_{sc}\sin(Z\pi/2)}\right)^{-1}. \quad (8)$$

The continuity in the momentum space variations of both SC and CFIDW gaps implies that on the border of regions I and II these gaps should be equal. In fact, if they were not equal and for example the SC gap in the region I side of the border is smaller than the CFIDW gap in the region II side of the border, the continuity of the gap variation would imply that the SC gap would be smaller than the CFIDW gap in a finite domain of region I sufficiently close to the border. If this was the case, then it would be energetically favorable for the system to have the larger CFIDW gap rather than the smaller SC gap on this finite border domain of region I. But region I is defined as the region occupied by the SC gap, and this would correspond in fact to a shift of the border. In conclusion, the equality in (8) fixes the relative extension Z of the CFIDW (for each L) and therefore $I_L^2[k_F\sin(Z\pi/2)]$ which then fixes the CFIDW gap Δ_{DW} and the critical temperature Δ_{DW} at which the CFIDW forms.

A graphic of Eq. (8) for Z is shown in Fig. 2(b). Surprisingly, there are two possible values of Z for a given Landau level configuration. Therefore, the Landau numbers L are not sufficient to index our quantum states. A *new quantum number* ζ, associated with the two possible momentum extensions Z for each L configuration, must be added. Physically ζ will index *the quantization of the superfluid density*. In fact,

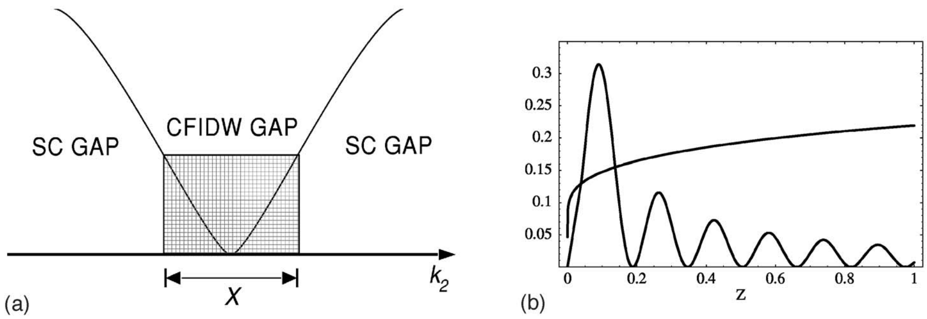

FIG. 2. (a) Schematic view of the SC-CFIDW competition. (b) Graphic solution of Eq. (8) in the $L=1$ configuration and a field of 3 T. Two different relative extensions Z $[X \approx k_F \sin(Z\pi/2)]$ of the CFIDW are possible.

each quantized value of Z corresponds to a different relative extension of the SC region over the FS and therefore to a different density of superfluid carriers.

IV. CFIDW AND THE MAGNETIC FIELD ANOMALIES IN HIGH-T_c CUPRATES

Using for our parameters values extracted from the experiments on HTSC and a conventional scattering $gN(E_F) \approx 1$ we obtain results like those reported in Figs. 3(a) and 3(b) in remarkable agreement with the data of Refs. 7 and 17. In Fig. 3(a) is reported the dependence of Δ_{DW} on the magnetic field in the various $|L,\zeta\rangle$ configurations. We also plot in this figure the experimental points of Refs. 7 and 17. In Fig. 3(b) we plot the corresponding magnetic field dependence of the accessible relative extensions Z of the CFIDW in each $|L,\zeta\rangle$ configuration for the same parameters. The higher values of Z for each L configuration appear to be more relevant. Indeed the smaller Z values would correspond to larger in real space cyclotron orbits and therefore would be discriminated by impurities or defects.

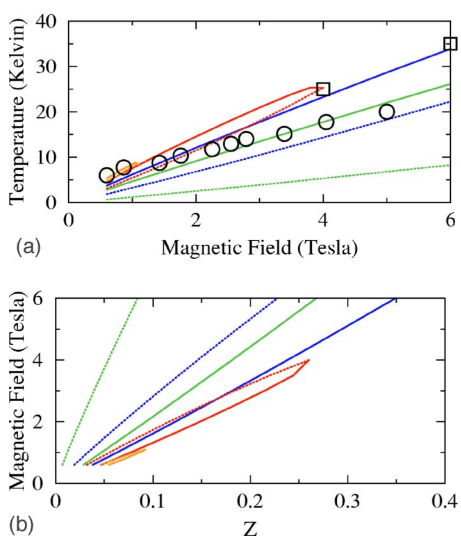

FIG. 3. (Color online) (a) Critical temperature T_{DW} versus critical field for the formation of a CFIDW state in the different quantum configurations $|L,\zeta\rangle$: $L=4$ (orange), $L=3$ (red), $L=2$ (blue), and $L=1$ (green). In all L configurations, full lines and dotted lines correspond to the two different ζ configurations (full lines to the higher Z solution). The $L=0$ lines are not shown for clarity. The open circles are the corresponding thermal transport experimental points of Krishana *et al.*[7] and the open squares are extracted from the penetration depth measurements of Ref. 17. (b) Relative extensions Z of the CFIDW over the FS, versus the magnetic field, for the various $|L,\zeta\rangle$.

Figure 3(a) indicates that when at a given temperature, for example at 20 K, we enhance gradually the field, at a field of a bit less than 3 T the $L=3$ configuration (with the higher ζ) is the first CFIDW state that develops. For a sample not sufficiently clean, we would expect the system to remain "locked" at that configuration even at higher fields because it corresponds to the larger momentum extension of the CFIDW [cf. Fig. 3(b)] at that temperature. However, for a very clean sample in which the mean free path is much larger than the cyclotron orbits, the system would jump to the first configuration that will become accessible at a higher field (the $L=3$ with the smaller ζ at a bit more than 3 T) because in that way, the CFIDW extension being smaller, the system will have on average a bigger gap over the regions I and II and therefore a lower free energy. At higher fields jumps to the other configurations [accessible by a horizontal cut in Fig. 3(a)] are expected until the effect of impurities becomes significant for very large cyclotron orbits (small momentum extensions).

A quantitative fit of the experiments as in Fig. 3 establishes that the orders of magnitude of the involved parameters are compatible with the experimental data. More importantly, there are distinct qualitative experimental facts which strongly support our picture. As one can see in Fig. 3(a), the T_{DW} versus critical magnetic field profile of the data in Ref. 7 (circles) show a "*reptation*" shape. The first two points have a bigger field slope than the next two points and so on. To the best of our knowledge, no explanation of the reptation behavior has been reported so far. Within our analysis this "reptation" profile is due to the *quantization* of the CFIDW states. Each slope corresponds to a different $|L,\zeta\rangle$ quantum configuration of the system. The higher the field is, the smaller is the field slope in agreement with the experiment. Moreover, if one associates the vortex solid to vortex glass transition with the SC to SC+CFIDW transition, one naturally understands *the unexplained vortex glass I to vortex glass II transition of Bouquet et al.*[6] *as a transition between two different* $|L,\zeta\rangle$ *configurations of the* SC+CFIDW *state*. The higher field $|L,\zeta\rangle$ state corresponds to a higher relative extension of the CFIDW state and therefore a less rigid vortex structure as is experimentally observed. Alltogether, this provides the first microscopic viewpoint for the origin of the vortex glass states. Moreover, recent thermal expansivity measurements report discontinuities at the vortex melting transition[37] indicating a major role played by the microscopic charge degrees of freedom as in density wave states like the ones we report.

The remarkable sensitivity of the occurence of this phenomenon on sample quality[11,13] further corroborates our picture. Within our analysis, a small magnetic field affects the large SC gap of HTSC creating CFIDW's in the node region *because of momentum confinement* which constrains the cyclotron orbits to be large in real space and consequently the involved flux is large as well. The occurrence of the CFIDW's *requires very clean samples* because the mean free path must be bigger than the cyclotron orbits. Samples which may appear of high quality from the usual criteria (width of the SC transition or magnitude of the SC T_c) may not be sufficiently clean to support large cyclotron orbits and show the CFIDW states. This explains the puzzling sample dependence of the occurence of the phenomenon. The minimum field at which the phenomenon is observable is also limited by sample defects because if fields are too small, momentum extensions of the CFIDW are also too small [see Fig. 3(b)] and consequently the required cyclotron orbits are too large. Our $d_{x^2-y^2}$ to $d_{x^2-y^2}$+CFIDW transition appears only above 1 T in Ref. 9 while it is already present at 0.6 T in Ref. 7 because samples in Ref. 7 are cleaner, admitting bigger cyclotron orbits. Because all $|L,\zeta\rangle$ configurations are nearly degenerate for the total system, the occurence of magnetic hysteresis on a dynamic probe like thermal transport will depend on the exact conditions of the magnetic cycle and on sample quality as well. In the magnetic cycle of Ref. 9 showing hysteresis, the field orientation is reversed when the field maxima are reached (the field passes through zero), while in Refs. 7 and 10 this is not the case and hysteresis is absent.

Our analysis is also the first to establish a natural relationship between the thermal transport[7] and penetration depth[17] puzzles. In Ref. 17 CFIDW's develop at a much higher T_{DW} for a given field than in Ref. 7 because the system is cooled in the presence of the magnetic field. By field cooling the sample, the first accessible $|L,\zeta\rangle$ configuration is the one with the higher T_{DW} which also corresponds to the higher Z [cf. Fig. 2(b)]. On the other hand, in the experiment of Ref. 7, the temperature is kept constant when the field varies. Not only do we reproduce simultaneously the experimental T_{DW} versus field profiles of both Refs. 7 and 17, but we also account for the reduction of the superfluid density reported in Ref. 17. As one can see in Fig. 2(b), in the regime 4–6 T explored in Ref. 17, the CFIDW occupy about a quarter of the FS ($Z\approx 0.25$ to 0.35) which is in very good agreement with the $\approx$15% to 25% reduction of the superfluid density reported in Ref. 17. We must note here that alternative explanations of the muon-spin rotation experiments of Ref. 17 that do not invoke the opening of a gap as we suggest have also been proposed in the literature.[38]

Furthermore, our CFIDW states correspond to a real space pattern that has all the characteristics of the one observed by STM.[5] Moreover, one of the most debated issues about the field-induced AFM moments reported by neutron experiments[2] is their incommensurate nature. Within our picture this incommensurability has a natural explanation. In fact, the characteristic wave vectors of our field-induced density waves are the nesting wave vectors of subsystem II, which are indeed expected to be incommensurate.[28] At this point we must stress that our analysis, as it stands, corresponds to the behavior of the optimally doped cuprates.[2] For the underdoped cuprates it would be interesting to explore in a future work the interplay of our mechanism for field-induced density waves with the various proposed pictures for the pseudogap that exists above the superconducting T_c.

Finally, in agreement with all the experiments, our CFIDW states appear *only for fields perpendicular to the planes* because for fields parallel to the planes cyclotron effects are irrelevant.

V. CONCLUSIONS

In conclusion, we have shown that in a superconductor with gap nodes, CFIDW states may develop over a finite portion of the FS around the nodes coexisting with the SC that occupies the rest of the FS. This leads to a number of novel macroscopic quantum phenomena related to the non-integer quantization of the relative extension over the FS of the CFIDW and SC states. We argue that these phenomena may be behind the unexplained features observed in the field behavior of high-T_c cuprates. For example, we show that characteristic anomalies of the thermal transport in the presence of a perpendicular magnetic field in these materials may be simultaneously understood with the penetration depth measurements that report a reduction of the superfluid density that accompanies the observed transition to a nodeless state. A series of additional seemingly unrelated puzzling phenomena may corroborate the relevance of our picture in the cuprates.

Moreover, similar magnetic field puzzling phenomena appear to be present in the quasi-two-dimensional synthetic compounds $\kappa-(BEDT-TTF)_2Cu(NCS)_2$ which have numerous similarities with the cuprates including indications for a d-wave gap.[39] For example, it is reported there as well the reduction of the superfluid density that accompanies the elimination of the gap nodes.[40] On the other hand, the absence of the phenomenon in a similar experiment on the same material by another group[41] may be simply explained within our picture by a lower sample quality that prevents the manifestation of our macroscopic quantum phenomena. We are confident that dedicated specifically designed experiments may find direct evidence of the quantization of the superfluid density and prove the validity of our picture in the above materials.

Our analysis demonstrates that CFIDW states are energetically plausible, and must therefore be taken into consideration as a possibility whenever we analyze field phenomena in superconductors with gap nodes.

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