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Quantum oscillations in the underdoped cuprate

M.A. Mojumder *

Flat No.201, First A Main, ST Bed Layout, Kormangala 4th Block, Bangalore 560034, India

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ABSTRACT

Quantum oscillations occur via Landau quantisation of the quasiparticle in a Fermi liquid at low temperature. In the light of currently popular notions their detection in the ortho-II-$YBa_2Cu_3O_{6.45}$ and $YBa_2Cu_4O_8$ crystals is inconsistent with this. We explain this in terms of multichannel Kondo model of the underdoped cuprate.

1. Quantum oscillation in the cuprate

de Haas–van Alfven oscillation (dHvA) experiments have been performed on two underdoped high-T_C cuprates (HTC), $YBa_2Cu_4O_8$ (YBCO:124), Ref. [1], and ortho-II-$YBa_2Cu_3O_{6.45}$ ($YBCO_{6.45}$), Ref. [2], at low temperature. Shubnikov–de Haas (SdH) experiments performed on the same crystals, YBCO:124, Ref. [3], and ortho-II-$YBa_2Cu_3O_{6.45}$, Ref. [4], gave generally consistent data. All the crystals used were more than usually disorder-free. The data of Ref. [1] and Ref. [3] for YBCO:124 do not agree well with those of the rest. An important finding is the indication [1] that the source of the oscillation signal is hole Fermi pockets for YBCO:124. The data for $YBCO_{6.45}$ shows [5] the source to be electronic Fermi pockets. These pockets, electronic or hole, appear in the four nodal directions but away from the nodes themselves. The consensus is that the electronic pocket is the general rule for the HTC while the hole pocket is an exception for YBCO:124. In general, the data have been interpreted successfully via the Liftshitz–Kosevich theory which shows quantum oscillations occurring in clean 2D Fermi liquids. The problem here is to find theoretically the Fermi pockets with appropriate charge in the underdoped pseudogap regime at low temperature. Conventional wisdom expects this regime to be a hole non-Fermi liquid. The detailed structure of the pseudogap where these experiments were performed has not been agreed upon in general. There are other problems too even if one accepts the presence of electronic Fermi pockets in the pseudogap.

The metal–nonmetal transition from the parent crystal at low temperature, say, T_M has been expected to lead to a hole Fermi liquid. This is a conventional (one channel) Kondo transition [6] at low energy found by numerical simulation if the parent crystal is taken to be a disordered paramagnet [7,8]. Evidence for the corresponding one channel Kondo fixed point (KFP) exists [9–12]. Evidence for coexisting two channel KFP [13–15] is mentioned in the sequel. Ref. [8] shows the actual crystal undergoing the metal–nonmetal transition to be a spinglass-like disordered paramagnet rather than an antiferromagnet. As a Fermi liquid cannot confront all the rest of the data that indicate non-Fermi liquid also we consider the transition to have a two channel Kondo component in the metal–nonmetal transition. This KFP is known to be a non-Fermi liquid. So one has here a case of coexistence of one and two channel KFPs at low temperature or a competition between the two fixed points for the ground state, a characteristic of electronic correlation. Of course, there are other approaches based on older theories of transition to the 'normal' state. Of these even the most popular ones are not up to the diverse and complex data that have accumulated over the years. In any case, we are unaware of a simple, unified and widely consistent approach based on the current theories that is able to deal with all the data.

The foregoing picture is not fully consistent with data. There is the further difficulty of the apparent violation [5] of the Luttinger sum rule which requires in this case the total carrier density to equal the total area of the 2D Fermi surface. From the oscillation frequency of 530 T found in the SdH experiment [5] with a particular crystal the calculated carrier density was 0.03 per planar Cu atom per electronic pocket. This number was equivalent to the carrier density of about 15% of the total of the four nodal electronic pockets. The four pockets have been detected by ARPES. A fraction of about 10% was expected here as the current Hubbard model-based theories would assume the number of delocalised Cu ions to equal the number of doped holes which is given by $p = 0.1$ in this case. In the Kondo theory-based approach that we propose here the former number may exceed the latter via the mechanism of

* Tel.: +91 80 25631655.
E-mail address: mamojumder@gmail.com.

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'exhaustion' [6] though possibly not as much [24] as was thought earlier. To our knowledge, no extra sheet of the Fermi surface has been detected which could enable an explanation of the difference between the two numbers in the conventional manner.

2. The two channel Kondo fixed point

The subject of two channel Kondo effect is not very well known nor it is usual to assume Kondo effect in the HTC. We include the following brief discussion of the notion and formalism of the effect as well as justify Kondo effect. We hardly use the formalism though we discuss it here briefly. For the late transition metal compounds that include the HTC, one can take [25] the local structure of the 3D open shell in a crystal field to have more dominant effect than the translation symmetry for energy scales of the order ~ 0.2–4 eV. Optical photoconductivity experiments for such compounds indicate strong local charge conservation. The d–d part of the optical spectra of the material has been found to be very similar to the optical spectra of ions in solution. It is believed that Kondo effect is due to the strong correlation in the HTC. Also, here the orbital effect is quenched by the crystal field. If Hubbard $U \approx D$ where D is the conduction band width Kondo effect is likely. The d-band compound LiV_2O_4 has been found with heavy fermion compound (HFC) behaviour. Considering the uncertainties one way is to look for experimental evidence. In view of the above there is at least a tentative justification in using the following equation (1) [13,14] for two channel Kondo model taking only the spin which is taken to be a local Kondo 'impurity',

$$H_2 = \sum_a \sum_{\sigma=1,2} \big[H_0\big(\psi^{\diamond}_{a\sigma}, \psi_{a\sigma}\big) + \sum_{i=x,y,z} J_i S^i \psi^{\diamond}_{a\alpha}(0)\sigma^i_{\alpha\beta}\psi_{a\beta}(0)\big],$$
$$\psi^{\diamond}_{a\alpha}(0)\sigma^i_{\alpha\beta}\psi_{a\beta}(0) \equiv \sigma^i. \tag{1}$$

This is a spin-only Hamiltonian which is accepted for the first transition series where the orbital effects are negligible. Here $a = (1,2)$ for doubly-degenerate conduction band with kinetic energy, $H_0(\psi^{\diamond}, \psi) = \sum_k \varepsilon_k \psi^{\diamond}_k \psi_k$; it is also the channel index of the 'impurity'. The usual 'dagger' symbol has been replaced here by the 'diamond' symbol for convenience. The second term in the square bracket is the Kondo term. $S = \frac{1}{2}$ is the pseudospin of the Cu^{2+} ion which is the 'impurity' here. σ is the spin of the conduction electrons and is 'up' or 'down'. The solution [13,14] of this Hamiltonian has been achieved for a single 'impurity' by a generalisation of the resonant-level model used earlier by Anderson and Yuval for the one channel Kondo model. The solution has been found only for a particular value of J_Z which corresponds to the Kondo scattering phase shift $= \pi/2$, the Emery–Kivelson (EK) point [13].

We have assumed the two channel Kondo transitions of the crystal at T_M, Fig. 1; there is evidence for simultaneous high temperature transition [26,27,19] of a single-site Kondo 'impurity', say, at $T_K \approx 1$ eV and higher. This high temperature would become considerably smaller [6,24,20], say, $\tilde{T}_K \approx 1500$ K at optimal doping for a coherent crystal of Kondo 'impurities', the Kondo lattice.

There being no intrinsic reason why the Kondo couplings of the two channels should be exactly symmetric, Eq. (1), the corresponding fixed point should be fully unstable. That is, the two channel KFP would not exist. But surprisingly, there are at least two important early pieces of experimental data that are quite compelling in favour of the effectiveness of the two channel KFP for the normal state once Kondo effect is accepted. They are (i) the detection [28,29] of the $\rho_{ab} \propto |\ln(T/\tilde{T}_K)|$ rule and its behaviour for change of the impurity level, (ii) the nature of the variation of an NMR parameter [30], say, $R \equiv 1/T^{63}T_1$ with temperature. The resistivity rule is the most well-known signature of two channel KFP. And R plotted against T shows a broad peak at low temperature which drops for both lower and higher temperatures. Since

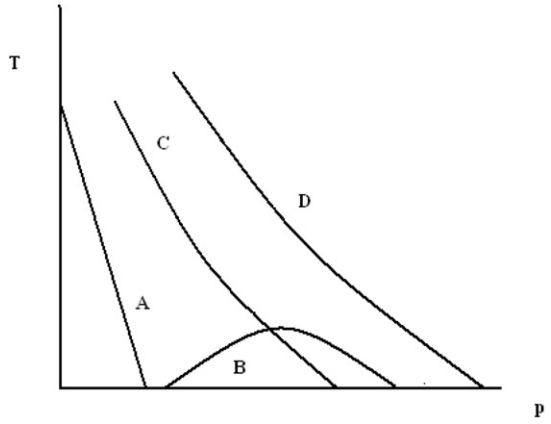

Fig. 1. Illustrative p–T phase diagram [16–22] of the cuprate. It shows the relevant transition lines and the KFP regimes. The symbols A, B, C, D have the following meanings: $A \equiv T_M$, $B \equiv T_C$, $C \equiv \tilde{T}^l_{KC}$, $D \equiv \tilde{T}_K$. The main evidence for the transition temperatures $\tilde{T}^l_{KC}$ and $\tilde{T}_K$ is Ref. [45]. This references provide the direct evidence; the indirect evidence are all discussed in Refs. [16–22]. The references rarely provide support for the full length of the transition curves. Such curves are either extrapolations or supported by other diverse data in the literature.

the higher temperature end is definitely known as a non-Fermi liquid the lower temperature end cannot be the same. It is usually a Fermi liquid. So a channel transition is strongly indicated if the two channel model is accepted. The primacy and robustness of local Coulomb scattering [31] between the carriers as well as between the carriers and doped holes suggests strong likelihood of the two channel Kondo effect under the circumstances [32]. However, the large number of outstanding data [16–23] that can be rationalised via the two channel model with varying levels of strength and specificity is possibly the best evidence [33] for the latter. A general comment in this reference in another context posits that even if no rigorous theoretical derivation can be given for a postulate it can still be justified by comparison with data much like the Fermi liquid theory.

We argue here that the two channel KFP is only weakly unstable and, therefore, effective. A pedestrian argument can be used [17] to show an enhancement of the energy scale $\tilde{T}_K$ due to defect disorder which would effectively render the symmetry-breaking model Hamiltonian, Eq. (2) below, insignificant. It has been shown [34] that even the nominally 'pure' common HTC crystal has a substantial amount of defect disorder which has the effect of enhancing the stability of the two channel KFP by raising $\tilde{T}_K$. The effectiveness of the two channel KFP has been emphasized [35] despite its expected instability. The important effective role of 'unstable' fixed points, the well-known examples being the Fermi liquid and the Kondo lattice, intervening between stable phases has been stressed [36]. A numerical study [37] of the two channel model in the manner of Wilson has shown the comparative stability of the model at higher temperatures. That strong correlation is due to Kondo effect appears to be gaining consensus. The two channel KFP that we advocate may thus be taken as a weakly unstable intermediate phase that is effective between the high temperature and low temperature stable paramagnetic phases. This weak instability leads to a very slow channel transition of the two channel KFP commencing at, say, $\tilde{T}^l_{KC} \approx 90$ K for close to but lesser than optimal doping, Fig. 1. $\tilde{T}^l_{KC}$ $(T = 0)$ has to be taken as a Kondo quantum critical point (QCP). The regime $T < \tilde{T}^l_{KC}(p)$, $p(T = 0) < 0.19$ is the pseudogap, Fig. 1.

The realistic two channel model has to take account of a suitable additional symmetry-breaking Hamiltonian enabling channel anisotropy that leads to the transition to the stable one channel model, i.e. the channel transition. Such a Hamiltonian that is added