Magnetic properties of lightly doped antiferromagnetic YBa$_2$Cu$_3$O$_y$.

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The present work addresses YBa$_2$Cu$_3$O$_y$ at doping below $x = 6\%$ where the compound is a collinear antiferromagnet. In this region YBa$_2$Cu$_3$O$_y$ is a normal conductor with a finite resistivity at zero temperature. The value of the staggered magnetization at zero temperature is $\approx 0.6\mu_B$, the maximum value allowed by spin quantum fluctuations. The staggered magnetization is almost independent of doping. On the other hand, the Neel temperature decays very quickly from $T_N = 420\,K$ at $x = 0$ to practically zero at $x \approx 6\%$. The present paper explains these remarkable properties and demonstrates that the properties result from the physics of a lightly doped Mott insulator with small hole pockets. Nuclear quadrupole resonance data are also discussed. The data shed light on mechanisms of stability of the antiferromagnetic order at $x < 6\%$.

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I. INTRODUCTION

It is well known that cuprates are layered compounds consisting of CuO$_2$ planes and there are no doubts that the generic physics of cuprates are related to the CuO$_2$ plane. In spite of the same generic physics specific properties of cuprates can be very different depending on crystal structure, ways of doping etc. The goal of the present work it to shed light on the generic physics via understanding of specific properties of lightly doped antiferromagnetic YBa$_2$Cu$_3$O$_y$ (YBCO).

Cuprates are essentially doped Mott insulators. It is well established that a Mott insulator possesses a long range antiferromagnetic (AF) order, therefore, one of the generic problems is how the AF order evolves with doping. Another generic problem is the shape of the Fermi surface. Are there small hole pockets as one expects for a very lightly doped Mott insulator, how the surface evolves with doping?

Cuprates are intrinsically disordered materials because of mechanisms of doping. Disorder complicates a theoretical analysis of experimental data usually masking the generic physics. YBCO is probably the least disordered part of a very weak logarithmic temperature dependence expected for a weak disorder. The heat conductivity also indicates delocalization of holes. This is very much different from La$_{2-x}$Sr$_x$CuO$_4$ where holes are localized and hence the compound is an Anderson insulator at $x \lesssim 0.15$. Ultimately, at the very low doping, $x \lesssim 0.01$, the disorder wins even in YBCO and it also becomes the Anderson insulator. It is helpful to have in mind an approximate empiric formula

$$x \approx 0.35(y - 6.20)$$

(1)

to relate the doping level $x$ and the oxygen content $y$ in underdoped YBCO at $x \lesssim 0.12$.

The static “staggered” magnetization in YBCO has been recently measured in the $\mu$SR experiment. The experimental plot of the zero temperature magnetization versus doping is shown in Fig. 1 (top). Remarkably the zero temperature magnetization is almost doping independent up to $x \approx 0.06$ and then it quickly decays. It is known from neutron scattering experiments that the static magnetization fully disappears at the Quantum Critical Point (QCP) $x \approx 0.09$ indicating transition

![Figure 1](image.png)
to a state without static magnetism. Importantly, the magnetism at $x > 0.06$ is incommensurate, this is why in the first sentence of this paragraph I put “staggered” in inverted commas. Value of the incommensurate wave vector $Q$ divided by $2\pi$ versus doping is plotted in Fig. 2.

![FIG. 2: (Color online). Incommensurate wave vector versus doping. The blue square, the red circle, and the red diamond show neutron scattering data. The solid line shows the theoretical value.](image)

While in the collinear antiferromagnetic phase the zero temperature staggered magnetization is almost independent of doping, the Neel temperature decays very quickly from $T_N = 420K$ at $x = 0$ to practically zero at $x \approx 6\%$. This is shown in Fig. 1 (bottom) copied from Ref. 8. The present paper explains these puzzling magnetic properties and shows that they are related to small hole pockets of lightly doped Mott insulator.

YBa$_2$Cu$_3$O$_y$ is doped via filling oxygen chains located above the CuO$_2$ planes. It has been argued that at $y = 6.5$, where the every second chain is full, the chain modulation causes the corresponding charge density wave (CDW) of in-plane holes. Nuclear quadruple resonance (NQR) for in-plane Cu is an excellent local probe of the hole density. Fig. 3 shows $^{63}$Cu NQR frequency sweeps from Ref. 18 for several values of oxygen content. There is a single narrow line at about optimal doping $y \approx 6.4$ indicating a very homogeneous hole density corresponding to completely filled chains. On the other hand, at $y \approx 6.5$ there are two distinct lines indicating a bimodal hole density distribution in agreement with Refs. 15-17. Importantly, the bimodal distribution is evident even at lower doping, $y = 6, 4, 6.45$, indicating the CDW induced by the oxygen chain superstructure. Below $y = 6.5$ the NQR lines are broader compared to $y = 6.5$. This is because the oxygen superstructure with every second chain filled cannot be perfect away from $y = 6.5$. It is worth noting that holes go to the CuO$_2$ plane only at $y > 6.2$, see Eq. (1). In the undoped case, $x = 0, y < 6.2$, there is only one NQR line with frequency $\nu_0 \approx 23.3 MHz$ independent of $y$, see Ref. 19. Comparing $\nu_0$ with frequencies of lines in Fig. 3 we see that the hole doping shifts the NQR frequency very strongly.

The present paper explains significance of the chain induced CDW for stability of the collinear antiferromagnetic phase at $x < 0.06$.

Structure of the paper is the following. The effective theory describing YBCO at low doping was formulated before in Ref. 14. Section II summarizes ideas of the effective theory. In Section III the theory is applied to calculate reduction of the staggered magnetization in the antiferromagnetic phase at zero temperature. Temperature reduction of the staggered magnetization at zero and nonzero doping, $0 < x < 0.06$, is calculated in Section IV. Interplay between the chain induced CDW, small hole pockets, and stability of the collinear antiferromagnetic phase is discussed in Section V. Section VI presents conclusions of the paper.

II. EFFECTIVE LOW ENERGY THEORY DESCRIBING LIGHTLY DOPED YBCO

This section summarizes the most important points of the effective low energy suggested in Refs. 14, 20 to describe YBCO at low doping. The analysis is based on the two-dimensional $t - t' - t'' - J$ model at small doping. The generic case of the single layer has been considered in Ref. 20. After integrating out the high energy fluctuations one comes to the effective low energy action of the model. The effective low-energy Lagrangian is written in terms of the bosonic $\vec{n}$-field ($\vec{n}^2 = 1$) that describes the staggered component of the copper spins, and in terms of fermionic holons $\psi$. The term “holon” is used instead of “hole” to stress that spin and charge are to large extent separated, see Ref. 20. The holon has a pseudospin that originates from two sublattices, so the fermionic field $\psi$ is the spinor in the pseudospin space. Minimums of the holon dispersion are at the nodal points $q_0 = (\pm \pi/2, \pm \pi/2)$. So, there are holons of two types corresponding to two pockets. The dispersion in a pocket is somewhat anisotropic, but for simplicity let us use here the isotropic approximation, $\epsilon (p) \approx \frac{1}{2} p^2$, where $p = q - q_0$. The lattice spacing is set to be equal to unity, 3.81 Å $\rightarrow$ 1. All in all, the effective Lagrangian...
for the single layer reads\(^1\)

\[
\mathcal{L} = \frac{\chi_\perp}{2} \vec{n}^2 - \frac{\rho_s}{2} (\nabla \vec{n})^2 + \sum_\alpha \left\{ \frac{i}{2} \left[ \psi_\alpha^\dagger D_t \psi_\alpha - (D_t \psi_\alpha)^\dagger \psi_\alpha \right] - \psi_\alpha^\dagger \mathcal{E}(\mathcal{P}) \psi_\alpha + \sqrt{2}g (\psi_\alpha^\dagger \vec{s} \psi_\alpha) \cdot [\vec{n} \times (e_\alpha \cdot \nabla) \vec{n}] \right\}.
\]

The first two terms in the Lagrangian represent the usual nonlinear \(\sigma\) model. The magnetic susceptibility and the spin stiffness are \(\chi_\perp \approx 0.53/8 \approx 0.066\) and \(\rho_s \approx 0.175\).\(^2\) Hereafter the antiferromagnetic exchange of the initial \(t-J\) model is set to be equal to unity,

\[ J \approx 130 \text{ meV} \rightarrow 1. \]

Note that \(\rho_s\) is the bare spin stiffness, therefore by definition it is independent of doping. The rest of the Lagrangian in Eq. (2) represents the fermionic holon field and its interaction with the \(\vec{n}\)-field. The index \(\alpha = a, b\) indicates the pocket in which the holon resides. The pseudospin operator is \(\frac{1}{2} \vec{\sigma}\), and \(e_\alpha = (\pm 1/\sqrt{2}, 1/\sqrt{2})\) is a unit vector orthogonal to the face of the magnetic Brillouine zone (MBZ), where the holon is located. The argument of \(e_\alpha\) in Eq. (2) and the time derivative of the fermionic field in the same equation are “long” (covariant) derivatives,

\[ \mathcal{P} = -i \nabla + \frac{1}{2} \vec{\sigma} \cdot [\vec{n} \times \nabla \vec{n}] \]

\[ D_t = \partial_t + \frac{i}{2} \vec{\sigma} \cdot [\vec{n} \times \nabla \vec{n}] \].

The covariant derivatives reflect gauge invariance of the initial \(t - t' - t'' - J\) model.

Numerical calculations within the \(t - t' - t'' - J\) model with physical values of hopping matrix elements give the following values of the coupling constant and the inverse mass, \(g \approx 1\), \(\beta \approx 2.4\). The value of the inverse mass \(\beta = 2.4\) corresponds to the effective mass \(m^* = 1.8m_e\). The dimensionless parameter

\[ \lambda = \frac{2g^2}{\pi \beta \rho_s} \]  \hspace{1cm} (3)

plays the defining role in the theory. If \(\lambda \leq 1\), the ground state corresponding to the Lagrangian (2) is the usual Néel state, the state is collinear at any small doping. If \(1 \leq \lambda \leq 2\), the Néel state is unstable at arbitrarily small doping and the ground state is a static or a dynamic spin spiral. The wave vector of the spiral is

\[ Q = \frac{g}{\rho_s}x. \]  \hspace{1cm} (4)

If \(\lambda \geq 2\), the system is unstable with respect to phase separation and/or charge-density-wave formation and hence the effective long-wave-length Lagrangian (2) becomes meaningless. The pure \(t - J\) model \((t' = t'' = 0)\) is unstable since it corresponds to \(\lambda > 2\).

To find parameters of the effective action (2) one can rely on calculations within the \(t - t' - t'' - J\) model or alternatively one can fit experimental data. Both approaches produce very close values of the parameters. The fit of elastic and inelastic neutron scattering data for \(La_{2-x}Sr_xCuO_4\) performed in Ref. (22) gives the following values, \(g = 1\), \(\beta = 2.7\) \((m^* = 1.5m_e)\), \(\lambda \approx 1.30\). The fit of data on magnetic quantum oscillations in \(YBa_2Cu_3O_y\) performed in Ref. (22) gives two possible sets,

\[ g = 1, \quad \beta = 2.78 \quad (m^* = 1.45m_e), \quad \lambda = 1.31; \]

\[ g = 1, \quad \beta = 2.95 \quad (m^* = 1.35m_e), \quad \lambda = 1.23. \]  \hspace{1cm} (5)

These values will be used in the present work.

It is very easy to understand the reason for instability of the commensurate AF order under doping. Assuming such an order one can calculate the magnon Green’s function

\[ G(\omega, q) \sim \frac{1}{\omega^2 - c^2 q^2 - \mathcal{P}(\omega, q) + i0}, \]  \hspace{1cm} (6)

where \(c = \sqrt{\rho_s/\chi_\perp} \approx 1.17\sqrt{2}J\) is the magnon speed in the parent Mott insulator and \(\mathcal{P}(\omega, q)\) is fermionic polarization operator. A well known peculiarity of the two-dimensional (2D) polarization operator is its independence of doping as soon as \(\omega = 0\) and \(q\) is sufficiently small. A straightforward calculation gives at \(q \rightarrow 0\), \(\mathcal{P}(0, q) = -\lambda c^2 q^2\). Hence, at \(\lambda > 1\) the Stoner criterion in (6) is violated, the Green’s function possesses poles at imaginary frequency indicating instability of the AF ground state at an arbitrary small doping.

In YBCO the AF order is commensurate at \(x < 0.06\), therefore the effective action (2) cannot be directly applied to this compound. To understand YBCO one can certainly assume that \(\lambda\) is doping dependent, \(\lambda < 1\) at \(x < 0.06\) and \(\lambda > 1\) at \(x > 0.06\). Purely theoretically it is hardly possible to have a significant \(x\)-dependence of \(\lambda\), but as a scenario one can consider this. However, in this scenario the incommensurate wave vector \(Q\) must jump from \(Q = 0\) at \(x < 0.06\) to \(Q\) given by Eq. (4) at \(x > 0.06\). This is not consistent with data, there is no a jump, the incommensurate wave vector evolves smoothly above \(x = 0.06\), see Fig 4.

A model describing the smooth evolution of \(Q\) with doping was suggested in Ref. (14). In addition to (4) the model incorporates two points. (i) Due to the bilayer structure the magnon spectrum in YBCO is split into acoustic and optic mode. The optic gap is about \(70 \text{meV}\)\(^3\) hence the optic mode does not influence the low energy dynamics, only acoustic magnons are important for these dynamics. (ii) The second point of the model is an assumption that the fermionic dispersion is split in two branches as it is shown in Fig 4(left). The splitting is \(\Delta_0\). The effective action that originates from
and incorporates these two points reads
\[
\mathcal{L} = 2 \left[ \frac{\Delta_0}{2} - \rho_s \frac{2}{2} \left( \nabla \tilde{n} \right)^2 \right] \\
+ \sum_{\alpha=\alpha, \beta=\pm 1} \sum_{\gamma=\pm 1} \left[ \frac{i}{2} \left( \psi_{\alpha, \gamma}^\dagger D_{\alpha, \gamma} \psi_{\alpha, \gamma} - (D_{\alpha, \gamma})^\dagger \psi_{\alpha, \gamma} \right) \right] \\
- \psi_{\alpha, \gamma} \left[ \epsilon_0 (\mathcal{P}) - \gamma \frac{\Delta_0}{2} \right] \psi_{\alpha, \gamma} \\
+ \sqrt{2} g (\psi_{\alpha, \gamma}^\dagger \sigma \psi_{\alpha, \gamma}) \cdot \left[ \mathbf{e}_\alpha \cdot \nabla \right] \tilde{n} \right]. \tag{7}
\]

Compared to (2), the first line is multiplied by two since the bilayer has the twice larger spin stiffness and magnetic susceptibility. In addition to the pocket index \( \alpha \), the holon field \( \psi_{\alpha, \gamma} \) gets an additional index \( \gamma = \pm 1 \) that indicates the branch of the split dispersion as it is shown in Fig. 4. Originally the paper\textsuperscript{14} suggested that the hole band splitting \( \gamma = \pm 1 \) was due to the hole hopping between layers inside the bilayer. So, \( \Delta_0 \) was the bonding-antibonding splitting. However, our recent analysis\textsuperscript{25} indicates that antiferromagnetic correlations forbid the bonding-antibonding splitting. So, contrary to the assumption in Ref.\textsuperscript{14} the interlayer hopping cannot contribute to \( \Delta_0 \). In Section VI of the present paper I argue that the splitting \( \Delta_0 \) is due to oxygen chains. For now let us accept the action (7) and study consequences of this action.

When doping is sufficiently small,
\[
x < x_0 = \frac{\Delta_0}{\pi \beta}, \quad \tag{8}
\]
only the \( \gamma = 1 \) band is populated, see Fig. 4(left). In this case the fermionic polarization operator is a half of that for the single layer case, \( \mathcal{P}(0, q) = -\frac{1}{2} \lambda c^2 q^2, q \to 0 \). Hence the Stoner stability criterion in Eq. (3) is fulfilled and the Neel order is stable. According to both neutron scattering data\textsuperscript{10,11,13} shown in Fig. 2 and to \( \mu \)SR data\textsuperscript{14} shown in Fig. 1 the value of \( x_0 \) is \( x_0 \approx 0.06 \). Hence, due to Eq. (3) the band splitting is
\[
\Delta_0 \approx 0.5 J \approx 65 \text{meV}. \tag{9}
\]
At \( x > x_0 \) fermions populate both \( \gamma = 1 \) and \( \gamma = -1 \) bands, Fig. 4(right), the polarization operator is doubled compared to the \( x < x_0 \) case, and the Stoner instability is there. As a result at \( x > x_0 \) the system develops the spiral with the wave vector\textsuperscript{14}
\[
Q = \frac{g \rho_s x - x_0}{3 - 2 \lambda}. \tag{10}
\]

The plot of \( Q/2\pi \) versus doping is shown in Fig. 2 by the solid line. The development of the spin spiral is driven by the pseudospin splitting of the fermionic bands \( \pm gQ \) as it is shown by solid and dashed lines in Fig. 4(right). Thus, \( x_0 \) is a Lifshitz point, where the \( \gamma = -1 \) band starts to populate, and where simultaneously the spin spiral starts to develop. In the present paper I consider quantum and thermal fluctuations in the Neel state, \( x < x_0 \). Quantum fluctuations in the spin spiral state at \( x > x_0 \) will be considered separately\textsuperscript{25}.

To summarize this section. Small hole pockets and associated spin spiral state are generic properties of all cuprates at low doping. The key point of the YBCO phenomenology is splitting of the hole pockets. This splitting together with splitting of magnon to the acoustic and the optic mode provides stability of the AF order up to 6% doping.

III. QUANTUM FLUCTUATIONS IN THE NEEL PHASE, REDUCTION OF THE ZERO TEMPERATURE STAGGERED MAGNETIZATION.

There are two magnons (two polarizations) in the Neel phase at \( x < x_0 \). The Green’s function of each magnon reads
\[
G(\omega, q) = \frac{(2 \chi_\perp)^{-1}}{\omega^2 - c^2 q^2 - \mathcal{P}_0(\omega, q) + i0}. \tag{11}
\]
Only the \( \gamma = 1 \) band, see Fig. 4(left), contributes to the polarization operator \( \mathcal{P}_0(\omega, q) \). Calculation of the polarization operator for the single layer was performed in Ref.\textsuperscript{20}. Comparing the single layer action (2) and the double layer action (7) and having in mind that at \( x < x_0 \) only the \( \gamma = 1 \) band is occupied one immediately concludes that in the double layer case the polarization operator is a half of that calculated in Ref.\textsuperscript{20}. Hence
Here $p_F$ is the Fermi momentum of the $\gamma = 1$ band and $\theta(x)$ is the usual step function. I’ve already pointed out above that at $q < 2p_F$, $P_0(0, q) = -\frac{1}{2}q^2$, so the Neel state is stable if $\lambda < 2$.

It is instructive to look at the magnon spectral function $-\text{Im} G(\omega, q)$ that describes inelastic neutron scattering. Spectral functions for $x = 0.05$ and for three values of the momentum $q$ are plotted in Fig. 5 by solid lines. Spectral functions for both sets of parameters from Eq. (5) are almost identical. To be specific I present functions for the second set. In the same Fig. 6 the dashed lines show spectral functions in the parent Mott insulator at the same values of momentum.

functions for both sets of parameters from Eq. (5) are almost identical. To be specific I present functions for the second set. In the same Fig. 6 the dashed lines show spectral functions in the parent Mott insulator [\(P_0(\omega, q) = 0\)]. The spectra demonstrate the low energy incoherent part that absorbs more than 50% of the spectral weight. The magnon quasiparticle peaks are still clearly pronounced. Their intensities are about half of that in the parent compound, and positions are slightly shifted up compared to the parent, the shift is proportional to the doping, $\delta \omega_q \propto x$. It is worth noting that while the reduction of the spectral weight is a reliable result, the upward shift is probably a byproduct of the low energy effective theory. The effective theory accurately accounts for the magnon “repulsion” from the particle-hole continuum that is below the magnon. The “repulsion” results in the upward shift. However, there is also a “repulsion” from very high energy excitations ($E \sim 2t \sim 6J$) that are related to the incoherent part of the hole Green’s function. This repulsion, unaccounted in the effective theory, leads to the downward shift of the magnon frequency that is also proportional to doping. More generally one can say that the chiral effective field theory employed in the present work allows controllable calculations of effects that are $x$-independent or scale as $\sqrt{x}$ or $x \ln(x)$. Quantities that scale as the first or as a higher than first power of $x$ are generally beyond the scope of the theory. Therefore, at this stage one can say only that position of the magnon is approximately the same as that in the parent compound, but the magnon spectral weight is significantly reduced.

Another point worth noting is the absence of the hourglass dispersion. The low energy incoherent part of the Green’s function clearly pronounced in Fig. 5 is transformed to the coherent hourglass only at $x > x_0$, beyond the Lifshitz point.

Quantum fluctuation of the staggered magnetization is given by the standard formula

$$\langle n_s^2 \rangle = -2 \sum_q \int \frac{d\omega}{2\pi} G(\omega, q) = -2 \sum_q \int \frac{d\omega}{2\pi} \text{Im} G(\omega, q)$$

(13)

The factor 2 comes from two polarizations. This expression must be renormalized by subtraction of the ultraviolet-divergent contribution that corresponds to the undoped $\sigma$-model. The integral in (13) can be calculated analytically with logarithmic accuracy

$$\langle n_s^2 \rangle \approx -2 \sum_q \int \frac{d\omega}{2\pi} G(\omega, q) \approx -2 \sum_q \frac{\lambda \beta x}{4p_s} \ln \left( \frac{\Lambda}{p_F} \right) = -2 \sum_q \frac{\lambda \beta x}{8p_s} \ln \left( \frac{\Lambda^2}{\pi^2x} \right).$$

(14)

There are two points to note. (i) In spite of the ultraviolet renormalization ($\sigma$-model subtraction) the fluctuation depends on the ultraviolet momentum cutoff $\Lambda \sim 1$. (ii) The leading logarithmic term, $x \ln(\Lambda^2/x)$, comes from momenta $p_F \ll q \ll \Lambda$.

The logarithm $\ln(\Lambda^2/x)$ is not large, the logarithmic accuracy is not sufficient. Fortunately a numerical integration of (14) is straightforward. The result is presented in Fig. 6 where $\langle n_s^2 \rangle$ is plotted versus doping. The second set of parameters from (5) is used, results are presented for two values of the ultraviolet cutoff $\Lambda$. Reduction of the static component of the n-field is

$$\mu/\mu_B = 0.615 \left( 1 - \frac{1}{2} \langle n_s^2 \rangle \right).$$

(15)
Here I take into account that the used regularization procedure corresponds to the normalization of the static component of the n-field to unity at zero doping when the staggered magnetization is 0.0615\(\mu_B\). The plot of the calculated staggered magnetization \(\mu\) versus doping together with experimental data is presented in Fig. 1(top). Dependence of the theoretical curve on \(\Lambda\) is pretty weak, to be specific the curve corresponding to \(\Lambda = 1\) is presented. Agreement between the theory and the experiment in the Neel phase is excellent. Thus, it is understood why quantum fluctuations only slightly reduce the staggered magnetization.

Note that the presented calculation is valid only in the Neel phase, \(x < 0.06\). Physics in the spin-spiral phase, \(x > 0.06\), is very much different because of the appearance of the soft “hourglass” dispersion and consequently because of greatly enhanced quantum fluctuations. The corresponding results will be published separately.

IV. TEMPERATURE DEPENDENCE OF THE STAGGERED MAGNETIZATION IN THE NEEL PHASE

A. Zero doping

It is well known that due to the Mermin-Wagner theorem the Neel temperature in a spin-rotationally-invariant 2D system is exactly zero, \(T_N = 0\). Cuprates are layered systems with a very small Heisenberg interaction, \(J_1 \lesssim 10^{-4}J\), between layers or bilayers. In spite of its smallness the interaction makes the system three dimensional and hence it makes the Neel temperature finite, \(T_N \sim J/\ln(J/J_1)\). Temperature dependence of the staggered magnetization in layered Heisenberg antiferromagnets has been intensively studied theoretically, for a review see Ref. 27. Unfortunately there is no a “small theoretical parameter” in the problem, therefore, while a qualitative behaviour is absolutely clear, there is no a universal quantitative description, different theoretical approaches give quite different results. In the present section I develop an effective description of the temperature dependence. This description certainly is not a rigorous solution of the layered Heisenberg antiferromagnet for all temperatures. This is a sort of interpolation between \(T \ll T_N\) regime and \(T \approx T_N\) regime. Importantly, the “interpolation” allows to describe quantitatively an undoped layered Mott insulator, and much more importantly it allows to move to the finite doping in the next subsection.

Let us start from the single layer case (La\(_2\)CuO\(_4\)) and rewrite Eq. (13) in the Matsubara technique at a finite temperature.

\[
\langle n^2_\perp \rangle = \frac{2T}{\chi_\perp} \sum_q \sum_s \frac{1}{\xi^2_s + \omega^2_q},
\]

where \(\omega_q = cq\) and \(\xi_s = 2s\pi T\), \(s = 0, \pm 1, \pm 2, ..., \) is the Matsubara frequency. Hence equation for \(n_z = 1 - \frac{1}{2}\langle n^2_\perp \rangle\) can be rewritten in the renormalization group (RG) form

\[
\frac{dn_z}{n_z d\ln(q)} = \frac{T}{2\pi \rho_{sq}} \sum_s \frac{\omega^2_s}{\omega^2_q + \xi^2_s},
\]

where \(\rho_{sq} = \rho_s(q)\) is the \(q\)-dependent spin stiffness. Eq. (17) assumes 2D geometry, so it is valid at \(q > q_{min}\), where the infrared cutoff \(q_{min} \propto \sqrt{J_1}\) is due to the Heisenberg coupling along the third dimension. To solve the RG problem one needs to add information how the spin stiffness scales with the magnetization. Let us write the relation between the magnetization and the spin stiffness as

\[
\frac{d\rho_{sq}}{\rho_s(q)} = \frac{r}{\pi} \frac{dn_z}{n_z}.
\]

It is known that one loop calculation valid at \(n_z \approx 1\) results in \(r = 1\) that implies \(\rho \propto n_z\). On the other hand, close to the Neel temperature when \(n_z \ll 1\) one should expect scaling very close to quadratic, \(\rho \propto n_z^2\). This is because the critical index \(\eta\) of the magnon quasiparticle residue is very small, see, e.g. Refs. 28, 29. For now I keep the power \(r\) as a parameter. Eqs. (17) and (18) are combined to

\[
\frac{d\rho_{sq}}{d\ln(q)} = \frac{rT}{2\pi} \sum_s \frac{\omega^2_s}{\omega^2_q + \xi^2_s}.
\]

To perform the ultraviolet renormalization let us introduce \(\rho_\Lambda\), the spin stiffness at the ultraviolet cutoff. Then due to Eq. (19) the finite temperature spin stiffness at \(q = 0\) reads

\[
\rho_{sT} = \rho_\Lambda - \frac{rT}{2\pi} \int_{q_{min}}^\Lambda \left( \sum_s \frac{\omega^2_s}{\omega^2_q + \xi^2_s} \right) \frac{dq}{q}.
\]

This expression can be renormalized by the condition that at zero temperature (more accurately at \(T \ll q_{min}\)) the spin stiffness is equal the standard value \(\rho_{s0} \approx 0.175J\) corresponding the \(\sigma\)-model originated from the spin 1/2 Heisenberg model. After the renormalization Eq. (20) is transformed to

\[
\rho_{sT} = \rho_{s0} - \frac{rT}{2\pi} \int_{q_{min}}^\infty \left( \sum_s \frac{\omega^2_s}{\omega^2_q + \xi^2_s} - \frac{\omega_q}{2T} \right) \frac{dq}{q}.
\]
The 3D interaction $J_\perp$ fixes value of the infrared cutoff $q_{\text{min}}$, however, one has to remember about scaling of the cutoff with the staggered magnetization $n_z$, see Ref. 27,

$$q_{\text{min}} = q_{\text{min}0}\sqrt{n_z},$$ \hspace{1cm} (22)

where, due to (18),

$$n_z = \left(\frac{\rho_{sT}}{\rho_{s0}}\right)^{1/2}. \hspace{1cm} (23)$$

Eqs. 21, 22, 23 can be easily integrated numerically. The Neel temperature is determined by zero of the spin stiffness 21. The infrared cutoff $q_{\text{min}0}$ is the only free parameter in the theory. Value of the parameter has to be tuned up to reproduce the measured Neel temperature. It has to be clear that $q_{\text{min}0}$ originates not only from $J_\perp$, relativistic anisotropies like Dzyaloshinskii-Moria etc, also contribute to $q_{\text{min}0}$. Let us recall that due to the used regularization procedure the staggered magnetization is $\mu = 0.615\mu_B n_z$, where $0.615\mu_B$ is the the staggered magnetization in the parent Heisenberg model 21. Staggered magnetization versus temperature in La$_2$CuO$_4$ is presented in Fig. 7(left). Red circles show neutron scattering data 29. The theoretical curve with $r = 2$ and $q_{\text{min}0} = 0.024$ is shown by the solid line and the theoretical curve with $r = 1$ and $q_{\text{min}0} = 0.004$ is shown by the dashed line. The curve with $r = 1$ corresponding to the single loop RG describes the data very poorly. This illustrates the known problem of poor accuracy of the single loop RG 27. However, the curve with $r = 2$ corresponding to the critical scaling of the spin stiffness describes the data very well.

In the double layer case (YBCO) the coefficient $\frac{r T}{\pi}$ before the integral in Eq. (21) has to be replaced by the twice smaller one, $\frac{T}{\pi}$. The point is that the optic magnon in YBCO has a gap $70$meV and therefore it does not contribute to the low energy dynamics. Only acoustic magnon is important, hence the effective number of magnons is twice smaller compared to LCO. Neutron scattering data 30 for YBa$_2$Cu$_3$O$_6$ are shown in Fig. 7(right) by red dots. Green squares show $\mu$SR data 22. The theoretical curve with $r = 2$ and $q_{\text{min}0} = 0.0085$ is shown by the solid line and the theoretical curve with $r = 1$ and $q_{\text{min}0} = 0.0004$ is shown by the dashed line. Again, the curve with $r = 1$ is not consistent with the data. The curve with $r = 2$ is quite good.

It is worth noting that for both LCO and YBCO the values of the infrared cutoff $q_{\text{min}0}$ for $r = 1$ are unrealistically small reflecting the same difficulty of single loop RG, see also 27. On the other hand, the cutoff values for $r = 2$ are quite reasonable, they indicate that the Neel temperature is determined by spin-wave dynamics at distances up to $1/q_{\text{min}0} \sim 100$ lattice spacing along the plane.

All in all, the conclusion is that the effective RG developed in this subsection describes undoped compounds pretty well. To achieve this description one needs to set $r = 2$, this corresponds to the critical scaling of the spin stiffness expected in the vicinity of the Neel temperature, $\rho \propto n_z^2$. In the next subsection the developed description will be applied to the nonzero doping case.

### B. Nonzero doping

To extend to the finite doping case one has to introduce in Eq. (21) the fermionic polarization operator

$$\rho_{sT} = \rho_{s0} \frac{T}{2\pi} \int_{q_{\text{min}}}^{\infty} \left\{ \sum_{\gamma = \pm 1} \frac{\omega_q^2}{\omega_q^2 + \xi_q^2 + P_0(i\xi, q)} - \frac{i\xi}{q} \right\} dq,$$

where the polarization operator $P_0(i\xi, q)$ is calculated at Matsubara frequencies. Expression for the polarization operator follows from the Lagrangian 27. One can use vertexes derived in Ref. 20 for the single layer case and rescale the vertexes by the factor $1/\sqrt{r}$ that follows from comparison of 22 and 27. The polarization operator reads

$$P_0(i\xi, q) = \pi \lambda \beta q^2 \text{Re} \sum_{\gamma = \pm 1} \sum_p \frac{f_p^\gamma - f_{p+q}^\gamma}{\epsilon_p - \epsilon_{p+q} + i\xi} = 2\pi \lambda \beta q^2 \text{Re} \sum_{\gamma = \pm 1} \sum_p \frac{f_p^\gamma}{\epsilon_p - \epsilon_{p+q} + i\xi} \hspace{1cm} (25)$$

Here $f_p^\gamma$ is the Fermi-Dirac distribution function

$$f_p^\gamma = \frac{1}{e^{(\epsilon_p - \gamma\Delta_0/(2-\mu))/T} + 1} \hspace{1cm} (26)$$

with chemical potential $\mu$ (do not mix it up with magnetic moment). Note that at $T \neq 0$ the $\gamma = -1$ band is also populated, see Fig. 4(left). This is why the summation in 23 is performed over both bands, $\gamma = \pm 1$. The chemical potential is determined by the condition

$$2x = 2 \times 2 \sum_{\gamma = \pm 1} \sum_p f_p^{\gamma^*} \hspace{1cm} (27)$$

that accounts for the double layer, the two pockets, and for the two psedospin projections. It is easy to check that

![Diagram](image-url)
Numerical evaluation of the polarization operator $\mathcal{P}_0$ is straightforward. Substitution of the polarization operator in the RG equation and solution of this equation together with (22) and (23) gives staggered magnetization at a given doping and temperature. The RG equation is solved with $r = 2$ and $q_{\text{min}} = 0.0085$ as it has been discussed in the previous subsection. These parameters are relevant to the n-field and they are independent of doping. Fermionic polarization operator is not very sensitive to the choice of parameters, to be specific I present results corresponding to the second set of parameters in Eq. (9) that is responsible for the position of the Lifshitz point, $x_0 = 0.06$. Plots of the staggered magnetization versus temperature for several values of doping are shown in Fig. 8. Theoretical curves are in agreement with data from Ref. 9 are presented in Fig. 9(bottom). Over-all agreement between the theory and experiment is very good.

The calculated Neel temperature versus doping is shown by large ired dots in Fig. 1(bottom). The calculated staggered magnetization versus temperature is plotted in Fig. 1(top) for several values of doping. Experimental curves from Ref. 9 are presented in Fig. 9(bottom). Over-all agreement between theory and experiment is very good.

It is worth stressing again that the calculation of the temperature dependence of the magnetization in the layered system is less reliable than calculations of zero temperature properties in section III. The complexity of the finite temperature case is due to the very large span of spacial scales involving in the problem with the largest scale about 100 lattice spacing. Only leading effects have been taken into account in the present calculation. Clearly there are subleading effects that also influence the magnetization. For example, usual disorder (impurities) must influence fermion dynamics at the scale ~100 lattice spacing and hence influence magnetization. In view of this comment the agreement between the theory and experimental data, see Fig. 1(bottom) and Fig. 9 is remarkable. Most importantly, the theory explains why the

\begin{equation}
\mathcal{P}_0(i\xi, q) = 2\pi\lambda^2\beta^2 \sum_{\gamma = \pm 1} \sum_p \frac{(\epsilon_p - \epsilon_{p+q})}{(\epsilon_p - \epsilon_{p+q})^2 + \xi^2 + \frac{\Gamma^2}{4}} (28)
\end{equation}

\begin{equation}
\Gamma = A\frac{T^2}{\epsilon_F}, \quad (29)
\end{equation}

where $\epsilon_F = \beta p_F^2/2 = \pi \beta x$ is the Fermi energy. I disregard the logarithmic $T$-dependence of the coefficient $A$, the dependence is beyond accuracy of the calculation. The coefficient $A$ will be used as a fitting parameter. Note, that generally the width $\Gamma$ depends on both temperature $T$ and Matsubara frequency $\xi$. The dominating contribution to Eq. (21) comes from the zero Matsubara frequency. Therefore, the width $\Gamma$ is important in the zero frequency term, $s = 0$, and it is completely negligible in $s \neq 0$ terms. Hence, the width $\gamma_{\text{in}}$ corresponds to the zero Matsubara frequency. Numerical evaluation of the polarization operator is not more difficult than evaluation of (23). Solution of RG equations gives the staggered magnetization $\mu(T, x)$ with account of the fermion lifetime. The best fit of the experimental dependence of the Neel temperature on doping is achieved at

\begin{equation}
A \approx 0.7. \quad (30)
\end{equation}

The calculated Neel temperature versus doping is shown by large ired dots in Fig. 1(bottom). The calculated staggered magnetization versus temperature is plotted in Fig. 1(top) for several values of doping. Experimental curves from Ref. 9 are presented in Fig. 9(bottom). Over-all agreement between theory and experiment is very good.

It is worth stressing again that the calculation of the temperature dependence of the magnetization in the layered system is less reliable than calculations of zero temperature properties in section III. The complexity of the finite temperature case is due to the very large span of spacial scales involving in the problem with the largest scale about 100 lattice spacing. Only leading effects have been taken into account in the present calculation. Clearly there are subleading effects that also influence the magnetization. For example, usual disorder (impurities) must influence fermion dynamics at the scale ~100 lattice spacing and hence influence magnetization. In view of this comment the agreement between the theory and experimental data, see Fig. 1(bottom) and Fig. 9 is remarkable. Most importantly, the theory explains why the
FIG. 9: Staggered magnetization versus temperature in YBa$_2$Cu$_3$O$_{y}$ for several values of doping $x$. Theoretical curves with account of the hole lifetime for $x = 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6$ are shown in the top figure. Experimental curves from Ref. 3 are presented in the bottom figure, the doping levels are $x = 0.001, 0.002, 0.005, 0.02, 0.029, 0.036, 0.039, 0.049, 0.061, 0.065$.

The Neel temperature drops down dramatically with doping, while the zero temperature magnetization is almost doping independent. This “contradictory” behavior is due to the band splitting, and due to different fillings of the split bands. The different filling is a fingerprint of small hole pockets. At zero temperature only the lower band is occupied while temperature populates the upper band as well. The “contradictory” behavior is closely related to the Lifshitz point at $x \approx 0.36$ and to the development of the spin spiral at $x \approx 0.65$. In other words, soft magnons included in the effective action (7) cannot induce a transition with the large momentum transfer. A careful analysis shows that the vertex vanishes after integration over $X$. In other words, soft magnons included in the effective action (7) cannot induce a transition with the large momentum transfer. A careful analysis shows that the vertex vanishes after integration over $X$.

Thus, contrary to the assumption in Ref. 14 the inter-layer hopping cannot contribute to $\Delta_0$. Another mechanism for splitting is necessary. In this section I argue that the splitting is due to oxygen chains. Let us first consider the case $y = 6.5$ when every second chain is fully filled. In this case chains produce the effective pseudopotential for in-plane holes

$$V_c(X) = -v_0 \cos(\pi X),$$

where $v_0$ is the amplitude of the potential and $X$ is the direction perpendicular to chains (I denote the distance by capital $X$ to make it different from the doping $x$). The hole dispersion in the antiferromagnetic background is shown in Fig. 10. The dispersion consists of two full pockets, the pocket $a$ and the pocket $b$. There is the perfect nesting condition between the pockets and the chain potential (31), therefore the two split bands are generated

$$\epsilon_p = -v_0 + \frac{\beta}{2} p^2, \quad \psi_+ = \frac{\langle a \rangle_p + \langle b \rangle_p}{\sqrt{2}} \cos \left( \frac{\pi}{2} X \right) e^{i p \cdot r},$$

$$\epsilon_p = +v_0 + \frac{\beta}{2} p^2, \quad \psi_- = \frac{\langle a \rangle_p - \langle b \rangle_p}{\sqrt{2}} \sin \left( \frac{\pi}{2} X \right) e^{i p \cdot r}$$

(32)

Here $p$ is the momentum with respect to the center of the pocket. Eqs. (32) represent exactly the $\gamma = \pm 1$ band splitting adopted in 7. Due to the exact nesting of small hole pockets a tiny pseudopotential $v_0 \approx 30 meV$ is sufficient to generate the splitting $\Delta_0 = 2v_0 \approx 65 meV$ that follows from the magnetic analysis, see Eq. (9).

There might be an impression that the splitting (32) is not quite equivalent to the effective action (7). For example, the question arises why there is no a spin-wave vertex that transfers $\psi_+ \rightarrow \psi_-$. The vertex carries a large momentum $\pi$, therefore the vertex vanishes after integration over $X$. In other words, soft magnons included in the effective action (7) cannot induce a transition with the large momentum transfer. A careful analysis shows that the splitting (32) with account of two layers is completely equivalent to (7).

According to (32) the wave function of the lower $\gamma = -1$ band is nonzero at $X=0, 2, 4, ...$ while the wave function of the upper $\gamma = +1$ band is nonzero at $X=1, 3, 5, ...$. Due to the splitting the bands are differently populated

\[\text{FIG. 10: Single hole dispersion in the AF background.}\]
and this results in the in-plane hole density wave with period of the two lattice spacing. Let us calculate the amplitude of the CDW. The oxygen content $y = 6.5$ corresponds to doping $x \approx 0.1$, see Eq. (33). This doping is within the spin-spiral phase, therefore to calculate fillings of bands one has to account the spin spiral as it is shown in Fig. (3) right). In the lower $\gamma = +1$ band both pseudospin projections are populated, while in the upper $\gamma = -1$ band only one pseudospin projection is populated. Populations of different subbands have been calculated in the analysis of magnetic quantum oscillations, see Eqs. (4) in Ref. 22. From these equations one concludes that populations of the upper and lower bands ($\gamma = \mp 1$) are

$$
\begin{align*}
  x_{-1} &= \frac{2 - \lambda}{2(3 - 2\lambda)}(x - x_0) \\
  x_{+1} &= x - x_{-1}.
\end{align*}
$$

(33)

Naturally, the population of the upper band vanishes at $x = 0$, this is the Lifshitz point. For $x = 0.1$, $x_0 = 0.06$, and $\lambda = 1.23$, one finds $x_{-1} = 0.03$ and $x_{+1} = 0.07$. Hence, the hole density per site at every even value of $X$ is $2x_{+1} = 0.14$, and at every odd value of $X$ it is $2x_{-1} = 0.06$. However, this is not the amplitude of the CDW yet.

All equations in the present paper are written in terms of holes dressed by magnetic quantum fluctuations (magnetic polarons). Hence $x_{\pm 1}$ are densities of the dressed holes. The dressed hole has a finite size, therefore, the charge density modulation is smaller than that naively given by $x_{\pm 1}$. It is known that the quasiparticle residue of the dressed hole is about $Z \approx 0.4$, see e.g. Ref. 33. This means that with the probability $Z \approx 0.4$ the hole resides at the same site as the quasihole and with the probability $(1 - Z)/4 \approx 0.15$ the hole resides at each of the four nearest Cu sites. Therefore, the real charge densities per site are

$$
\begin{align*}
  \rho_{+1} &= 2 \left[ \left( Z + \frac{1 - Z}{4} \right) x_{+1} + \frac{1 - Z}{4} x_{-1} \right] \approx 0.12 \\
  \rho_{-1} &= 2 \left[ \left( Z + \frac{1 - Z}{4} \right) x_{-1} + \frac{1 - Z}{4} x_{+1} \right] \approx 0.08
\end{align*}
$$

(34)

This gives the amplitude of the CDW. The estimate of the amplitude is based purely on magnetic data, it depends mainly on the position of the Lifshitz point, $x_0 = 0.06$.

NQR was not used in the estimate. Nevertheless the estimate is pretty much consistent with NQR data presented in Fig. 5. The NQR frequency shift with respect to the frequency of the undoped sample, $\nu_0 = 23.3 MHz$, is proportional to the local hole concentration $\rho$

$$
\nu_Q = 23.3 MHz + B\rho.
$$

(35)

The higher frequency NQR line at $y = 6.56$ is $\nu_2 \approx 30.3 MHz$, see Fig. 5. According to Eq. (34) the line corresponds to $\rho \approx 0.12$. Hence, the constant $B$ in Eq. (35) is $B \approx 58 MHz/\text{hole}$. Interestingly, the value of $B$ is significantly larger than that in La$_{2-x}$Sr$_x$CuO$_4$, $B \approx 20 MHz/\text{hole}$, and in HgBa$_2$CuO$_{4+\delta}$, $B \approx 30 MHz/\text{hole}$. Assuming that optimal doping corresponds to $\rho \approx 0.14$ and using Eq. (35) one finds the optimal doping NQR frequency $\nu \approx 31.4 MHz$. This value is pretty close to $\nu_{opt} \approx 31.6 MHz$ that follows from Fig. 5 at $y \approx 7$. According to (34) the lower frequency NQR line at $y \approx 6.5$ corresponds to $\rho \approx 0.08$. Substituting this value in Eq. (35) one finds the frequency $\nu \approx 27.9 MHz$. Again, this value is pretty close to the lower frequency line at $y \approx 7$.8 MHz that is shown in Fig. 5 at $y = 6.56$. Thus, the amplitude of the CDW determined from the position of the Lifshitz point is fully consistent with the NQR data.

The simple potential is literally applicable only to $y = 6.5$. Obviously, there is no any modulation at $y = 7$ as the rightmost Fig. 3 indicates. Away from $y = 6.5$ more complex oxygen superstructures can appear. Assumption important for the present work is that at $0 < x < 0.1$ (6.20 < $y$ < 6.5) the superstructure is dominating. NQR data for $y = 6.4$ and $y = 6.45$ presented in Fig. 6 support this assumption: there are only two NQR lines that are only slightly broader than the lines at $y = 6.5$.

VI. CONCLUSIONS

Small hole pockets and the associated spin spiral state are generic properties of all cuprates at low doping. The key point of the YBCO phenomenology additional to the generic properties is splitting of the hole pockets into the lower band and the upper band. This splitting together with splitting of magnon to the acoustic and the optic mode provides stability of the collinear aniferromagnetic order at doping below the Lifshitz point at $x \approx 0.06$. At doping below the Lifshitz point only the lower band is populated. At higher doping the upper band starts to populate and simultaneously the spin spiral starts to develop.

At doping below the Lifshitz point the doping induced spin quantum fluctuations are pretty weak. This explains why the zero temperature staggered magnetization is close to $0.6 \mu_B$, the maximum value allowed by quantum fluctuations of localized spins. The developed theory perfectly reproduces the weak decrease of the staggered magnetization with doping observed experimentally.

While the zero temperature staggered magnetization is almost doping independent, the Neel temperature decays very quickly from $T_N = 420K$ at $x = 0$ to practically zero at $x \approx 0.06$. This quick decay is a consequence of the closeness to the Lifshitz point. Again, the theory reproduces very well the doping dependence of the Neel temperature as well as the observed temperature dependence of the staggered magnetization at a given doping.

The band splitting (the hole pocket splitting) is in-
duced by the modulation of oxygen chains. The main period of the modulation is two lattice spacing. Because of the perfect nesting between the small hole pockets and the period of the modulation, a small pseudopotential caused by the chains is sufficient to induce the band splitting about 60meV. The splitting causes the in-plane charge density wave with a significant amplitude dependent on doping.

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