Commensurate magnetic excitations induced by band splitting and Fermi surface topology in n-type cuprates

H Y Zhang\textsuperscript{1}, Y Zhou\textsuperscript{1}, H Q Lin\textsuperscript{2} and C D Gong\textsuperscript{1,3}

\textsuperscript{1} National Laboratory of Solid State Microstructure, Department of Physics, Nanjing University, Nanjing 210093, People’s Republic of China
\textsuperscript{2} Department of Physics and the Institute of Theoretical Physics, Chinese University of Hong Kong, Hong Kong, People’s Republic of China
\textsuperscript{3} Center for Statistical and Theoretical Condensed Matter Physics, Zhejiang Normal University, Jinhua 321004, People’s Republic of China

E-mail: zhouyuan@nju.edu.cn

Received 24 December 2012, in final form 2 February 2013
Published 19 March 2013
Online at stacks.iop.org/JPhysCM/25/155603

Abstract
The antiferromagnetic correlation plays an important role in high-$T_c$ superconductors. Considering this effect, the magnetic excitations in n-type cuprates near the optimal doping are studied within the spin-density-wave description. The magnetic excitations are commensurate in the low-energy regime and further develop into spin-wave-like dispersion at higher energy, consistent with the inelastic neutron scattering measurements. We clearly demonstrate that the commensurability originates from the band splitting and Fermi surface topology. The commensurability is a normal state property and has nothing to do with d-wave superconductivity. Our results strongly suggest the essential role of antiferromagnetic correlations in the cuprates.

(Some figures may appear in colour only in the online journal)

1. Introduction

The parent compounds of the high-$T_c$ superconductors are antiferromagnetic (AFM) Mott insulators. Superconductivity (SC) emerges when charge carriers (holes or electrons) are doped into the CuO$_2$ planes. It is well known that clear electron–hole asymmetry is found in the phase diagram. For the hole-doped case, the AFM and superconducting phases are separated by a spin glass phase. In contrast, the AFM phase extends over a much wider range of doping and even coexists with SC in the electron-doped cuprates \cite{1}. Due to the proximity of antiferromagnetism and SC, it is generally believed that there exists an intrinsic link between the two phases. Studies of the spin dynamics in n-type and p-type cuprates will shed light on the mechanism of superconductivity.

One of the most commonly available techniques to study spin dynamics is inelastic neutron scattering (INS), which directly measures the magnetic excitations (MEs). Compared with the well studied p-type cuprate \cite{2, 3}, investigations on the MEs in n-type cuprates \cite{4–10} are much fewer due to technical reasons. A robust feature of MEs in n-type cuprates, i.e. the commensurate spin response, has been revealed by these INS measurements. The commensurability, characterized by the strongest intensity peaked at $Q = (\pi, \pi)$, covers a wide low-energy region near the optimally doped Nd$_{2−x}$Ce$_x$CuO$_4$ (NCCO) \cite{4} and Pr$_{1−x}$LaCe$_x$CuO$_{4−δ}$ (PLCCO) \cite{6}. Further detection shows that such commensurability in n-type cuprates exists for a wide doping range from underdoping to heavy overdoping \cite{8, 9}. More importantly, the commensurate MEs persist well above the superconducting critical temperature $T_c$, indicating its non-superconducting origin. There gradually develops a spin-wave-like dispersion centered on the $Q$ point at higher energy, analogous to its undoped parent compound \cite{5}. In contrast, the well known ‘hourglass’ type magnetic dispersion...
has been discovered in the p-type cuprates, where the commensurate peak is only found at the resonance energy. Therefore, the two types of cuprates exhibit distinct spin response, indicating the intrinsic particle–hole asymmetry. The energy of the spin-density-wave (SDW) description. The main n-type cuprates near optimal doping within the framework of response, indicating the intrinsic particle–hole asymmetry. The commensurate peak is only found at the resonance energy. Additionally, as we mentioned above, the AFM correlation may not exist [7].

2. Hamiltonian and formula

A SDW description is adopted to investigate the n-type cuprates near the optimal doping. Such a description was first suggested by Armitage et al based on the ARPES measurements on NCCO [18]. The underlying Fermi surface disappears around the hot-spot near the optimal doping, where the long-range antiferromagnetism is absent, strongly suggesting the existence of a $Q = (\pi, \pi)$-scattering. Parker et al further proposed an effective energy band with $\epsilon^i_k = \epsilon^i_k + \eta \epsilon^j_k + V_{\pi,\pi}^2$ ($n = 1$ and $-1$ for the upper and lower band, respectively) [19], where $V_{\pi,\pi}$ is the strength of the effective $Q$-scattering, representing the influence of the SDW. $\epsilon^i_k$ and $\epsilon^j_k$ is the inter- and intra-lattice hopping term. This description well reproduces the $\sqrt{2} \times \sqrt{2}$ band folding and Fermi surface reconstruction [20, 21], and its applications on the temperature evolution of optical conductivity [22] and the Hall coefficient [23] give qualitative agreement with experiments. Now, the model Hamiltonian is expressed as

$$H = \sum_{k\sigma} \epsilon^i_k (d^+_k \sigma \epsilon_k + e^{+i}_{k\sigma} \epsilon_k) + \sum_{k\sigma} \epsilon^j_k (d^+_k \sigma \epsilon_k + \text{h.c.}) - \sum_{k\sigma} \sigma V_{\pi,\pi} (d^+_k \sigma \epsilon_k - e^{+i}_{k\sigma} \epsilon_k),$$

(1)

where the two sublattices $D$ and $E$ with respective fermionic operators $d$ and $e$ are introduced due to SDW$^4$ $\epsilon^i_k = -2t(\cos k_x + \cos k_y)$ and $\epsilon^j_k = -4t' \cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y) - \mu$ with $t$, $t'$, and $t''$ are the fitting parameters for nearest-neighbor (NN), second-NN, and third-NN hopping. The summation is restricted in the AFM Brillouin zone. The quasi-particle dispersion $\epsilon^i_k$ can be obtained by the rotation transformation. The corresponding weight factor $W^0 = \frac{1}{2}(1 + \eta \sin 2\theta_k)$ with $\cos 2\theta_k = \frac{V_{\pi,\pi}}{\sqrt{\epsilon^j_k + V_{\pi,\pi}^2}}$ and $\sin 2\theta_k = -\frac{4t'}{\sqrt{\epsilon^j_k + V_{\pi,\pi}^2}}$.

Here we would like to emphasize that the long-range AFM order disappears near the optimal doping. As pointed out by Motoyama et al, the Néel temperature detected above $x = 0.134$ in NCCO originates from the regions of samples that were not fully oxygen-annealed [7]. This means that the genuine long-range antiferromagnetism does not coexist with superconductivity. However, the two-dimensional AFM correlation remains. Unlike only several lattice-distant lengths in p-type cuprates [24], the AFM correlation is about ten lattice distances in the optimal electron-doped cuprates [7]. In this sense, the AFM correlations in the n-type cuprates are similar to the long-range AFM order, at least in the small scaling. Therefore, using a slowly fluctuating SDW order to describe the long-range AFM correlation is a treatment worth considering [25, 26]. Though the present SDW description is analogous to the form in the AFM phase [14], the physics behind it is essentially different.

The spin susceptibility under the random phase approximation is

$$\chi_q(\omega) = \frac{\chi_q^0 - U(\chi_{q,0}^0 \chi_{q+Q,0}^0 - \chi_{q+Q,0} \chi_{q,0}^0)}{(1 - U\chi_{q,0}^0)(1 - U\chi_{q+Q,0}^0) - U^2 \chi_{q+Q,0}^0 \chi_{q+Q,0}^0}$$

(2)

$^4$ Any order with characteristic wavevector $Q$ would reproduce such band structure, but the SDW is most likely.
with $U$ being a reduced Coulomb interaction due to the screening effect [27]. The bare spin susceptibilities are

$$
\chi_{q,q}^0 = \sum_k \sin^2 \left( \theta_{k+q} + \theta_k \right) \left( F_{--} + F_{++} \right) + \sum_k \cos^2 \left( \theta_{k+q} + \theta_k \right) \left( F_{--} + F_{+-} \right)
$$

$$
\chi_{q,q+Q} = \sum_k \left( \cos 2\theta_k - \cos 2\theta_{k+q} \right) \left( F_{--} - F_{++} \right)
$$

where

$$
F_{\eta\eta'} = \frac{1}{4} \left( f_{\eta q}^0 - f_{\eta' q}^0 \right) \left( \frac{1}{\omega - \xi_{\eta q}^0 + \xi_{\eta' q}^0} \right),
$$

with $F_{\eta\eta'}$ given by

where $f_k = 1/(1 + e^{\xi_k/T})$ is the Fermi distribution function. Numerically, the doping level is fixed at $x = 0.15$, near the AFM quantum critical point [7]. $t = 250$ meV, $t' = -50$ meV, and $t'' = 20$ meV are adopted [19]. The best fitting effective $Q$-scattering strength is $V_{\pi,\pi} = 100$ meV, and will be adjusted as necessary. The temperature is fixed at $T = 0.2$ meV. We adopt a broadening factor $\Gamma$ to calculate the spin susceptibility. The reduced Coulomb interaction is about 600–760 meV, which is about 2–3 times $U$. For example, when $U = 760$ meV, the magnetic resonance energy $\omega_{res}$ of 70 meV for $q = \pi$. From left to right we have $U = 660$ meV, 700 meV, and 760 meV, respectively. The effective $Q$-scattering potential is $V_{\pi,\pi} = 100$ meV and the damping rate $\Gamma = 5$ meV. All data have been renormalized by setting the strongest intensity at given $\omega$ as unity, denoted by the white lines.

3. Results and discussions

The typical energy evolution of the MEs $\Im \chi_q(\omega)$ is shown in figure 1. In the low-energy regime below 18 meV (figures 1(a), (b)), the MEs are incommensurate with strong intensity in diagonal directions. Simultaneously, the intensity near $Q$ is gradually enhanced. In the intermediate-energy regime, the strongest intensity is located at the $Q$ point, leading to the so-called commensurability (figures 1(c), (d)). It is maintained up to a critical energy of about 88 meV (figure 1(e)), where the strongest intensity $\Im \chi_{Q\pi}(\omega)$ in the normal state can be found, and is referred to as the magnetic resonance $\omega_{res}^M$. The total energy range for the commensurability is approximately 70 meV for $\Gamma = 10$ meV. This magnetic resonance is directly related to the fact that the real part in the denominator of the RPA formula (equation (2)) reduces to zero. Subsequently, it evolves into a ring-like incommensurability in the high-energy region with its radius expanding with the further increased energy (figure 1(f)). For high enough energy, the MEs are incommensurate with strong intensity in the vertical directions (not shown).

Such features can be clearer in the dispersion of the MEs at high symmetry scanning lines, as shown in figure 2. A wide energy regime with commensurability exists for all selected $U$, manifesting its universal nature. The low-energy incommensurability increases slightly with $\omega$; this is consistent with a recent study [28]. Hence the commensurability cannot be viewed as the overlap of two incommensurate peaks. It is an intrinsic feature of n-type cuprates. The low-energy incommensurability may be suppressed and even absent with enhanced $U$. For example, when $U = 0.76$ V (figure 2(c)), the MEs are still commensurate at low enough energy. Correspondingly, the magnetic resonance energy $\omega_{res}^M$ decreases down to 30 meV for $\Gamma = 5$ meV. The experimentally discovered commensurability in NCCO [4] and PLCCO [8, 9, 29] near the optimal doping is more likely similar to this case. The value of $U = 760$ meV is near the AFM stability, consistent with the fact that the optimal doping is near the AFM quantum critical point [7].
The possible energy range of commensurability is mainly determined by the effective $Q$-scattering potential $V_{\pi,\pi}$. For $V = 100 \text{ meV}$ and $\Gamma = 5 \text{ meV}$, it is about 48 meV. This energy range decreases down to 10 meV when $V = 50 \text{ meV}$. However, the realistic energy range of commensurability may be substantially reduced for strong $U$ due to the proximity of the AFM stability. It is only 30 meV for stronger $U = 760 \text{ meV}$. For strong enough $U \geq 770 \text{ meV}$ at given $V = 100 \text{ meV}$, the commensurability is entirely suppressed and only the ring-like magnetic feature remains. This situation is indeed an AFM state. Therefore, the ring-like feature at the high-energy regime in the electron-doped cuprates shares the same origin as that in their parents’ compounds. In fact, those theories based on the long-range AFM order [14, 15] cannot account for the commensurability found in NCCO [4] and PLCCO [8] due to Stoner instability at $\omega = 0$ [17], unless some special control parameter is adopted. The energy range of commensurability also depends on the broadening factor $\Gamma$—compare the data in figure 1 and figures 2(e) and (f). However, this phenomenon is still present even if a small $\Gamma = 1 \text{ meV}$ is adopted, which is less than the instrument resolution. Hence, the commensurability is an intrinsic and universal property of the electron-doped cuprates in the normal state.

The main difference in the present work from the previous theoretical investigation by Krüger et al [11] is that the influence of the AFM correlation is taken into account. The SDW description takes the place of the single-band description, producing a splitting into two bands. Therefore, the commensurability is a direct result of the band splitting. This can also be seen from the fact that the commensurate energy region diminishes with the reduced $V_{\pi,\pi}$ as we have shown before. We know that the AFM correlation weakens with doping [30]. In the heavy overdoping range, the AFM correlation vanishes, i.e. $V_{\pi,\pi} = 0$, leading to the absence of band splitting. Our result is then the same as the work of Krüger et al, the MEs become incommensurate, which is consistent with INS measurements [8].

The Fermi surface topology is also essential for commensurate MEs. It is well known that the Fermi surface of n-type cuprates evolves from the small electron pocket centered at $(\pi, 0)$ in underdoping to a large-three-pieced structure centered at $(\pi, \pi)$ near the optimal doping [18]. The hot-spot region is fully gapped as shown in figure 3, leading to the excitations of particle–hole pairs with momentum transfer $(\pi, \pi)$. Both the magnetic resonance and commensurate MEs reside below the particle–hole continuum. Therefore, both the band splitting and Fermi surface topology are important in the universal commensurability in the n-type cuprates. As we stressed before, they both originate from the AFM correlation. Together with the previous theoretical works on the band structure [20, 21] and transport properties [22, 23], we conclude that the AFM correlation plays essential roles in the cuprates.

The commensurate MEs remain in the presence of superconductivity. We introduce a phenomenological BCS-like pairing term $\sum_{\Delta k} \Delta_k (d_{\uparrow k} e^{-i k \cdot x} + e^{i k \cdot x} d_{\downarrow -k})$ with standard d-wave symmetry $\Delta_k = \Delta (\cos k_x - \cos k_y)$ [26]. In fact, our main results are insensitive to the detailed form of d-wave pairing. The resultant MEs change little, consistent with the INS observations. Therefore, the commensurability in n-type cuprate is a normal state property, and has nothing to do with SC. The commensurability has also been obtained in a single-band description with d-wave superconductivity [12, 13], though the d-wave pairing produces two bands. However, the superconducting gap in the optimal doped n-type cuprates is only 3–4 meV [32, 33], too small to account for the wide energy range commensurability. It seems that the commensurability comes from the strong peaked factor $U_q [12]$ or $J_q [13]$ rather than the d-wave superconductivity in these theoretical investigations. More importantly, the commensurability is a normal state property, which can also be discovered well above the superconducting transition temperature $T_C$.

4. Conclusion

In conclusion, the magnetic excitations near the optimal doped n-type cuprates are studied within a SDW description. We adopt a slowly fluctuating SDW to account for the antiferromagnetic correlations in the n-type cuprates. The main features of magnetic excitations in the normal state are well established. Our analyses clearly demonstrate that the band splitting and the Fermi surface topology are the key for commensurability in n-type cuprates. This strongly suggests that the antiferromagnetic correlation plays important roles in cuprates. We emphasize that the commensurability is a normal state property and has nothing to do with superconductivity. The qualitative agreement between the theoretical calculations and experimental data also suggests the validity of the SDW description near the optimal doping where the long-range antiferromagnetic order is absent.

The pairing symmetry in n-type cuprates is an open issue. It was argued that the nonmonotonic d-wave nature can be reproduced by the simple-d-wave symmetry if the SDW is considered; see for example [31].
Acknowledgments

This work was supported by NSFC Project No. 11274276 and a project funded by the Priority Academic Program Development of Jiangsu Higher Education Institutions. Gong CD acknowledges 973 Project No. 2011CBA00102. Lin HQ acknowledges RGC grant from HKSAR, Project No. HKUST3/CRF/09.

References

[1] Armitage N P, Fournier P and Greene R L 2010 Rev. Mod. Phys. 82 2421
[2] Fujita M, Hiraka H, Matsuura M, Tranquada J M, Wakimoto S, Xu G and Yamada K 2012 J. Phys. Soc. Japan 81 011007 (and reference therein)
[3] Brinckmann J and Lee P A 1999 Phys. Rev. Lett. 82 2915
[4] Yamada K, Kurahashi K, Uefuji T, Fujita M, Park S, Lee S-H and Endoh Y 2006 Nature 442 59
[5] Wilson S D, Li S, Chi S, Kang H J and Lynn J W 2006 Nature 445 186
[6] Fujita M, Matsuda M, Lee S-H, Nakagawa M and Yamada K 2008 Phys. Rev. Lett. 101 107003
[7] Zhao J et al 2011 Nature Phys. 7 719
[8] Krüger F, Wilson S D, Shan L, Li S, Huang Y, Wen H-H, Zhang S-C, Dai P and Zaanen J 2007 Phys. Rev. B 76 094506
[9] Ismer J-P, Eremin I, Rossi E and Morr D K 2007 Phys. Rev. Lett. 99 047005
[10] Li J X, Zhang J and Luo J 2003 Phys. Rev. B 68 224503
[11] Yuan Q S, Lee T K and Ting C S 2005 Phys. Rev. B 71 134522
[12] Chen C P, Jiang H M and Li J X 2010 J. Phys.: Condens. Matter 22 035701
[13] Rowe W, Knolle J, Eremin I and Hirschfeld P J 2012 Phys. Rev. B 86 134513
[14] Schrieffer J R, Wen X G and Zhang S C 1989 Phys. Rev. B 39 11663
[15] Armitage N P et al 2001 Phys. Rev. Lett. 87 147003
[16] Park S R, Roh Y S, Yoon Y K, Leem C S, Kim J H, Kim B J, Koh H, Eisaki H, Armitage N P and Kim C 2007 Phys. Rev. B 75 060501(R)
[17] Ikeda M et al 2009 Phys. Rev. B 80 014510
[18] Matsu H, Terashima K, Sato T, Takahashi T, Wang S-C, Yang H-B, Ding H, Uefuji T and Yamada K 2005 Phys. Rev. Lett. 94 047005
[19] Zimmers A, Tomczak J M, Lobo R P S M, Bontemps N, Hill C P, Barr M C, Dagan Y, Greene R L, Millis A J and Homes C C 2005 Europhys. Lett. 70 225
[20] Das T, Markiewicz R S and Bansil A 2006 Phys. Rev. B 74 020506(R)
[21] Luo H G and Xiang T 2005 Phys. Rev. Lett. 94 027001
[22] Zhou Y, Lin H Q and Gong C D 2010 Phys. Lett. A 374 4065
[23] Das T, Markiewicz R S and Bansil A 2012 Phys. Rev. B 85 064510
[24] Fujita M, Matsuda M, Nakagawa M and Yamada K 2008 Phys. Soc. Japan 75 093704
[25] Zhou Y, Lin H Q and Gong C D 2008 Phys. Rev. B 77 092510
[26] Yuan Q, Yuan F and Ting C S 2006 Phys. Rev. B 73 054501
[27] Shan L, Wang Y L, Huang Y, Li S L, Zhao J, Dai P and Wen H H 2008 Phys. Rev. B 78 014505
[28] Dagan Y, Qazilbash M M, Bontemps N, Hill C P, Barr M C, Dagan Y, Greene R L, Millis A J and Homes C C 2005 Europhys. Lett. 70 225
[29] Zimmers A et al 2007 Phys. Rev. B 76 064515
[30] Dagan Y, Qazilbash M M, Hill C P, Kulkarni V N and Greene R L 2004 Phys. Rev. Lett. 92 167001
[31] Kastner M A, Birgeneau R J, Shirane G and Endoh Y 1998 Rev. Mod. Phys. 70 897
[32] Das T, Markiewicz R S and Bansil A 2012 Phys. Rev. B 85 064510
[33] Fujita M, Matsuda M, Nakagawa M and Yamada K 2008 J. Phys. Soc. Japan 75 093704
[34] Zhou Y, Lin H Q and Gong C D 2008 Phys. Rev. B 77 092510
[35] Yuan Q, Yuan F and Ting C S 2006 Phys. Rev. B 73 054501
[36] Shan L, Wang Y L, Huang Y, Li S L, Zhao J, Dai P and Wen H H 2008 Phys. Rev. B 78 014505
[37] Dagan Y, Qazilbash M M and Greene R L 2005 Phys. Rev. Lett. 94 187003