Quasiparticle interference in antiferromagnetic parent compounds of Fe-based superconductors.

I.I. Mazin, Simon A.J. Kimber, and Dimitri N. Argyriou

1 Code 6393, Naval Research Laboratory, Washington, DC 20375, USA and
2 Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner Platz 1, Berlin 14109, Germany

Recently reported quasiparticle interference imaging in underdoped Ca(Fe$_{1-x}$Co$_x$)$_2$As$_2$ shows pronounced C$_2$ asymmetry that is interpreted as an indication of an electronic nematic phase with a unidirectional electron band, dispersive predominantly along the $b$-axis of this orthorhombic material. On the other hand, even more recent transport measurements on untwinned samples show near isotropy of the resistivity in the $ab$ plane, with slightly larger conductivity along $a$ (and not $b$). We show that in fact both sets of data are consistent with the calculated ab initio Fermi surfaces, which has a decisively broken C$_4$, and yet similar Fermi velocity in both directions. This reconciles completely the apparent contradiction between the conclusions of the STM and the transport experiments.

PACS numbers: 74.20.Pq,74.25.Jb,74.70.Xa

The Fe-based superconductors present a new paradigm for high-$T_C$ superconductivity as here Cooper-pairs appear to emerge upon chemical doping from a metallic ground state as opposed to a Mott insulator as found in the celebrated High-$T_C$ cuprates. Despite this difference of parent ground state of the Fe- and Cu-based superconductors, similarities lie in that in both cases superconductivity emerges after the suppression of static ordered magnetism. Although band theory has correctly predicted the unusual antiferromagnetic (AFM) order in the parent compounds of the Fe-based superconductors, it consistently overestimates the tendency to magnetism and underestimates the electronic mass, so there is no doubt that electronic interactions can not be ignored in quantitative descriptions, and that they play a different role compared to cuprates. The exact role of correlations, especially once the parent phase of the Fe-superconductors is doped, has been the focus of much debate and controversy.

An almost universal feature of the Fe-superconductors is that in the parent phases, there is a tetragonal to orthorhombic structural phase transition that is closely associated with the onset of antiferromagnetic order. Upon chemical doping $x$, the onset of the structural and magnetic transitions ($T_S$ and $T_N$ respectively) decrease with $x$ and superconductivity emerges. The physical nature of the cross over from antiferromagnetic order to superconductivity varies between specific materials. In some cases both $T_S$ and $T_N$ coincide while in others $T_S$ is a few degrees higher than $T_N$.

Band structure calculations have suggested that the AFM ordering is accompanied by a strong restructuring of the Fermi surface, with the Fermi surface area being reduced by roughly an order of magnitude. This has been confirmed by optical and Hall measurements that register a drastic reduction of the carrier concentration in the AFM state. The calculated AFM Fermi surface consists of several small pockets, which are arranged in the Brillouin zone in a way that strongly breaks the tetragonal symmetry, but each of them is rather isotropic. This led to a prediction of small transport anisotropy. An alternative point of view, that associates the orthorhombic transition with orbital (charge) degrees of freedom, suggests a double exchange (metallic) ferromagnetic interaction along one crystallographic direction and a superexchange along the other direction. This picture is also consistent with the observed AFM direction and naturally suggests a metallic conductivity along the ferromagnetic chains and a substantially reduced conductivity in the other direction.

Recent experiments on detwinned single crystals support the former point of view: they demonstrate a small anisotropy with the AFM direction being more, not less metallic. However, transport measurements are integrated probes, and also involve possibly anisotropic scattering rate, therefore experiments directly probing the topology of the Fermi surface in the AFM state are highly desirable.

One such experiment has been recently performed by Chuang et al. They have reported quasiparticle interference (QPI) imaging of a lightly cobalt doped sample of CaFe$_2$As$_2$ compound. They interpreted their result in terms of a quasi-1D (“unidirectional”) electronic structure, metallic only along the FM, consistent with above-mentioned orbital picture. On the other hand, their argumentation was rather indirect, based largely on the fact that directly measured dispersion of the QPI maxima (which was indeed 1D) coincided with the ARPES-measured band dispersion along the the same direction.

In this paper we show that in reality the data of Ref. are consistent with the calculated ab initio Fermi surfaces, and not with the implied in that work 1D bands. This reconciles completely the apparent contradiction between the conclusions of Ref. and the transport measurements on untwinned samples.

The reported STM examination shows a QPI pattern in the momentum space that breaks completely the $C_4$ symmetry, the main features being two bright spots along the $y$ (crystallographic $b$) direction, with no counterparts along $x$ (note that $y$ is the ferromagnetic direction, and...
x in the antiferromagnetic one). Ref. 1 insists “that the scattering interference modulations are strongly uni-
directional, which should occur if the k-space band sup-
porting them is nematic”. However it should be kept in
mind that this occurs in that part of the phase diagram
where the long-range antiferromagnetic order is fully es-
lished, as reflected by the fact that the lattice sym-
metry is orthorhombic, and the $C_2$ symmetry is already
completely broken. Indeed the size of the orthorhombic
distortion is not “minute”, as Ref. 1 posits, with $b/a ~ 1%$, and is instead comparable with distortions seen in
various iron oxides systems. For instance, in the Verwey
transition the Fe-O bond dilation is $\sim 0.6\%$ with Fe atoms
in the same tetrahedral symmetry as in the ferropnictide
superconductors, and this is usually considered to be
a strong distortion. Similarly, in the antiferromagnetic
phase of FeO, where the cubic symmetry is completely
broken, the structural effect is also on the same order.

Since the sample under study is orthorhombic it is mis-
leading to call its electronic structure nematic, as the lat-
tice orthorhombic distortion here is substantial. Nematic
phases are frequently found in organic matter. The defin-
ing characteristic of these phases is orientational order in
the absence of long range positional order, resulting in
distinctive uniaxial physical properties. It has also been
proposed that nematic order exists in some electronic sys-
tems, and may even play a role in mediating high tem-
perature superconductivity. Borzi et al demonstrated the
presence of another interesting phase in $\text{Sr}_3\text{Ru}_2\text{O}_7$ at millikelvin temperatures and high magnetic fields, which
has also been called nematic. In this case, the crystallo-
graphic planes were shown to remain strictly tetragonal
(withing $0.01\%$) with $C_4$ structural symmetry, while a
pronounced $C_2$ asymmetry in electronic properties was
measured. This breaking of the electronic symmetry
compared to that of the underlying lattice is now con-
ventionally referred to as electronic nematicity (in fact,
even in those cases one has to be careful to distinguish
between nematic physics and simply an unusually weak
electron-lattice coupling, but this goes beyond the scope
of this paper, and in any event is not a concern for Fe
pnictides where this coupling is strong).

Since the tetragonal symmetry is decisively broken at
the onset of the magnetic order in this ferropnictide, it
is clear that the symmetry of the electronic structure
defining the structural distortion is also completely bro-
den. What is more important is that while the observed
QPI pattern does violate the $C_4$ symmetry, it is clearly
not one-dimensional, in the sense that it varies equally
strongly along $k_x$ and $k_y$ directions. Thus, interpretation
of the data in terms of a 1D electron band does not ap-
pear to be possible. To understand this experiment one
needs to start with a realistic model for the electronic
structure and actually calculate the QPI pattern.

Such calculation has recently been presented by Knolle
et al. They used a weak-coupling theory that inter-
prets the antiferromagnetic state as resulting from a spin-
Peierls transition, with a correspondingly small magnetic
moment. Knolle et al have been able to describe quali-
tatively the experimental data obtained by Chuang et al
in the sense that their calculated QPI pattern strongly
breaks the $C_2$ symmetry, while the band dispersion, on
average, remains fairly isotropic in plane. Note that one
should not be looking for a quantitative interpretation,
since the STM experiment in question did not detect any
Ca atoms on the surface, so the sample surface is likely
charged with up to 0.5 hole per Fe, and thus any bulk
calculation can only be applied to this experiment in a
qualitative way. Besides, it was recently shown that
Fe pnictide systems feature surface states quite different
from the bulk that should undoubtedly affect the STM
spectra.

However, this result, as mentioned, has been obtained
in a weak coupling limit, corresponding to small magneti-
ization, while in this system the ordered magnetic mo-
tions are on the order of 1 $\mu_B$, and local moments even
larger. Not surprisingly, their Fermi surface is rather
far from that measure recently on untwinned samples by
Wang et al, while the LDA Fermi surface reproduces
it quite well. Indeed, this is a known problem in the
weak coupling approach: while being physically justified
for the paramagnetic parts of the phase diagram, the Fe
magnetism in the ordered phases is driven by the strong
local Hund rule coupling, and not by the Fermi surface
nesting, as assumed in the weak coupling models.

Therefore we have calculated the QPI images for anti-
ferromagnetic $\text{CaFe}_2\text{As}_2$ entirely from first principles7 ,
using the Local Density Approximation (LDA) magnetic
moment (somewhat larger that the experimental mo-
tment at zero doping). We used the standard linear
augmented plane wave method as implemented in the
WIEN2k code12. The corresponding Fermi surface is
shown in Fig. 1. We see that the magnetism has a dras-
tic effect on the Fermiology, and the resulting Fermi sur-
faces are completely breaking the $C_4$ symmetry. Apart
from small quasi-2D tubular pockets, originating from
Dirac cones, there is one hole pocket around $Z (0,0,\pi/c
or 2\pi/a,0,0)$ and two electron pockets between $Z$ and
$0,\pi/b,\pi/c$. It is immediately obvious that the QP scat-
tering between these pockets must exhibit strong interfer-
ence for scattering along $b$, but not $a$. 

![FIG. 1: (Color online) Calculated LDA Fermi surface for $\text{CaFe}_2\text{As}_2$ in the antiferromagnetic state.](image.png)
Indeed, we have calculated the QPI function $Z$, using the known expression (Ref. 19, Eq. S9)

$$|Z(q, E^\prime)|^2 \propto \int \frac{dE^\prime}{E - E^\prime} \sum_k \delta(E - E_k)\delta(E^\prime - E_{k+q}), \quad (1)$$

where we assumed a constant in-purity scattering rate and a constant tunneling matrix elements. This approximation is sufficient for a qualitative or semiquantitative comparison. As explained above, given that the surface in the experiment in question was charged compared to the bulk, a quantitative comparison is meaningless.

A calculated pattern (there is some dependence on $q_z$ and $E$, but we are interested in the qualitative features only) are shown in Fig. 2. One can see immediately that, very similarly to the patterns obtained in Ref. 11, two sharp maxima appear at $q = 0, \pm \xi, 0$, where $\xi \sim \pi/4b$. The origin of these QPI features is obvious from the Fermi surface (Fig. 1). Note that these LDA calculations have no adjustable parameters, and yet are in excellent qualitative agreement with the QPI images.

It is also worth noting that while the calculated Fermi surfaces completely break the tetragonal symmetry, which is fully reflected in the QPI images, the individual pockets are very three-dimensional, so that the calculated conductivity is comparable for all three directions. While experimentally there is up to a 20% $a/b$ charge transport anisotropy, close to tetragonal to orthorhombic phase boundary in CaFe$_2$As$_2$, it is much less than what would be predicted for a quasi 1D electronic band, and of the opposite sign.

It may be worth at this point to explain at some length while a quantitative comparison between a Fourier transform of a tunneling current map, and theoretical calculations, whether ours or any other, is impossible at this stage. Quasiparticle interference, as discussed in many papers, manifests itself in tunneling in a very indirect way. In a sense, it is a multistage process. First, a defect existing near the metal surface, is screened by the conducting electrons. This creates Friedel oscillations in the real space. This oscillations are formed by all electrons (mostly those near the Fermi surface, but not only). In a multiband system, it includes electrons originated from different atomic orbitals, such as $xy, xz, yz, z^2$ and $x^2 - y^2$. As is well known in the theory of tunnelling, the rate at which electrons tunnel through vacuum depends drastically on their orbital symmetry, especially on their parity (see, e.g., Ref. 21). Indeed tunnelling through a wide barrier mainly proceeds through electrons with zero momentum projection onto the interface plane (such electrons have to travel the shortest length in the subbarrier regime). If such electrons belong to an odd 2D representation (for d-electrons, all but $z^2$, if $z$ is the normal direction), the tunneling rate is suppressed. This effect is well known in spintronics, where it can drastically change the current spin polarization. On the other hand, for a thin barrier the tunneling conductance depends on the number of the conductivity channels, which is given by the density of states (DOS) times normal velocity. In both cases, it is not just the density of quasiparticles, as assumed in Eq. 1 (and in Ref. 11), but the DOS weighed by a strongly $k$-dependent, unknown function.

Nothing is known about the nature of the scattering centers, producing the above mentioned Friedel oscillations. In this particular experiment they may be magnetic or nonmagnetic defects, twin domain boundaries, antiphase domain boundaries, remaining surface Ca ions, and more. Some of these scatterers are strongly anisotropic by nature, others are strongly dependent on the orbital character. We have dropped the scattering matrix elements completely form our consideration. Knolle et al instead have chosen a specific model for the scattering centers. We believe that without any knowledge about the actual scattering centers in the system any QPI using a particular model is more obscuring the actual physics, compared to the simplest constant matrix elements approximation, rather than clarifying it.

Finally, there are several issues specific for this particular experiment: (1) unknown, but strongly different from the bulk, charge state. As opposed to Ba122, and Sr122, where 1/2 of the alkaline earth atoms stay on the surface, providing charge neutrality, in Ca122 STM does not detect any Ca on the surface, suggesting a strongly charged surface. A corollary of that is appearance of a surface reconstruction (as indeed observed), of a surface relaxation, and, importantly (since tunneling proceeds largely through the surface states), of surface bands (as demonstrated, for instance, in Ref. 22).

While the above considerations preclude a quantitative comparison and extracting quantitative analysis of the experiment in question, we see, particularly when comparing our calculations with those of Knolle et al, that the $C_2$ QPI structure observed in Ref. 1 is a very universal consequence of the long-range stripe-type antiferromagnetic ordering. Indeed, Knolle et al calculations were

FIG. 2: (Color online) Quasiparticle interference pattern (in arbitrary units) for zero bias and $q_z \sim 0$, calculated using the same electronic structure as in Fig. 1 and Eq. 1.
built upon a basically incorrect band structure and fermi surfaces, an used a weak coupling nesting scenario for the antiferromagnetism, while in reality the magnetism in pnictides is a strong coupling phenomenon; yet, their calculations produced a “unidirectional” QPI pattern just as well. Together with the strong-coupling LDA calculations, this span a large range of possible models, indicating that the $C_4$ symmetry is strongly broken in QPI images with simply by virtue of the long range AFM order, whatever the the origin of this order.

Last but not least, we can also predict, from our calculations, that this symmetry will be also broken, although the peaks are likely to be substantially broaden, in the truly nematic phase (see review for a discussion), that is to say, the phase between the long-range magnetic transition and the structural orthorhombic transition.

1. T.-M. Chuang, M. P. Allan, J. Lee, Y. Xie, N. Ni, S. L. Bud’ko, G. S. Boebinger, P. C. Canfield, J. C. Davis, Science, 327, 181 (2010).
2. M.A. Tanatar, E. C. Blomberg, A. Kreyssig, M. G. Kim, N. Ni, A. Thaler, S. L. Bud’ko, P. C. Canfield, A. I. Goldman, I. I. Mazin, and R. Prozorov, Phys. Rev. B 81, 184508 (2010).
3. P.A. Lee, N. Nagaosa, X.-G. Wen, Rev. Mod. Phys. 78, 17 (2006).
4. I. I. Mazin, Nature, 464, 183 (2010).
5. D.C. Johnston, Adv. in Phys., 59, 803 (2010).
6. W. Z. Hu, J. Dong, G. Li, Z. Li, P. Zheng, G. F. Chen, J. L. Luo, and N. L. Wang, Phys. Rev. Lett. 101, 257005 (2008); L. Fang, H. Luo, P. Cheng, Z. Wang, Y. Jia, G. Mu, B. Shen, I. I. Mazin, L. Han, C. Ren, and H.-H. Wen, Phys. Rev. B 80, 140508 (R) (2009); F. Rullier-Albenque, D. Colson, A. Forget, and H. Alloul, Phys. Rev. Lett. 103, 057001 (2009).
7. J. P. Wright, J. P. Attfield, and P. G. Radaelli, Phys. Rev. Lett. 87, 266401 (2001).
8. D.G. Isaak, R. E. Cohen, M. J. Meh, and D. J. Singh, Phys. Rev. B 47, 7720 (1993).
9. S.A. Kivelson, E. Fradkin, and V.J. Emery, Nature 393, 550 (1998).
10. R. A. Borzi, R. A. Borzi, S. A. Grigera, J. Farrell, R. S. Perry, S. J. S. Lister, S. L. Lee, D. A. Tennant, Y. Maeno, A. P. Mackenzie, Science, 315, 214 (2006).
11. J. Knolle, I. Eremin, A. Akbari, R. Moessner, Phys. Rev. Lett. 104, 257001 (2010).
12. E. van Heumen, J. Vuorinen, K. Koepernik, F. Massee, Y. Huang, M. Shi, J. Klei, J. Goedkoop, M. Lindroos, J. van den Brink, M. S. Golden, http://arxiv.org/abs/1009.3493 (unpublished).
13. I.I. Mazin and J. Schmalian, Physica C, 469, 614-627 (2009).
14. M.D. Johannes, I.I. Mazin, D.S. Parker, Phys. Rev. B 82, 024527 (2010).
15. M.D. Johannes and I.I. Mazin, Phys. Rev. B 79, 220510(R) (2009).
16. Q. Wang, Z. Sun, E. Rotenberg, F. Ronning, E.D. Bauer, H. Lin, R.S. Markiewicz, M. Lindroos, B. Barbiellini, A. Bansil, D.S. Dessau, arXiv:1009.0271 (unpublished).
17. Compared to Ref.12, both $\beta 1$ and $\beta 2$ bands are present, their nontrivial crescent shape is reproduced, their size and location (around the $Z$ point) are consistent with the calculation. Not that these $\beta$ pockets are mainly responsible for the QPI peak in our Fig. 2. The flattish $\gamma$ pocket is also in excellent agreement with the calculation, although in the experiment it is split into $\gamma 3$ and $\gamma 4$ (probably an effect of the surface reconstruction). The claimed experimental bands ($\alpha 1$, $\alpha 2$, $\gamma 1$ and $\gamma 2$) along Z-X are quite messy. The calculations predict small pockets there located roughly where ARPES sees some bands. These are formed by the famous “Dirac cones”. The only feature that does not find any correspondence in the calculation is the long segment “$\gamma2$” stretched along $k_y$. This may be a surface state similar to those discovered in Ref.12 (note that this band is drawn rather speculatively, the corresponding signal is really weak). This agreement is even more impressive given that the Fermi surface reproduced here was published 7 months ago (Ref.12), well before any untwinned ARPES data became known, from 1D bands.
18. P. Blaha et al., computer code WIEN2K, Technische Universität Wien, Austria, 2001;
19. T. Hanaguri, T. Hanaguri, Y. Kohsaka, M. Ono, M. Matsu, P. Coleman, I. Yamada, M. Azuma, M. Takano, K. Ohishi, and H. Takagi, Science 323, 923 (2009).
20. Measurement of charge transport in Co-doped BaFe$_2$As$_2$ reported by J-H. Chu, J. G. Analytis, K. De Greve, P. L. McMahon, Z. Islam, Y. Yamamoto, and I. R. Fisher, Science 329, 824 (2010), show a larger $a/b$ anisotropy close to the orthorhombic transition, which we believe not to be representative of the CaFe$_2$As$_2$ upon which the STM measurements of Ref.1 were taken. Regardless, the values of a factor of 2 anisotropy for doped samples in that study still remain too low to be associated with the large anisotropies expected from unidirectional band structure suggested in Ref.1 and are of the opposite sign.
21. I. I. Mazin, Europhys. Lett., 55, 404, 2001.
22. E. van Heumen, J. Vuorinen, K. Koepernik, F. Massee, Y. Huang, M. Shi, J. Klei, J. Goedkoop, M. Lindroos, J. van den Brink, M. S. Golden, http://arxiv.org/abs/1009.3493 (unpublished).