Available online at www.sciencedirect.com
ScienceDirect
Journal of Electron Spectroscopy and Related Phenomena 159 (2007) 91–93
JOURNAL OF ELECTRON SPECTROSCOPY and Related Phenomena
www.elsevier.com/locate/elspec

Short communication

From tunneling to photoemission: Correlating two spaces ☆

A.A. Kordyuk [a,b,*], V.B. Zabolotnyy [b], D.S. Inosov [b], S.V. Borisenko [b]

[a] *Institute of Metal Physics of National Academy of Sciences of Ukraine, 03142 Kyiv, Ukraine*
[b] *Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, 01069 Dresden, Germany*

Received 14 September 2006; accepted 13 February 2007
Available online 20 February 2007

Abstract

Correlating the data measured by tunneling and photoemission spectroscopies is a long-standing problem in condensed matter physics. The quasiparticle interference, recently discovered in high-T_c cuprates, reveals a possibility to solve this problem. Application of modern phase retrieval algorithms to Fourier transformed tunneling data allows to recover the distribution of the quasiparticle spectral weight in the reciprocal space of solids measured directly by photoemission. This opens a direct way to unify these two powerful techniques and may help to solve a number of problems related with space/time inhomogeneities predicted in strongly correlated electron systems.

PACS: 42.30. −d; 79.60. −i; 68.37. −d; 74.72. −h

Keywords: Photoemission spectroscopy; Tunneling spectroscopy; Fermi surface; Fourier transformation

1. Introduction

The electronic inhomogeneity in high-T_c cuprates (HTSC) seen by scanning tunneling spectroscopy (STS) [1] has attracted much interest from the scientific community because of its clear relation to a central problem of HTSC—the mechanism of their evolution with hole doping from the antiferromagnetic insulator to superconductor. Recent breakthrough in the development of STS technique to a level where the Fourier transformed (FT) STS images have been crystallized into well-defined symmetric patterns [2] has revealed the existence of regular inhomogeneities which could relate the HTSC problem to self-ordering phenomena in correlated electron systems. An important step in this direction has been made by identifying the essential part of these inhomogeneities with rather trivial quasiparticle interference (QI) through an impurity scattering hypothesis [2–4], which says that the FT STS function, $\mathbf{F}S(\mathbf{r})$, is proportional to a joint density of states $C(\mathbf{q})$ which, in turn, is just an autocorrelation (AC) of the quasiparticle spectral function $A(\mathbf{k})$. However, a reason for the remaining non-QI inhomogeneities, as well as the scattering hypothesis by itself, is yet to be understood. This is due, in part, to lack of deep understanding of the scattering phenomenon, but mainly due to an absence of a direct transition from the joint $\mathbf{q}$-space of FT STS to the reciprocal $\mathbf{k}$-space where the distribution of the quasiparticle spectral function, $A(\mathbf{k})$, is known from the angle resolved photoemission spectroscopy (ARPES) with a tremendous accuracy [5]. The AC procedure gives an attractive possibility to compare the FT STS images to the AC ARPES data but evidently suffers from the absence of a direct transformation from the joint to plain reciprocal spaces: due to presence of experimental factors such as matrix elements the process of fitting $A(\mathbf{k})$ to $C(\mathbf{q})$ is time consuming and, more important, does not give a unique solution [6,7]. Here, we suggest a procedure to uniquely recover $A(\mathbf{k})$ from $S(\mathbf{r})$, shifting the problem of STS and ARPES correlation to ARPES domain.

To understand the essence of the concept, let us rewrite the above mentioned impurity scattering hypothesis in a symbolic way:

$$|\mathbf{F}S| = \mathbf{AC}\, A = C. \tag{1}$$

The AC is defined as

$$\mathbf{AC}\ \ A(\mathbf{k}) = \int A(\mathbf{k})A(\mathbf{k}+\mathbf{q})\,\mathrm{d}\mathbf{k} = C(\mathbf{q}), \tag{2}$$

and is therefore an irreversible and time consuming operation.

☆ The project is part of the Forschergruppe FOR538.
* Corresponding author. Tel.: +49 351 4659 566; fax: +49 351 4659 440.
E-mail address: kordyuk@gmail.com (A.A. Kordyuk).

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doi:10.1016/j.elspec.2007.02.017

Nevertheless, we have found that both problems can be solved using the Wiener-Khinchin theorem [8], which sets an extremely important relationship between AC and FT:

$$\mathbf{AC}\, A = \mathbf{F}^{-1}|\mathbf{F}A|^2. \tag{3}$$

The fast Fourier routine essentially speeds up the calculations, but more important is that the theorem shows the way to reverse the autocorrelation procedure and derive $A(\mathbf{k})$ from $S(\mathbf{r})$. With Eq. (3), the impurity scattering hypothesis can be rewritten as

$$|\mathbf{F}A| = \sqrt{\mathbf{F}|\mathbf{F}S|}, \tag{4}$$

and the problem is reduced to recovering of a function from its Fourier amplitude $R(\boldsymbol{\rho}) = |\mathcal{R}(\boldsymbol{\rho})| = |\mathbf{F}A(\mathbf{k})|$.

Fortunately, similar problem arose in applied optics and a number of phase retrieval algorithms (PRA) were developed [9]. These algorithms involve iterative Fourier transformation back and forth between the object and Fourier domains with application of the known constraints.

Fig. 1 (top row) shows $A(\mathbf{k})$—a gaped quasiparticle density of states of an optimally doped CuO-bilayer—as well as the real part of its Fourier image, $\mathrm{Re}(\mathbf{F}A)$, and the result of its autocorrelation, $\mathbf{AC}\, A$. $A(\mathbf{k})$ is simulated at 20 meV binding energy based on experimentally determined parameters of the bare band dispersion for an optimally doped Bi-2212 compound [10] taking into account a d-wave superconducting gap $\Delta = \Delta_0(\cos k_x - \cos k_y)/2$ with $\Delta_0 = 40$ meV. We note, that $\mathrm{Im}(\mathbf{F}A) = 0$ due to even symmetry of the spectral function, $A(\mathbf{k}) = A(-\mathbf{k})$, so, the problem can be reduced to recovering of a *real* smooth function from its modulus. It seems that such a procedure can be realized, in principle, but should evidently suffer from finite resolution and unavoidable uncertainty of the experiment.

In turn, the PRA are essentially discrete. Their uniqueness, in case of positive and spatially confined object, has been proved theoretically while the stability to noise and speed of convergence are the issues of continues development [9]. The recovering of $A(\mathbf{k})$ from $|\mathbf{F}A|$ by means of PRA is illustrated by Movie 1 [11]. Here, we used a modified "input–output" algorithm [9], the n th iteration of which can be formulated as follows:

$$\mathcal{R}_n = \mathbf{F}A_n, \tag{5}$$

$$\mathcal{R}'_n = R\,\exp[i\arg(\mathcal{R}_n)], \tag{6}$$

$$\mathcal{A}'_n = \mathbf{F}^{-1}\mathcal{R}'_n, \tag{7}$$

$$A_{n+1} = \begin{cases} \mathrm{Re}(\mathcal{A}'_n) & \text{if } \mathrm{Re}(\mathcal{A}'_n) \geq 0, \\ \mathrm{Re}(A_n - \beta\mathcal{A}'_n) & \text{if } \mathrm{Re}(\mathcal{A}'_n) < 0, \end{cases} \tag{8}$$

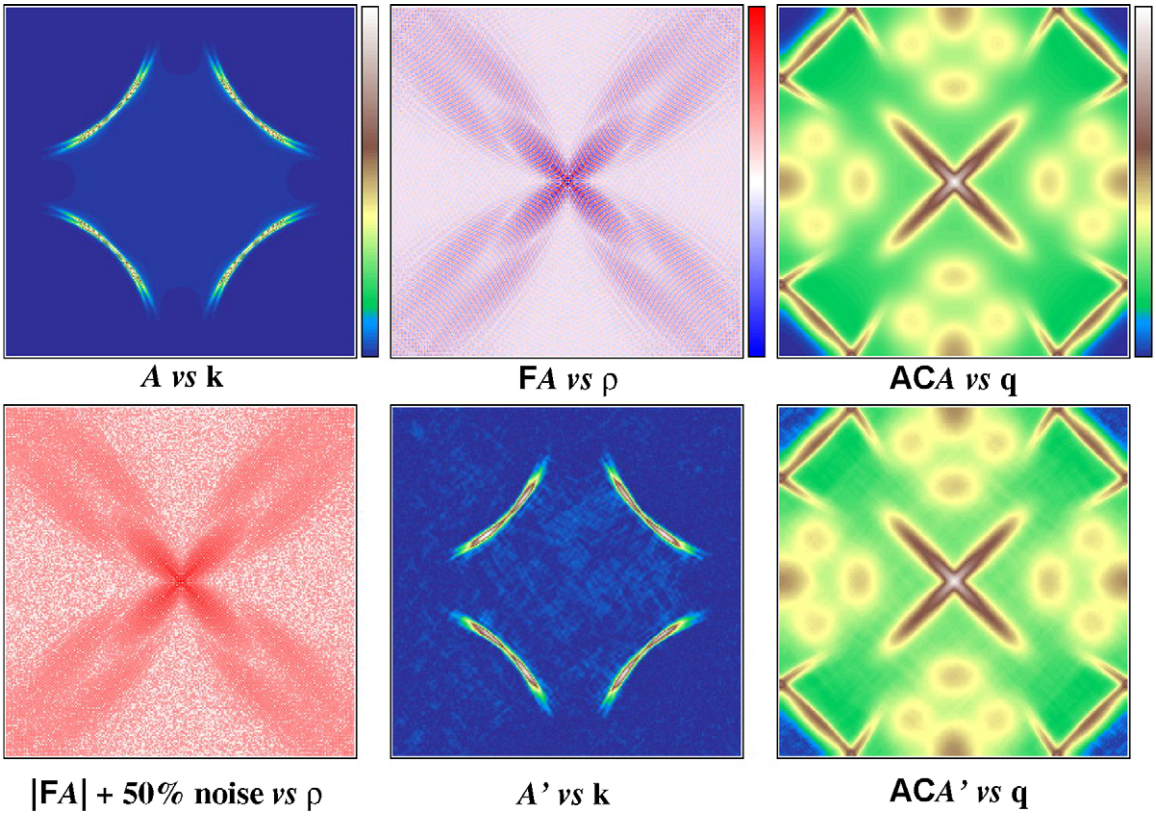

Fig. 1. Representations of quasiparticles in different spaces of high-T_c cuprates: the spectral function A in the reciprocal space $\mathbf{k}$, the real part of its Fourier image $\mathbf{F}A$ in a joint real space $\boldsymbol{\rho}$, and a joint spectral weight $C = \mathbf{AC}\, A$ in a joint reciprocal space $\mathbf{q}$. The reverse transformation $C \rightarrow A$ is possible by means of PRA (see Movie S1). The bottom row illustrates the stability of PRA to experimental uncertainty—a noise has been added to $|\mathbf{F}A|$ (see also Movie S2). $A(\mathbf{k})$ is simulated at 20 meV binding energy based on experimentally determined parameters of the bare band dispersion for an optimally doped Bi-2212 compound [10] taking into account a d-wave superconducting gap $\Delta = \Delta_0(\cos k_x - \cos k_y)/2$ with $\Delta_0 = 40$ meV; $\mathbf{k}$- and $\mathbf{q}$-images cover exactly the 1st Brillouin zone.

where $R(\boldsymbol{\rho})$ is a "source" function, and β is a constant which we choose between 1 and 2 as a compromise between speed of convergence and stability of the algorithm. As an initial guess we used a Gaussian distribution with random noise: $A_0(\mathbf{k}) = \exp(|\mathbf{k}|^2/w^2) + noise$.

Bottom row of Fig. 1 illustrates the robustness of PRA to experimental uncertainty: $A'(\mathbf{k})$ is recovered from a noisy $|\mathbf{F}A|$ (the noise has been simulated by a random value from a Gaussian distribution such that the standard deviation of an infinite number of such values would be 50% of the average value of $|\mathbf{F}A|$). The work of RPA in this case is illustrated by Movie 2 [11].

Finally, we discuss the existent attempts to compare the STS and ARPES data in the **q**-domain [4,6,7]. It has been shown that the intensity maps measured by ARPES, when autocorrelated, does not result in so distinct spots as observed in FT STS images [4]. The correspondence can be made better assuming better energy resolution in ARPES [4], or **k**-dependent matrix elements in STS [6]. We believe that both effects should be taken into account together with the gaped and highly anisotropic quasiparticle self-energy, but, in this paper, we do not purpose to define a region of parameters which result in spot patterns seen in FT STS. Instead, we suggest the approach to recover $A(\mathbf{k})$ from FT STS, shifting this problem to ARPES domain. Comparing $A(\mathbf{k})$, measured directly by ARPES, to $A'(\mathbf{k})$, determined from STS by means of the suggested approach, will clarify the intriguing problem between ARPES and STS data. Namely, the question whether or not the ordered inhomogeneities seen by STS can be detected by ARPES (see ref. [12] and references therein). This will provide an insight into the nature of these inhomogeneities. We also believe that such a comparison will resolve other inconsistencies between ARPES and STS data. In particular, it will help to understand the discrepancy in the values of the quasiparticle self-energies determined from STS and ARPES experiments on high-T_c cuprates [13], and clarify the problem of tunneling matrix elements [13].

In summary, we have proposed a procedure to derive the distribution of the quasipartical spectral weight in plain reciprocal space of a crystal from STS measurements and demonstrated its robustness to experimental uncertainty. When applied to STS data, this procedure will give an ultimate check for the validity of the impurity scattering hypothesis and open a direct way to unify STS and ARPES techniques. Such a unification has two evident prospects: (i) to reveal any inconsistencies between real and reciprocal manifestations of electronic world of crystals, and (ii) to combine, when the inconsistencies are understood, the power of the momentum resolution of ARPES with extremely low energy resolution of STS.

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