Slow fracton modes in antiferromagnetic correlations of high-\(T_c\) superconductors

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(Dated: December 7, 1999)

In cuprate superconductors superconductivity develops as a unique crossover between the two extremes characterizing these compounds, an antiferromagnetic (AF) Mott insulator phase, on one side, and a non-superconducting itinerant metal on the other. The hole doping tunes a cuprate inside such a broad spectrum of phases. Numerous inelastic neutron scattering studies on underdoped samples shows most directly that the static AF order of the parent phase does not disappear by doping but transforms in such a way that at least fluctuating and local AF order persists, coexisting with superconductivity. Structurally, the model of stripe-type correlations accounts for the coexistence while their genuine dynamics might hides the most interesting physics of cuprates, including the pairing mechanism. Indeed, there is an impressive accumulation of knowledge in favour of AF correlations underlying the pairing. Some crucial properties of these correlations have recently been pointed out: they should involve small velocity collective modes of the wave vector identical to that of the static AF order, while their energy scale (< 50 meV) should be rather low compared with any other involved. Here we show on phenomenological ground that the latter dynamics originates, irrespective of structural details of stripe order, from general geometrical constraints known to characterize the problem of disordered interpenetrated phases. In particular, we show that dynamics of the Euclidean-to-fractal crossover introduces a new (10-50 meV) energy scale, associated with slow (or almost localized) and well-defined fracton modes, and provides a consistent and natural interpretation for redistribution of spectral weight and other inelastic neutron scattering observations. We conclude therefore that the fracton excitations substantially contribute to pairing interactions in high-\(T_c\) cuprates.

High-resolution studies of dissipation in weak link network of polycrystalline cuprates have recently identified a fractal dissipative regime inside which a self-organized current-carrying medium is an object of fractal geometry. Taking into account that the Josephson-coupled disordered medium represents a good description of the problem of phase coherence not only between the \(\text{CuO}_2\) planes but also inside them (due to stripes and/or other forms of charge separation and clustering, filamentary fragmentation, etc.) the presence of fractal geometry in self-organized structures of \(\text{CuO}_2\) planes seems rather plausible as well. In this work we investigate elastic modes in such a hypothetical (but still physically justified) two dimensional (2D) fractal lattice. In particular, we study AF spin fluctuations inside a model which allows a fractal geometry of the relevant AF cluster; the latter, being sample-sized and homogeneous in the parent compound, gets progressively more ramified by hole doping. (The liquid-crystal-like stripe phases represent of course a closely related visualization).

Generally, the dynamical features of such a problem are well-known: instead of extended modes (phonons or magnons) of elastic quasi-continuum the vibrational modes in fractal lattices are localized excitations, known as fractons. The fractality of real lattices depends on wave vector of the considered excitation so the fracton modes start to dominate only above some critical wave vector, i.e., above the frequency of phonon-to-fracton crossover. Also, there is a considerable accumulated knowledge about fractons specifically in classical diluted antiferromagnets both in their theoretical and experimental aspects. In these classical systems the magnetic component responsible for static AF order (e.g., \(\text{Mn}^{2+}\) ion in \(\text{MnF}_2\) or in \(\text{RbMnF}_3\)) is substituted at random by non-magnetic substituent (e.g., \(\text{Zn}^{2+}\) or \(\text{Mg}^{2+}\), respectively). Inelastic neutron scattering studies on samples comprising substituent in concentrations approaching threshold concentration (above which there would be no magnetic order) revealed dynamical features consistent with predictions for AF fractons. However, besides some doubts regarding proper assignment of specific experimental features there are still some uncertainties about the proper analytical form of the dynamical structure factor to be applied in modeling fractal antiferromagnets.

Applying this knowledge to the problem of underdoped cuprates we first simplify our elaboration by limiting ourselves to the case of localized magnetic moments (spins associated to \(\text{Cu}^{2+}\) ions) only. There is a consensus now that this is entirely appropriate for the spin wave phase of parent AF compounds but also equally inappropriate for the overdoped non-superconducting systems being compatible with itinerant electron description. The present work explores primarily the underdoped range. Localized description certainly makes sense for low hole concentration but becomes questionable close to optimal doping. There is however an increasing number of arguments pointing...
out the localized nature of incommensurate magnetism even in optimally superconducting samples (oxygen doped La$_2$CuO$_{4+y}$), so one could expect that the model we elaborate here may be applied at least to a reasonably wide range of underdoped concentrations. Now we define our ‘building block’ which, playing the role of a non-magnetic ion in diluted antiferromagnets, are to be placed at random in the initially homogeneous and antiferromagnetic CuO$_2$ plane. The fluctuating stripe correlations are certainly the most convincing interpretation for the incommensurate magnetism in superconducting cuprates and the local stripe order seems to be an inevitable element of cuprate physics. Our building blocks are therefore the regions with stripe order, disordered in sizes and, possibly, in other features. By ‘stripe order’ we mean, in accordance with the localized magnetism of the present model, the original pattern of ‘the three spins wide AF stripes separated by non-magnetic antiphase domain boundary’. The internal structure of the building block complicates somewhat the geometrical percolation scenario of the diluted antiferromagnets; thus, we do not attempt to define the threshold hole concentration here. However, one expects that the main qualitative elements of an crossover to fracton dynamics, in increasing hole concentration, remain valid.

Qualitatively, the scenario for underdoped cuprates would be the following: With no holes added the magnetic collective modes are high-velocity ($h\nu = 650$ meVÅ, typically) regularly damped spin waves (Fig.1a) characterized by dominantly 2D dynamics. The latter follows from the very high inplane superexchange (100 meV, typically) compared with the interplane one. Added holes introduce random obstacles for spin waves localizing them into fracton modes at short wave lengths ($q > q_c$), i.e., above the hole-concentration-dependent cross over energy $h\nu_c = h\nu_{qc}$. This takes place when ramified AF cluster becomes self-similar (fractal) on all spatial scales smaller than 1/q$_c$, subsequently, the crossover frequency progressively decreases as hole concentration (thus cluster fractality) increases.

Quantitatively, all of these dependencies must obey specific power-laws involving several static and dynamical exponents (e.g., correlation length and dynamical one, fractal and AF fracton dimensions) which are, at least approximately, known. The dynamical structure factor $S(q, \omega)$ has to include these power-laws and to assure known asymptotic behaviour characterizing the homogeneous ($\omega \ll \omega_c$) and the fractal ($\omega \gg \omega_c$) regime. The problem of dynamical structure factor for AF fractons has been treated by many approaches most of which are founded on the effective-medium considerations. Out of several probably equivalent results for $S(q, \omega)$ in this work we use the form of Polatsek and Entin-Wohlman as it explicitly demonstrates the localization features of fracton modes (Fig.1b). Although the latter result suffers from general shortcomings of all effective medium approaches, why it cannot quantitatively be correct in all details, its general Green’s function background assures its basic usefulness. This form has been successfully used in studies of fractons in silica aerogel and, more recently, in fused silica. Therefore, the form we propose to determine the scattering cross section of AF spin waves in cuprate CuO$_2$ planes of increasing fractality reads as

$$S(q, \omega) = \left[ \frac{v(\omega)q}{\omega^2} \right] \frac{\Gamma(\omega)}{(\omega - v(\omega)q)^2 + \Gamma^2(\omega)} - \frac{\Gamma(\omega)}{(\omega + v(\omega)q)^2 + \Gamma^2(\omega)},$$

where $v(\omega)$ and $\Gamma(\omega)$ are velocity of spin waves and damping (lifetime) function, respectively. The frequency dependence of these two quantities makes the present $S(q, \omega)$ different, together with its prefactor, from standard Lorentzian ‘shape functions’ generally used in scattering problems and, particularly, in the inelastic neutron studies on diluted antiferromagnets. The asymptotic forms of $v(\omega)$ and $\Gamma(\omega)$ are precisely known. At low $\omega$ ($\omega < \omega_c$), $v = v_0$, the magnon velocity, while at high $\omega$ ($\omega > \omega_c$), in fractal regime, it must obey $v(\omega) \propto \omega^z$ ($z$ is dynamical exponent). In the same limits the damping $\Gamma(\omega)$ crosses over from the phonon (magnon)-like Rayleigh law ($\Gamma(\omega) \propto \omega^{d+1}/\omega$), $d$ is Euclidean dimension) to the localized Ioffe-Regel ($\Gamma(\omega) \propto \omega^d$) regime, where both the dispersion and the wave vector description becomes ill-defined. For the specific frequency dependence of $v$ and $\Gamma$ we use the heuristic expressions of Courten et al. shown to work well in different fractal systems. Taking into account a predominantly 2D nature of magnetism in CuO$_2$ planes the expressions are:

$$v(\omega) = v_0 \left[ 1 + (\omega/\omega_c)^m \right]^{2/m}, \quad \Gamma(\omega) = \Gamma_0 \omega_c (\omega/\omega_c)^3 \left[ 1 + (\omega/\omega_c)^m \right]^{-2/m},$$

where $m$ characterizes the sharpness of the crossover. Most of the features of the present model have a weak dependence on the choice of $m$ and the ‘traditional’ value $m = 4$ has been used. Also, in calculation of $z = d_f/d_{a,f}$, where $d_f$ is the fractal and $d_{a,f}$ the AF fracton dimension, a well-accepted value $d_f \approx 1.9$ and $d_{a,f} \approx 0.9$ have been used. We note however that our results depend very little, at least qualitatively, on the fine tuning of exponents. Fig.1 visualizes $S(q, \omega)$ of Eq.1 taking into account real physical parameters of YBCO superconductor.

Now we compare $S(q, \omega)$ with the experimental results for imaginary part of generalized susceptibility $\chi'(q, \omega)$ on cuprates which determines the scattering cross section. These results are summarized in, e.g., Refs. 19,20. Results at fixed $q$ ($\omega$-scan) or at fixed $\omega$ ($q$-scan) depend very much on convolution with instrumental resolution $\Gamma$, involving the integration of intrinsic $S(q, \omega)$ inside usually a sizable resolution ellipse. Hence, a better defined experimental
quantities are momentum- or energy-integrated $\tilde{\chi}(q, \omega)$. The local (Brillouin zone averaged) susceptibility $\chi_{2D}(\omega) \propto \int \chi(q, \omega) dq$ is particularly well investigated\cite{21,22}. In hole doped samples $\chi_{2D}(\omega)$ shows a characteristic maximum (Fig.2b,c) in the range of 20-50 meV while the parent compounds reveal approximately energy independent $\chi_{2D}$, in agreement with $S^{SW}(q, \omega)$ for spin waves. It is important to note that a sizable area of $\chi_{2D}(\omega)$ peaks is positioned, in graphs involving absolute calibration, above the spin wave level. The latter reflects a substantial redistribution of spectral weight in frequency domain as the holes are added to the planes. The present model for $S(q, \omega)$ readily accounts for the redistribution. The 2D integration of our model's $S(q, \omega)$, Eq.1, gives:

$$S_{2D}(\omega) \equiv \int_{B.z.} S(q, \omega) dq = \frac{2\pi \Gamma}{\omega^2 v^2} \left[ \Gamma A(\omega) \left( \frac{\omega^2}{\Gamma^2} - 1 \right) + \omega \ln \left( \frac{(vQ - \omega)^2 + \Gamma^2}{\omega^2 + \Gamma^2} \right) - \frac{(vQ + \omega)^2 + \Gamma^2}{\omega^2 + \Gamma^2} \right]$$

where $Q$ is Brillouin zone boundary and

$$A(\omega) = \arctg \frac{vQ - \omega}{\Gamma} - \arctg \frac{vQ + \omega}{\Gamma} + 2\arctg \frac{\omega}{\Gamma}.$$  

We note again that $v$ and $\Gamma$ are $\omega$-dependent (Eq.2). The result for $S_{2D}(\omega)$, which makes a central result of this paper, is shown in Fig.2a for one particular choice of parameters together with the level which would characterize magnons propagating with velocity $v_0$. Except behaviour just above the origin there is a full reproduction of experimental curves. The physical reason for the redistribution in our model is clear immediately from Fig.1: For very small energies the magnetic modes start to propagate as magnons but soon, by approaching $\omega_c$, slow down and accumulate in the region around $\omega_c$, taking away the spectral weight that magnons would have in the hole-free lattice up to high energies. We discover therefore that $\hbar \omega_c$ represents a natural new scale of energy characterizing the AF correlations in cuprates. $S_{2D}(\omega)$ of Eq.3 perfectly models most of the experimental results by choosing $\hbar \omega_c$ from the interval $10-50 \text{meV}$. The present model attributes the experimental peaks in $\chi_{2D}$ (and also in $\chi''(q, \omega)$, see below) to dynamics of crossover quantified, in this work, by Eqs.2,3. One should note, however, that the main features are not determined by some special choice of spectral function $S(q, \omega)$, such as the one of Eq.1; instead, the features stem from universal principles of matching the two different regimes characterized by different geometrical constraints. In our model there is no principal difference between the narrow ‘resonant’ peaks\cite{22} setting-in below $T_c$, and the broad off-resonant $\omega$ peaks as they both reflect the dynamics of crossover. The experimental differences may come primarily from the involved parameters, such as the damping scale $\Gamma_0$. Indeed, it seems very plausible that the macroscopic superconductivity of the optimum-doped samples allows higher level of fractal self-organization accompanied with the increased value of $\Gamma_0$. One easily verifies that the increased $\Gamma_0$ induces, in turn, a more pronounced peak in $S_{2D}(\omega)$. 

Now we analyze results for fixed fixed $q$-scans) or at fixed $\omega$ (q-scans) in the light of our model, Fig.3. In literature, there are many data for $\chi''$ with $q$ fixed at AF wave vector, $q = (0.5, 0.5)$ in reciprocal lattice units ($\text{rlu}$), measured on a variety of underdoped and optimally doped samples (no significant magnetic correlations has been observed in overdoped range). These results reveal a pronounced peak with the maximum positioned usually inside the interval 20-50 meV but with other details (e.g., temperature dependence, energy width) being dependent on the sample family and the extent of doping. In particular, the resonant peak remains as the only magnetic contribution to $\chi''$ in optimally doped samples (not yet observed in La$_{2-x}$Sr$_x$CuO$_4$ family). In our model the region of Brillouin zone which belongs to the close vicinity of $q = (0.5, 0.5)$ (say, for $0.5 \text{rlu} < q < 0.6 \text{rlu}$, Fig.3) is subject to an abrupt transformation of modes from a purely dispersive (spin wave) to almost localized (fracton) ones. A $\omega$-scan taken nominally at $q = (0.5, 0.5)$ actually integrates the neighbouring region in which this transformation takes place. In the integration, the dispersive mode gives an $\omega$-independent background contribution while the modes accumulating close to $\omega_c$ contribute to the net $\omega$-dependence of $\chi''((0.5, 0.5), \omega)$. This is illustrated and further commented in Fig.3.

Finally, we discuss the q-scans. The neutron data have shown that there is a characteristic linear relationship between the q-space width of $\chi''(q, \omega)$ and $T_c$ at constant $\omega$. The slope of this dependence, having the dimension of velocity, has been used as an evidence for the slow excitation, perhaps with a crucial contribution to formation of the superconducting state. In our model, a pronounced q-width of $\chi''(q, \omega)$ is a natural consequence of progressive slowing down and localization of magnetic modes close to $\omega_c$. The peak k-width depends on the value of $\omega_c$ determined, in turn, by the hole concentration. Fig.4 illustrates the increase of the q-width by decreasing $\omega_c$ demonstrating that an approximately linear relationship is well-obeyed in a broad range of crossover frequencies.

We conclude therefore that there is a high level of agreement between the present model and the experimental results for imaginary susceptibility and that the slow fracton modes could provide a basis for interpretation of the neutron studies. We also claim that these modes could provide a basis for understanding pairing in high-$T_c$ superconductors. Generally, the fracton-mediated superconductivity has been treated theoretically in framework of quasi-crystals by solving an appropriate Eliashberg equation. On other hand, the coupling of carriers to 40 meV resonant spin...
excitations’ has recently been recognized as strong enough to account for high values of $T_c$ in cuprates. The present work demonstrates that the fracton modes possibly underly these excitations and we believe that they could be a clue for ‘uncovering the nature of slow moving charge objects’, thus providing ‘a crucial step for our understanding of high-$T_c$ superconductivity’.

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Acknowledgements. Discussions with D. Pavuna, S. Tomić, D. Djurek and A. Siber are gratefully acknowledged.
FIG. 1: Dynamical structure factor $S(q, \omega)$ for inelastic neutron scattering by cuprates’ AF correlations of this model, Eqs. 1, 2. The two asymptotic dynamics is shown: dispersive spin waves (shown in a)) and localized fractons (shown in b)). Lattice parameters of YBCO superconductor have been assumed. Known velocity of spin waves $v_0$ has been used as a parameter. Some reduction of $v_0$ by hole doping has been both observed and expected. The form of Eq. 2 has been used for damping; however, in a) the damping was somewhat additionally suppressed in order to visualize the spin waves. The main physical parameter is the crossover frequency $\omega_c$. It decreases by hole doping and defines the energy scale of localizing fracton modes. The feature of localization is reflected by vanishing wave vector dependence for $\omega > \omega_c$, where the mode extension becomes parallel to q-axis.
FIG. 2: Integrated (local) dynamical structure factor $S_{2D}(\omega)$ of Eqs.3,4, normalized to $S_{2D}$ of AF magnons characterizing the Euclidean parent phase, is shown in a) (full black line). A peak develops as a result of accumulating modes with frequencies close to the crossover ($\omega_c$) one. Numerical integration of Eq.1 has also been performed (open circles). Disagreement for small energies represent an artifact of numerical integration of very sharp functions. Experimental results for local susceptibilities of doped superconducting cuprates are shown in b), Ref.23, and c), Ref.24,26 on the same energy scale. Thick gray lines in all panels represent the level associated to propagating spin waves.

FIG. 3: $\omega$-dependence of $S(q, \omega)$, Eqs.1,2, for five fixed wave vectors close to the AF zone center at $q_{AF} = 0.5$. The numbers near the curves designate the parametric values of $q$ in reciprocal lattice units $2\pi/a \propto 1.63 \text{Å}^{-1}$. A crossover to a weak $q$-dependence (i.e., localization) obviously takes place in this interval of $q$. Thick gray line is the average of curves. Depending on parameters, there are sharp propagating magnon peaks (not shown) immediately above $q_{AF}$ (0.5 < $q$ < 0.55, typically). Inset: experimental result on underdoped superconductor, Ref.26.
FIG. 4: Dependence of the relative $q$-width of $S(q, \omega)$ on doping-dependent parameter $\omega_c$. Inset shows a set of $\omega$-scans of $S(q, \omega)$, Eqs.1,2, for $q$ fixed at $q = 0.6$ differing only in the designated choice for $\omega_c$. The amplitude of $S(0.6, \omega)$, taken at $\hbar \omega = 25\text{meV}$, has been chosen as a relative measure for the $q$-width. One notes a broad range of $\omega_c$ characterized by approximately linear behaviour of $q$-width. Full line is a guide for the eye.