Linking the pseudogap in the cuprates with local symmetry breaking: A commentary

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In the last 2 decades, increasingly precise measurements have established that the cuprate high-temperature superconductors exhibit numerous ordering tendencies. In addition to the "big 2"—Néel antiferromagnetism (AF) and d-wave superconductivity (SC)—a variety of other orders have been observed, especially in the enigmatic "pseudogap" regime of the phase diagram. The term pseudogap denotes a suppression of the density of states between a doping-dependent crossover temperature, $T^*(p)$, and the (lower) SC transition temperature, $T_c(p)$. Thus, for doping less than $p^* \approx 0.19$ [above which $T^*(p)$ vanishes], the pseudogap is the "normal state" out of which SC emerges.

Mukhopadhyay et al. (1), in PNAS, venture a bold proposition as to the origin of the pseudogap on the basis of a careful examination of high-resolution scanning tunneling spectroscopy on $Bi_2Sr_2CaCu_2O_{8+x}$ (Bi-2212). They focus on 2 distinct forms of order: charge density wave (CDW), the breaking of lattice translation symmetry; and nematicity, the breaking of lattice rotational symmetry. Both of these have been identified in well-defined regimes of the phase diagrams of all hole-doped cuprates. By measuring tunneling conductance over a large field of view, performing a Fourier transform, and analyzing data from distinct regions of momentum space, Mukhopadhyay et al. identify energies Δ^*, E_{max}^D, and E_{max}^N characterizing the pseudogap, CDW, and nematicity, respectively. Measured on samples whose doping spans the pseudogap regime, these energies are, within experimental error, identical.

On the basis of this result, Mukhopadhyay et al. (1) argue that the pseudogap is a consequence of a tendency toward a unidirectional density wave that, if long-range–ordered, would break both translation and rotation symmetry. In the presence of disorder, translation symmetry breaking cannot occur (unless the CDW is commensurately locked to the lattice). However, a phase with "vestigial nematic" order (2, 3), i.e., rotational symmetry breaking, survives to a

critical disorder strength. The transition temperature for this nematic order would then provide a sharp definition for T^*.

In brief, the pseudogap is due to density-wave correlations rendered short-range by disorder. These correlations produce a "vestigial" nematic phase, whose transition temperature determines T^*.

While the arguments leading to this conclusion are highly suggestive, several subtleties and challenges remain to be addressed. In the remainder of this article, we discuss some of the most significant—not as a critique but as a road map for further investigation.

How Definitive Is the Spectroscopic Evidence?

To establish the link between CDW and nematic orders and the pseudogap, Mukhopadhyay et al. (1) compared 3 separate spectroscopic measurements. Each relies on data from nonoverlapping regimes of Fourier space: the CDW spectrum, $D^Z(\mathbf{Q}, E)$, from near the ordering vectors $\mathbf{Q} = \mathbf{Q}_x^D \approx (0.25, 0)$ and $\mathbf{Q} = \mathbf{Q}_y^D \approx (0, 0.25)$; the nematic $N^Z(E)$ from the reciprocal lattice vectors $\mathbf{Q} = \mathbf{Q}_x^B = (1, 0)$ and $\mathbf{Q} = \mathbf{Q}_y^B = (0, 1)$; and the averaged ($\mathbf{Q} = 0$) density of states $\rho(E)$. However, all are based on single-particle spectra and so, to some extent, are sensitive to the density of states. We thus have to ask whether the coincidence of the maxima in the CDW and nematic spectra with Δ^* might be less meaningful than it seems. We do not know a quantitative way to address this. However, while the drop of all 3 quantities with decreasing E for $E < \Delta^*$ might be simply a density of states effect, both $N^Z(E)$ and $D^Z(\mathbf{Q}, E)$ drop much more rapidly with increasing $E > \Delta^*$ than does $\rho(E)$. This strongly suggests that these orders are tied to the pseudogap.

Other Orders

Just as nematic order can serve as an avatar for CDW order, there may be other ordering tendencies for which the presence of one can serve as indirect evidence of another. Indeed, Mukhopadhyay et al. (1)

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note that the CDW could be a subsidiary order, reflecting a primary tendency toward a spatially modulated superconducting order known as pair density wave (PDW) (4). The evidence for PDW is not yet conclusive, but the notion that the pseudogap involves local SC pairing is both theoretically plausible and supported by experiment (5–8). Moreover, at very low doping, the pseudogap is associated with the growth of the AF correlation length beyond a few lattice constants (9–11), although the AF correlation length is less than a lattice constant in the pseudogap regime of near-optimally doped $YBa_2Cu_3O_{7-x}$ (YBCO) and Bi-2212 (12).

Accordingly, the pseudogap may not have just one cause. On the other hand, "all of the above" is an unsatisfactory answer to the question of the pseudogap. Indeed, exploring the validity of the proposed unifying perspective should stimulate future experiments. For instance, the suggested relation between nematicity and T^* implies that uniaxial strain should be a fruitful knob to turn.

Ascribing a spectroscopic pseudogap to fluctuations of an order parameter is an inherently imprecise notion. A system illustrating this point (5) is a 1-dimensional system with a Luther-Emery liquid ground state. At high temperatures, the system behaves as a Luttinger liquid, with gapless charge and spin excitations. At a crossover temperature T^*, a spin gap opens. For $T < T^*$, both CDW and SC correlations grow strongly. An array of such systems weakly coupled together will order at some temperature $T_o \ll T^*$, but whether as an SC or CDW state depends on a variety of details. This is a solved problem without a straightforward intuitive understanding. Viewing the spin gap (essentially a pseudogap) as due to CDW fluctuations is reasonable, but an equally good case exists for SC fluctuations, and neither perspective fully captures the underlying physics.

Ambiguity Concerning the $\vec{Q} = \vec{0}$ Order

The T^* line in the central phase diagram presented by Mukhopadhyay et al. (1) shows points at which various probes have provided evidence for the uniform ($Q = 0$) breaking of a symmetry. (Several other studies merit inclusion here, such as refs. 13–15.) These experiments provide evidence that numerous symmetries are broken at T^* (a logical possibility, although one requiring fine tuning). If so, the authors' proposal that T^* is a nematic transition is incomplete. Of course, it may eventually turn out that all of these experiments are detecting the same transition, one of primarily nematic character.

Material-Specific Differences

One of the appeals of the present proposal is its universality. Because the building blocks of the high-T_c cuprates are similar nearly square CuO planes, it is generally accepted that the essential physics is the same for all "families" of these materials. However, many properties, including some directly relevant to Mukhopadhyay et al.'s (1) proposal, differ substantially between families, and an overarching understanding may require incorporating this diversity. Specific differences are as follows:

1) The CDW wavelength is not universal. The sign of its doping dependence varies among families, and its value ranges from roughly 3 lattice constants (as in YBCO) to 4 (as in Bi-2212). The CDW may even be commensurate in some materials (16), in principle permitting long-range order.
2) Spin density wave (SDW) order is often observed, and its interplay with CDW strongly depends on the material. For instance, in $La_{2-x}Sr_xCuO_4$, the CDW and SDW orders are mutually commensurate and appear to cooperate: Wherever CDW is observed, SDW appears at a lower temperature. In contrast, in YBCO, the SDW and CDW are mutually incommensurate, and apparently compete so ferociously that they never coexist.
3) Quenched disorder is essential to the authors' proposal. Almost all the cuprates form nonstoichiometric crystals, so some disorder is unavoidable. However, since the character of the disorder varies between families of materials, so too may disorder's effects on the CDW.

These complexities should not be barriers to a single synthetic perspective, but may be crucial when applying this perspective to individual materials.

Is the CDW Order "Strong" Enough?

Since CDW order has been observed by many different experimental probes, its presence in the pseudogap regime is uncontroversial. It also has been established from numerous studies that it is one of the leading ordering tendencies of paradigmatic models studied in this context, such as the Hubbard (17) and $t - J$ (18) models. Moreover, the CDW order is strong enough to significantly suppress T_c under certain circumstances (19).

However, CDW order does not appear as strongly as in conventional CDW materials such as the rare-earth tritellurides (RTe_3) (20). In comparison with RTe_3, the CDW peaks observed in hard X-ray diffraction studies of the cuprates are several orders of magnitude weaker, and signatures of band reconstruction in angle-resolved photoemission are, at best, much more subtle (21). Thus, there is a question whether the CDW order in the cuprates is "strong" enough to account for the pseudogap.

It is not clear how to quantify this issue. In contrast to the above evidence of weakness, the modulations in the local density of states observed in STM are large—order 1 effects—for energies near Δ^*. Moreover, estimates from NMR (22) yield charge density variations of order 0.03 e per Cu atom, which is substantial.

Perspective

High-temperature SC was discovered in the cuprates more than 30 y ago. Initially, it was thought that it would admit an elegant "solution"—although there was considerable disagreement about whose proposed solution that would be. Since then, through a combination of remarkable advances in material perfection, experimental probes, and computational methods, we have uncovered a plethora of phenomena of interest in their own right, and which reveal the complexity of the problems at hand. Perhaps the most significant aspect of the Mukhopadhyay et al. (1) paper is that it refocuses attention on the big questions. We have raised above a number of issues to be reconciled with their proposition. However, in such a complex system, the failure of a theory to account for some observed behaviors—so long as they are, in some sense, "inessential"—is a shortcoming that is expected and should be tolerated (23).

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