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 \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) (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 \( \Delta^* \), \( E_{\text{max}}^0 \), and \( E_{\text{max}}^N \) characterizing the pseudogap, CDW, and nematicity, respectively. Measured on samples whose doping spans the pseudogap, Mukhopadhyay et al. (1) compared 3 separate spectroscopic measurements. Each relies on data from nonoverlapping regimes of Fourier space: the CDW spectrum, \( D^2(Q, E) \), from near the ordering vectors \( Q = Q_0^D \approx (0.25,0) \) and \( Q = Q_0^N \approx (0,0.25) \); the nematic \( N^2(E) \) from the reciprocal lattice vectors \( Q = Q_0^N = (1,0) \) and \( Q = Q_0^y = (0,1) \); and the averaged \( (Q = 0) \) 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 \( \Delta^* \) 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 \( N^2(E) \) and \( D^2(Q, E) \) drop much more rapidly with increasing \( E > \Delta^* \) than does \( \rho(E) \). This strongly suggests that these orders are tied to the pseudogap.

How Definitive Is the Spectroscopic Evidence?

To establish the link between CDW and nematic orders and the pseudogap, Mukhopadhyay et al. (1) propose a road map for further investigation. However, while the drop of all 3 quantities with decreasing \( E \) for \( E < \Delta^* \) might be simply a density of states effect, both \( N^2(E) \) and \( D^2(Q, E) \) 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)
Ambiguity Concerning the $\vec{Q} = \vec{0}$ Order

The $T^\ast$ line in the central phase diagram presented by Mukhopadhyay et al. (1) shows points at which various probes have provided evidence for the uniform ($\vec{Q} = \vec{0}$) 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 $T^\ast$ (a logical possibility, although one requiring fine tuning). If so, the authors’ proposal that $T^\ast$ 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$_x$Cu$_4$O$_8$, 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$_2$) (20). In comparison with RTe$_2$, 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 $\Delta^\ast$. 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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