QUANTUM MATERIALS

Waves divide the Fermi sea

The discovery of charge density waves in a heavily doped cuprate strengthens proposals that these symmetry-breaking modulations play a role in the anomalous electronic properties of high-temperature superconductors.

Mark P. M. Dean

Although the fundamental Coulomb interactions between electrons in materials are well-known and relatively simple, experiments frequently reveal unexpected emergent phenomena that arise when many electrons interact strongly. The copper oxide — cuprate — superconductors are a touchstone in the quest to understand this phenomenon. Now, writing in *Nature Communications*, Charles Tam and colleagues establish the presence of periodic charge modulations in the heavily doped cuprate $Tl_2Ba_2CuO_{6+\delta}$, which has a particularly well-understood electronic structure, through an X-ray scattering study[1]. They suggest that these modulations alter the material's electronic properties and explain a sudden change in the density of charge carriers.

According to band theory — the conventional theory of how weakly interacting electrons behave in solids — cuprates should be metals with a large number of current-carrying electrons. The locus of points in reciprocal space that these electrons occupy is called the Fermi surface, and in this material band theory predicts that it should look like a large cylinder. In fact, the electrons in undoped cuprates repel each other so strongly that they jam and form an insulating state, meaning that there is no Fermi surface. Doping this insulator with a moderate number of charge carriers produces the so-called underdoped phase of cuprates, which is metallic but with surprising and unconventional properties.

Experiments measuring underdoped cuprates detect far fewer charge carriers than expected. Hints of a Fermi surface remain, however, with the detection of small Fermi pockets containing fewer electrons than predicted by band theory[2]. At the same time, electrons in underdoped cuprates show a tendency to self-organize into regular periodic charge modulations, or charge density waves (CDWs). This has motivated many researchers to suggest that there may be a link between these CDWs, the small Fermi pockets, and the electronic properties of cuprates more generally. But this idea has been hard to confirm because of the difficulty in identifying CDWs in cuprates with well-understood electronic structure in which to do detailed comparisons.

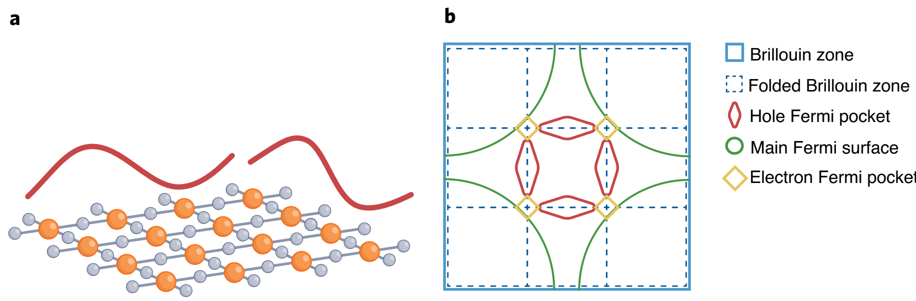

Fig. 1 | Charge density wave and proposed Fermi surface reconstruction in $Tl_2Ba_2CuO_{6+\delta}$. a, Illustration of the charge density wave (red line) reported by Tam and collaborators[1]. This modulates the electron density with a period of three lattice units in both directions of the plane of copper (orange) and oxygen (grey) atoms that appear in cuprate superconductors. **b**, Schematic of the quasi-two-dimensional electronic structure of heavily doped cuprates, shown as a two-dimensional cut and plotted within the standard Brillouin zone in blue. The green quarter circles centred around the corners represent the main well-established Fermi surface. The periodic repetition of the Brillouin zone ensures that they join up to create a full circle, which extends to make a cylinder in the out-of-plane direction. Dotted blue lines represent the Brillouin zone that is created by a period-three modulation consistent with a charge density wave and which creates, among other features, the electron and hole pockets, shown in yellow and red, respectively.

Tam and colleagues used a technique called resonant inelastic X-ray scattering — a sensitive tool for showing the presence of CDWs — to observe a diffraction signal. Fig. 1a illustrates the structure of these CDWs, which involve modulations in the valence charge density with a period of approximately three lattice units. The first question raised by this observation is why a CDW is present in heavily doped $Tl_2Ba_2CuO_{6+\delta}$ at all? A frequently invoked concept for CDW formation is 'nesting', in which electrons order at wave vectors that connect parallel (or quasi-parallel) pieces of the Fermi surface. The Fermi surface of $Tl_2Ba_2CuO_{6+\delta}$ (plotted in green in Fig. 1b) shows no obvious possibilities for nesting, however, excluding this as a plausible formation mechanism.

Instead, strongly correlated mechanisms, which relate to the balance between Coulomb interactions and kinetic energy, might be at play. By clustering together on neighbouring atoms in the copper oxide layers, doped carriers can break fewer magnetic bonds than they would if they spread out evenly. Countering this energy gain is the increased Coulomb repulsion and kinetic energy reduction caused by such clustering. A plausible means to establish the overall minimum energy solution of this complicated situation may involve a modulated clustering: a CDW. This mechanism could be relevant in $Tl_2Ba_2CuO_{6+\delta}$, but if so, there remains the challenge of explaining why other heavily doped cuprates have CDWs with somewhat different properties[3,4].

At a fundamental level, the presence of a CDW defines a new periodicity within a material. Fig. 1b shows the shape of the Fermi surface in heavily doped cuprates, which consists of cylinders centred around the corners of the Brillouin zone (green). The presence of a CDW with a wavelength of three unit cells results in a new inverse periodicity in the Brillouin zone. Therefore, the Brillouin zone folds into thirds, creating new electron and hole Fermi pockets. Tam and colleagues note that these new Fermi surfaces are predicted to vanish at a doping were the CDW is measured to disappear. This also draws appealing links to other cuprate superconductors such as $YBa_2Cu_3O_{6+x}$ for which electron pockets have been detected directly and linked to CDW formation[1,5]. Although prior quantum oscillation[6] and photoemisson[7] measurements did not observe electron pockets in $Tl_2Ba_2CuO_{6+\delta}$, the results of Tam and colleagues motivate efforts to revisit these experiments. A further challenge is to explain how the weak CDW can impart a strong enough electrostatic potential modulation to justify the band folding.

The CDW in $Tl_2Ba_2CuO_{6+\delta}$ adds to a picture in which charge correlations exist over a strikingly large fraction of the cuprate phase diagram. Whether CDWs play a lead role or are merely extras in the strange metal and superconducting phenomena in the cuprates remains controversial, but their sheer ubiquity points towards their importance. Indeed, evidence for CDWs in another superconducting family, the low-valence nickelates, appeared very recently[8–10]. ❐

Mark P. M. Dean ✉
Condensed Matter Physics and Materials Science Division, Brookhaven National Laboratory, Upton, NY, USA.
✉*e-mail: mdean@bnl.gov*

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Competing interests

The author declares no competing interests.