Inhomogeneity, Dynamical Symmetry, and Complexity in High-Temperature Superconductors: 
Reconciling a Universal Phase Diagram with Rich Local Disorder

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A model for high-temperature superconductors incorporating antiferromagnetism, \(d\)-wave superconductivity, and no double lattice-site occupancy can give energy surfaces exquisitely balanced between antiferromagnetic and superconducting order for specific ranges of doping and temperature. The resulting properties can reconcile a universal cuprate phase diagram with rich inhomogeneity, relate that inhomogeneity to pseudogaps, give a fundamental rationale for giant proximity effects and other emergent behavior, and provide an objective framework for separating essential from peripheral in the superconducting mechanism.

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High-temperature superconductivity was discovered more than two decades ago \([1]\), but its interpretation remains controversial \([2]\). We believe that this lack of theoretical consensus may be attributed to two fundamental, and related, issues: (1) Most models emphasize a limited aspect of the (complex) problem; as a result, there are few solvable models that capture a sufficient range of essential physics. (2) The complex behavior of these compounds obscures the superconducting mechanism because, in the absence of solvable models incorporating a wide enough range of physics, it is difficult to separate essential features from secondary ones using only data.

For example, high-temperature superconductors exhibit a variety of spatial inhomogeneities such as stripes or checkerboards, particularly in the hole-underdoped region and near magnetic vortex cores \([3, 4, 5, 6, 7]\). The relationship of this inhomogeneity to the unusual properties of these systems is unsettled. Does it lead to superconductivity (SC), does it oppose SC, or is it a sideshow? Particularly vexing is that this rich variety of inhomogeneity would at first glance seem to be inconsistent with broad evidence for a cuprate phase diagram that is rather universal, particularly for hole-doped compounds. How does one reconcile a seemingly universal phase diagram with a bewildering array of inhomogeneity for individual compounds?

Dopant atoms play a dual role in high-temperature superconductors: they support SC globally by enhancing charge carrier density, but may suppress SC locally through atomic-scale disorder. McElroy et al \([8]\) found strong disorder in atomically-resolved scanning tunneling microscope images of the SC gap for Bi-2212. They concluded that this disorder derives primarily from dopant impurities and that charge variation between nanoregions is small, implying that inhomogeneity is tied to impurities need not couple strongly to charge.

We show here that such inhomogeneities are a generic consequence of perturbations on the antiferromagnetic (AF) and SC correlations, largely independent of specifics and not necessarily coupled to charge variation. Further, we show that these properties are consistent with a global cuprate phase diagram, are tied intimately to the nature of pseudogap states, and imply a linkage among pseudogaps, inhomogeneity, and emergent behavior. Thus we provide a testable hypothesis for separating primary from derivative features in the rich high-temperature superconductor data set.

The SU(4) model \([9, 10, 11, 12, 13, 14]\) is a fermion many-body theory that incorporates AF and SC order on an equal footing, conserves spin and charge, and implies no double occupancy on the lattice (Mott insulator ground state at half filling). The effective SU(4) Hamiltonian can be expressed as

\[
H = H_0 - \tilde{G}_0 \left( (1 - \sigma) D^+ D + \sigma \tilde{Q} \cdot \tilde{Q} \right) + g' \tilde{S} \cdot \tilde{S},
\]

where \(H_0, \tilde{G}_0\) and \(g'\) are constants, \(D^+\) creates \(d\)-wave singlet pairs, \(\tilde{Q}\) is the staggered magnetization, \(\tilde{S}\) is spin, \(\sigma = \sigma(x)/\chi(x)\), and \(\tilde{G}_0 = \chi(x) + G_0(x)\), and \(G_0(x)\) and \(\chi(x)\) are effective SC and AF coupling strengths. Doping is characterized by a parameter \(x = 1 - n/\Omega\) for an \(n\)-electron system, with \(\Omega\) the maximum number of doped holes (or doped electrons for electron-doped compounds) that can form coherent pairs, taking the normal state at half filling as the vacuum. Generally, \(P \approx 0.25x\), where \(P\) is the standard hole-doping parameter, normalized to the number of copper sites \([10]\).

Three dynamical symmetry limits have exact solutions \([9]\). The SO(4) limit (\(\sigma = 1\)) is a collective AF state, the SU(2) limit (\(\sigma = 0\)) is a collective SC state, and the SO(5) limit (\(\sigma = 1/2\)) is a critical dynamical symmetry interpolating between the SC and AF limits \([9]\). For other values of \(\sigma\) an approximate solution can be obtained using generalized coherent states. We characterize AF in these solutions by the staggered magnetization \(Q \equiv \langle Q_z \rangle\), or by \(\beta\) defined through

\[
Q = 2\Omega \beta (n/(2\Omega) - \beta^2)^{1/2},
\]

and singlet \(d\)-wave pairing through \(\Delta = \langle D^+ D \rangle^{1/2}\).

Total energy surfaces are obtained from the expectation value of Eq. \([1]\) in coherent state approximation \([9]\). To relate them to data we use the variation of \(\sigma\) with doping, which was determined by fitting to cuprate data and given in Fig. 1 of Ref. \([11]\a. Figure\([1]\) shows SU(4) energy surfaces as functions of AF order \(\beta\), SC order parameter \(\Delta\), and doping \(x\). These energy surfaces exhibit two fundamental instabilities that may play a large role in the properties of cuprate superconductors.
The first is an instability against condensing pairs when the system is doped away from half-filling infinitesimally. This instability is similar to the Cooper instability for a normal superconductor, but generalized to a doped Mott insulator, and accounts for the remarkably rapid development of superconductivity with hole doping in the cuprates \([12]\). In this paper we concentrate on the properties and implications of a second fundamental instability that occurs in the underdoped region.

The energy surfaces at constant doping fall into three general classes: AF+SC (e.g., \(x = 0.1\)), SC (e.g., \(x = 0.9\)), and critical (e.g., \(x = 0.6\), which marks a quantum phase transition). Curves in the AF+SC class have minima at finite and large \(\beta_0\), and small but finite \(\Delta_0\), where the subscript zero denotes the value of the order parameter at the minimum of the energy surface. Curves in the class SC are characterized by \(\beta_0 = 0\) and finite \(\Delta_0\). Of most interest here are surfaces near critical in Fig. 1 which correspond to broken SU(4) \(\supset\) SO(5) dynamical symmetry \([9]\) and are flat over large regions of parameter space. This implies that there are many states lying near the ground state with very different values for \(\beta\) and \(\Delta\). Thus the surface is critically balanced between AF and SC order, and small perturbations can drive it from one to the other. This defines a critical dynamical symmetry of the SU(4) algebra \([9]\); we shall term this situation dynamical criticality.

The extreme sensitivity of critical surfaces to perturbations is illustrated in Fig. 2. Each set of curves is associated with a fixed value of doping \(x = 0.6\) (equivalently, \(P = 0.15\)), with the solid line corresponding to \(\sigma = 0.6\), the dashed line to a 10% increase in \(\sigma\) (AF perturbation), and the dotted line to a 10% reduction in \(\sigma\) (SC perturbation). The effect on the energy surface versus \(\Delta\) (not shown) is significant but less dramatic: \(\Delta_0\) is shifted, but remains finite in all three cases. We see that this small fluctuation in \(\sigma\) can alter the energy surface between AF+SC (finite \(\beta_0\) and \(\Delta_0\)) and SC (\(\beta_0 = 0\) and finite \(\Delta_0\)). This sensitivity is specific to the critical (broken SU(4) \(\supset\) SO(5)) dynamical symmetry. The AF region near \(x = 0\) and the \(d\)-wave superconducting region at larger hole doping (see Fig. 1) are very stable against such perturbations.

The AF instability displayed graphically in Fig. 2 may also be understood analytically. From the \(T = 0\) solution for \(Q\) given by Eqs. (24a) and (14) of Ref. \([11]\), we find

\[
\frac{\partial Q}{\partial x} \bigg|_{x = q_x} = \frac{1}{4} \frac{x_q + x_q^{-1} - 2 x_q}{(x_q - x)(x_q^{-1} - x)^{1/2}} \bigg|_{x = q_x} = -\infty, \tag{3}
\]

and a small change in doping will cause a large change in anti-ferromagnetic correlations near \(x = q_x\). This is a consequence of SU(4) symmetry, which requires that \(Q\) vanish for \(x \geq x_q\) and be finite for \(0 < x < x_q\).

It is not hard to conjecture mechanisms altering the ratio of AF to SC coupling locally. For example, Ref. \([8]\) found that nanoscale disorder is tied to influence of dopant impurities. Nunner et al \([15]\) (see also \([16]\)) compared these results with Boboliubov–de Gennes calculations and proposed that out-of-plane dopant atoms can modulate pairing on a scale comparable to the lattice spacing, through lattice-distortion modification of electron–phonon coupling or superexchange.

States associated with critical dynamical symmetry may be termed chameleon states: their variational energy surfaces are flat over large regions of parameter space and their intrinsic collective properties may be changed qualitatively by a small perturbing background that alters the AF–SC competition. Figure 1 suggests that underdoped cuprates have near-critical energy surfaces. Thus, chameleon states are central to the discussion of inhomogeneity and to the general issue of understanding pseudogap states in underdoped cuprates.

Figure 3 is constructed from the expectation value of \(\sigma\) in coherent state approximation, assuming a 1-D spatial perturbation, \(\sin(2\pi L)\), with \(\sigma = 0.6\). It illustrates schematically how a small (10%) periodic fluctuation in the AF and SC coupling for a critically symmetric underdoped compound can...
lead to inhomogeneity. In this example, 1-dimensional spatial variations of the coupling ratio $\sigma$ give fluctuations in order parameters leading to stripes in which AF+SC ($\sigma > 0.6$) and SC ($\sigma < 0.6$) are favored alternately. Also shown are the responses of AF fluctuations $d\beta/dL$ to this variation in $\sigma$. (We do not intend this as a realistic model of a stripe phase, but as a cartoon indicating how such a model could be built.)

Figure 3 indicates that a small spatial variations in the coupling ratio $\sigma$ can produce regions having large AF and weaker SC order, interspersed with regions having significant SC correlations but no AF order. Although not plotted, the AF+SC regions also exhibit small triplet pair densities, which vanish in the SC regions. The primary fluctuation between stripes is in the AF order, which can jump between zero and the maximum allowed by the SU(4) model between adjacent stripes; the pairing order changes are much smaller and pairing is finite in both the SC and SC+AF regions. The variation of $d\beta/dL$ indicates that appreciable softness in AF and SC may occur on the boundaries between regions.

The expectation value of the charge $M$ is not a function of the coupling ratio $\sigma$ in the SU(4) coherent state, so the critical energy surface fluctuations responsible for alternating AF+SC and SC stripes in Fig. 3 cause no charge variation ($\Delta M = 0$). Data indicate that the relative charge variation for Bi-2212 surface nanoscale patches is less than 10%, implying heterogeneity not strongly coupled to charge [8]. This view is supported by analyses of heat capacity and NMR data on Bi-2212 and YBCO that find a universal phase behavior for cuprates, with little static charge modulation [17,18].

Of course, the variation in $\sigma$ could itself be due to a charge modulation. From the preceding discussion, we may expect that if a charge modulation occurs in either the AF region near half filling or the SC region at larger doping, its effect will be small because the energy surfaces are not critical there. However, if a charge modulation occurs in the underdoped region where the energy surfaces are near critical its effect could be amplified by dynamical criticality even if $\sigma$ is not altered significantly, since this is equivalent to a doping modulation. Thus, we suggest a mechanism for producing strong inhomogeneity without necessarily invoking charge fluctuations as the cause, but that can in particular cases for under-doped compounds be produced by a charge modulation. Such a mechanism could make understandable strong inhomogeneity in the face of a universal phase diagram, and resolve competing experimental claims regarding the role of charge variation in producing inhomogeneity.

As an aside, inhomogeneity without charge modulation has an analog in astronomy. We might assume, erroneously, that density in the bright arms of a spiral galaxy (a form of “stripe order”) is much larger than that between the arms. Actually, spiral arms are prominent because the mass (gravitational charge) there is more visible: galactic dynamics generates many hot, luminous stars in the spiral arms. In analogy, the structure in Fig. 3 is not due to charge variation but rather to modulation of the charge “visibility” by (quantum) dynamics.

The minimal patch size that can support SU(4) coherent states is crucial to the present argument. Experience (e.g., Ref. [19]) suggests that dynamical symmetry can be realized in fermion valence spaces having as few as several particles. This would be consistent with inhomogeneities on scales comparable to atomic dimensions, as required by data [8].

Inhomogeneity caused by electronic self-organization is often contrasted with that caused by dopant impurities. Our discussion implicates both as sources of nanoscale structure. The proximate cause may be impurities that perturb the SU(4) energy surface but the criticality of that surface, which greatly amplifies the influence of impurities, results from the self-organizing, doped Mott insulator encoded in the SU(4) algebra. Note a recent analysis [16] suggesting, from a different perspective, that intrinsic amplification of impurity effects is required to explain nanoscale structure in Bi-2212.

Critical dynamics may also produce inhomogeneities near magnetic vortices and magnetic impurities. A magnetic field should suppress SC relative to AF, so distance from a vortex $d$ may be expected to alter the average value of $\sigma$, just as changing the doping $P$ would. Therefore, we may expect a region near magnetic vortices or impurities where the symmetry is critical and exhibits sensitivity to perturbations similar to that exhibited in Fig. 2 with $d$ modulating $\sigma$ rather than $P$.

Giant proximity effects are observed in the cuprates where non-SC copper oxide material sandwiched between superconducting material can carry a supercurrent, even for a thickness much larger than the coherence length [20]. Phenomenology indicates that pre-existing nanoscale SC patches can precipitate such effects [21]. We find similar possibilities on fundamental grounds, but also suggest that the inhomogeneity need not pre-exist. Dynamical criticality renders even a homogeneous pseudogap phase unstable against large fluctuations in the AF and SC order. Thus, proximity of superconducting material to pseudogap material coupled with perturbations from background impurity fields can trigger dynamical nucleation of nanoscale structure and giant proximity effects, even if no static inhomogeneity exists beforehand.

In experiments with one unit cell thickness La$_2$CuO$_4$ AF barrier layers between superconducting La$_{1.85}$Sr$_{0.15}$CuO$_4$
samples, Bozovic et al. [22] found that the two phases did not mix, with the barrier layer completely blocking a supercurrent. These results were interpreted to rule out many models of high-temperature superconductors, in particular models in which SC and AF phases are nearly degenerate like the SO(5) model [23]. The absence of a proximity effect between the AF and SC phases (but presence of a strong proximity effect between pseudogap and SC material) is plausibly consistent with the SU(4) model: the AF phase is not rotated directly into the SC phase but rather evolves with increased doping into a mixed SC and AF phase, which then is transformed into a pure SC state at a critical doping point near optimal doping, where the AF correlations vanish identically [11].

The spontaneous appearance of properties that do not preexist in a system’s elementary components is termed emergence; systems with emergent behavior are said to exhibit complexity (see Dagotto [24] for a review). Complexity can occur when the choice between potential ground states is sensitive to even weak external perturbations. The amplification effect implied by SU(4) dynamical criticality can facilitate emergent behavior and complexity. The giant proximity effect that implements AF and highly universal character, both follow directly from a model cuprate phase diagram (including pseudogaps) that exhibits [11], and a quantitative description of fermi arcs [13]. Therefor, the propensity of the pseudogap state to a broad variety of induced inhomogeneity, and a quantitative model of the emergent behavior and complexity. The giant proximity effect implied by SU(4) dynamical criticality can facilitate emergent behavior and complexity. The giant proximity effect and the perturbatively-induced structure of Fig. 3 are examples. More generally, critical dynamical symmetry may represent a fundamental organizing principle for complexity in strongly-correlated fermi systems. For example, critical dynamical symmetries are known in nuclear physics [25].

The SU(4) coherent state method that yields the variational energy surfaces discussed here admits quasiparticle solutions that generalize the BCS equations, giving a rich, highly universal character of induced inhomogeneity, and a quantitative model of the cuprate phase diagram (including pseudogaps) that exhibits highly universal character, both follow directly from a model that implements AF and \(d\)-wave SC competition in a doped Mott insulator. This natural coexistence of a universal phase diagram with a rich susceptibility to disorder could reconcile many seemingly disparate observations in the cuprate superconductors. For example, since the SU(4) pseudogap state has both pairing fluctuations and critical dynamical symmetry, it could support Nernst vortex states as perturbations on a homogeneous phase having incipient nanoscale heterogeneity.

In summary, competing antiferromagnetism and \(d\)-wave pairing, constrained by no double site occupancy, can lead to energy surfaces in hole-underdoped cuprates that are critically balanced between antiferromagnetism and superconductivity. These surfaces can be flipped between dominance of one or the other by small changes in the ratio of the antiferromagnetic to pairing strength. Therefore weak perturbations in the underdoped region, and near vortex cores or magnetic impurities, can produce amplified inhomogeneity having the spatial dependence of the perturbation but the intrinsic character of an SU(4) symmetry. (The symmetry defines the possible states; the perturbation selects among them.) Our results show that such effects could, but need not, imply spatial modulation of charge. More generally, we have suggested that critical dynamical symmetry may be a fundamental principle of emergent behavior in correlated fermion systems.

The generality of our solution implies that any realistic theory describing superconductivity competing with antiferromagnetism should contain features similar to those discussed here. In particular, similar phenomena may be possible in the new iron-based high-temperature superconductors [20]. Then the existence of complex inhomogeneities for compounds having (paradoxically) universal phase diagrams suggests that (1) properties of superconductors in the pseudogap state, and near magnetic vortices and impurities, are largely determined by critical dynamical symmetry, and (2) inhomogeneity is a strong diagnostic for the mechanism of high-temperature superconductivity but it is only consequence, not cause.

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