Topological Doping of Correlated Insulators

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Abstract

A material which is an insulator entirely because of interaction effects is called a correlated insulator. Examples are trans-polyacetylene and the cuprate high temperature superconductors. Whereas doping of a band insulator results in a shift of the chemical potential into the conduction or valence band, doping of a correlated insulator produces fundamental changes in the electronic density of states itself. We have found that a general feature of doping a correlated insulator is the generation of topological defects; solitons in one-dimension and anti-phase domain walls in higher dimensions. We review the well known features of this process in polyacetylene, and describe the experimental evidence that the analogous features are seen in the cuprate superconductors. We also distinguish the case in which the doping-induced features can be viewed as a Fermi surface instability, as in polyacetylene, and the more usual case in which they are a consequence of a Coulomb frustrated electronic tendency to phase separation.

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I. INTRODUCTION

Perhaps the most intensively studied problem in condensed matter physics in recent years is the doping of a Mott insulator, a system with one electron per unit cell, which is insulating rather than metallic by virtue of the strong electron-electron repulsion. This long-standing unsolved problem has been revitalized by the discovery, almost a decade ago, of the cuprate high temperature superconductors, which are themselves doped Mott insulators. The scale of temperatures below which a system is insulating is set by the gap in the charge excitation spectrum; the interactions are sufficiently strong that this scale is much larger than the temperature of any transition to an electronically-ordered state. Nonetheless, at least on a bipartite lattice, such systems typically exhibit ordered ground states in which the size of the unit cell doubles. Of course, the most-studied example has a ground state with Néel, or antiferromagnetic order, as in the high temperature superconductors.

This problem is a subclass of the somewhat broader problem of doping a correlated insulator, which is relevant for a host of synthetic metals that have been studied in the past three decades. By a correlated insulator, we simply mean a material that would be a metal in a single-electron theory, but is rendered insulating by interaction effects [1]. As with the Mott insulator, the commensurability between the density of conduction electrons and the underlying lattice is important. Frequently the unit cell contains one conduction electron or hole in the high-temperature phase, and is doubled in the broken symmetry state.

It is our contention that a certain more or less universal motif, which we have named “topological doping”, characterizes the evolution of the electronic structure of such materials. The basic idea is that it is energetically favorable for the system to maintain the local commensurate insulating structure even when lightly doped, and for the additional charges to be incorporated as local defects. Moreover we find, quite generally, that the preferred defects are topological, in that the commensurate structure experiences a phase shift across the defect. When there is one conduction electron or hole per unit cell, the phase shift is equal to $\pi$. In one dimension such defects are $\pi$ solitons, while in higher dimensions they
are the various forms of discommensuration, familiar from studies of the commensurate-incommensurate transition [2]. It is a natural consequence of this view that, as the doping is increased, there is a crossover from a “doped insulator” regime, where the defects are far separated, to an “overdoped” or more or less conventionally metallic regime, when the spacing between defects is comparable to their width [3].

Many materials display the characteristics of topological doping, and it is useful to take a broad perspective in order to understand what they have in common. In this paper, we use the language of topological doping to describe the well known polyacetylene story, whose understanding was largely based on the work of A. J. Heeger and collaborators [4]. We then show that analogous considerations govern the evolution of the electronic structure of the high temperature superconductors.

II. TRANS-POLYACETYLENE

The Undoped State: Undoped trans-polyacetylene [4] has a half-filled $\pi$ band on the order of $10$ eV wide, and it would be a rather good metal were it not for the Peierls instability that causes it to dimerize; thus it is a prime example of a correlated insulator. The dimerized state is insulating and characterized by a broken symmetry, i.e. the dimerization itself, which can be observed as a Bragg peak in X-ray scattering. (The existence and magnitude of the static dimerization also has been inferred from fancy NMR techniques.) The undoped polymer exhibits a gap to both charge and spin excitations. The charge gap can be seen, for example, in the optical absorption spectrum and also has been measured by electrochemical means. The existence of a spin gap can be deduced from the vanishingly small value of the spin susceptibility [5], although its magnitude has been obtained only by indirect means, such as third-harmonic generation spectroscopy [6]. The gap in the excitation spectrum of a single electron, which of course combines charge and spin, also has been measured by photoemission spectroscopy [7]. All of these measurements are more or less consistent with a semiconducting model of the insulating state with a gap of order $1.8$ eV. There are, however,
two features of the insulating state that suggest the inadequacy of the semiconductor model: 

i) Long sub-gap tails, observed by for example optical absorption spectroscopy, suggest that there are excitations which have a substantially lower energy and are weakly accessible in the insulating state. These tails are now thought to be due to the direct photoproduction of soliton pairs, and are weak since they rely on the existence of virtual solitons as quantum fluctuations in the ground state. 

ii) There are remarkable photo-induced changes in the electronic structure as seen, for example, in photo-absorption experiments. These changes are known to be directly analogous to the dopant-induced changes in the electronic structure, and hence these experiments can be viewed as exploring the effects of photodoping the polymer.

*The Doped Insulator:* Upon doping, the conductivity of trans-polyacetylene rises by many orders of magnitude, signifying that there is no longer a gap (or at most a very small gap) in the charge excitation spectrum. This can be seen in more detail from the dopant-induced changes in the optical absorption spectrum. Here, it is found that, upon doping, the spectral weight of the features associated with the insulating gap is transferred continuously (and rapidly) to a broad “mid-gap” absorption feature, with substantial weight extending to much lower frequencies. At the same time, the spin susceptibility remains very small, suggesting that the gap in the spin excitation spectrum is not destroyed. As far as we know, the symmetry of the ground state is restored even at the lowest doping levels.

The basic explanation of these features was set forward in the seminal paper by W-P. Su, J. R. Schrieffer, and A. J. Heeger in 1979. They realized that doping does not proceed uniformly, as in a semiconductor, but rather it is energetically favorable to destroy the dimerization, and hence the gap, in local “defect” regions, associated with antiphase domain walls or discommensurations in the dimerization order. These are the famous solitons in polyacetylene. The local nature of the dopant-induced changes in the dimerization is responsible for most of the salient features of the doping of polyacetylene: 1) The spin gap remains intact because the dimerization (hence the gap) persists between solitons. 2) In the core of the soliton, the dimerization vanishes, hence there exists a zero energy (midgap)
of density of states into the middle of the insulating gap and hence to the associated peak in the optical absorption, with weight proportional to the dopant concentration. (The fact that all bound states are either fully occupied or unoccupied implies that there are no low-energy spin excitations associated with the soliton cores.) 3) Low energy collective charge excitations are associated with the translational motion of the domain walls and appear in the far infrared absorption spectrum with oscillator strength proportional to the dopant concentration.

It is a more subtle matter to deduce the topological character of the dopant-induced defects directly from experiments. Soliton doping (as opposed to, for example, bipolaron doping) produces different distributions of states in the gap, although this is complicated by interaction effects and disorder. But, most importantly, the rapid restoration of the symmetry of the ground state upon doping is a consequence of the topological character of the defects; dopant-induced non-topological defects would produce only a modest reduction in the magnitude of the order parameter in proportion to the dopant concentration. One additional consequence of the topological character of the solitons is that they are anomalously one-dimensional, since a single soliton cannot tunnel between two polymer chains. This is a form of “confinement”, and is a general feature of the one-dimensional electron gas in the spin gap regime [10]. Confinement has not been directly observed experimentally, but it is fair to say that no evidence of three-dimensional quantum mechanical coherence has ever been observed in these materials, despite the fairly substantial magnitude of the wave function overlap between adjacent polyacetylene chains.

Of course, as a consequence of the dynamics of the solitons, the above picture of an inhomogeneous dopant-induced state is valid only at intermediate time scales and length scales. In the absence of disorder, and for weak enough interchain coupling, thermal and quantum fluctuations of the soliton positions produce a “soliton liquid” state [11]. Here, dimerization is completely absent in the static structure factor, but would be evident at intermediate times (or frequencies). In the more realistic case in which disorder plays a
dominant role, the solitons are pinned at random positions, producing a “soliton glass” state \[12\]. In either case, all configuration-averaged static correlation functions ultimately are translationally invariant or, equivalently, the dimerization order parameter is zero when averaged over distances long compared to the mean spacing between solitons.

Finally, we observe that the conductivity of lightly-doped polyacetylene, although enormous compared to the undoped polymer, is still considerably too small to be thought of as metallic in the usual sense, since it violates the so-called Ioffe-Regel criterion \[13,14\]. Basically, the idea is that the smallest value of the conductivity consistent with Boltzmann transport theory occurs when the mean-free-path, \(\ell\), is equal to the Fermi wavelength, \(\lambda_F = \frac{2\pi}{k_F}\), and this constitutes a sort of minimum conductivity, \(\sigma_m\), for a conventional metal. Any material with a smaller conductivity cannot be understood in terms of the occasional scattering of coherently propagating quasiparticles. For a quasi one-dimensional material, such as polyacetylene, \(\sigma_m = 4(e^2/\hbar)(n_\perp/k_F) \approx 1.5\, \text{m}\Omega - \text{cm}\), where \(n_\perp\) is the areal density of polyacetylene chains. In the entire doped-insulator regime, the conductivity at room temperature is substantially smaller than \(\sigma_m\), and it decreases with decreasing temperature. This poor conductivity is a consequence of soliton doping. The fact that the solitons are confined to one dimension implies that they are easily pinned by disorder. This is exacerbated by their local character, in that the majority of the electrons remain more or less condensed in the insulating state, and hence cannot participate in screening the impurity potential. If, by contrast, doping suppressed all dimerization entirely, the room temperature conductivity would be large \[15\], as it is in the overdoped regime.

*The Overdoped Metal:* All of the above properties are features of the lightly-doped polymer which one can think of as a “doped insulator”. Clearly, there is a characteristic dopant concentration \(y_c\), which is roughly equal to the reciprocal of the soliton width, at which the defects begin to overlap. For higher dopant concentrations, one expects a crossover or transition to new physics. This crossover is clearly evident in the abrupt destruction of the spin gap above a critical dopant concentration which is of order \(y_c \approx 5\%\), although it depends on the dopant species. The overdoped polymer behaves grossly like a three-dimensional
Fermi liquid [15]: 1) It has a Pauli susceptibility and a T-linear term in the specific heat of roughly the magnitude that would be expected from band theory. 2) Its D.C. conductivity can be as large as that of typical metals, and certainly much larger than $\sigma_m$. 3) It exhibits three dimensional coherent transport, as seen for instance in the measured negative magnetoresistance [16].

The essential known features of the topological doping of trans polyacetylene are summarized in Table I.

**III. COULOMB FRUSTRATED ELECTRONIC PHASE SEPARATION**

In a series of previous publications, we have worked out the theory of topological doping of correlated insulators in higher dimensions, with special emphasis on the high temperature superconductors [17–22]. While the ideas are quite general, we shall use language specific to the high temperature superconductors in summarizing the basic ideas, *i.e.* we will take the commensurate insulating state to be an ordered spin 1/2 Heisenberg antiferromagnet, and the doping to be p-type, *i.e.* hole doping:

1) Given a short-range model of a doped antiferromagnet, such as the $t-J$ model, we have shown that the most common behavior at low doping concentrations is phase separation. That is to say, the system separates into two macroscopically distinct regions: a commensurate ordered insulating region and a hole-rich metallic region. It is important to recognize that the driving force for this electronic phase separation is kinetic; it derives from the fact that the hole motion is frustrated in the antiferromagnetic state. Thus, phase separation is the best compromise between the hole kinetic energy and antiferromagnetic ordering. Since superexchange is itself a kinetic process, the strongly-correlated system has chosen phase separation as a means of minimizing the total zero-point energy. Elsewhere we have reviewed the set of model systems which can be proven to exhibit phase separation, and the experimental evidence that this physics is operative in the high temperature superconductors [17]. Among other things, high temperature superconductors exhibit macroscopic
phase separation whenever the dopants are mobile enough to counterbalance the effect of the long-range Coulomb interaction, as in the case of photodoping or oxygen doping. In other words “turning off” the long-range Coulomb interaction reveals the microscopic tendency to phase separation in these materials.

2) In the presence of long-range Coulomb interactions, the short-range tendency to phase separation is frustrated. So long as the Coulomb interaction is not too strong, this always results in a state which is inhomogeneous on intermediate time scales or length scales, *i.e.* the material forms a state consisting of a mixture of local undoped antiferromagnetic regions and heavily-doped metallic regions. While many mesoscopic motifs can result from this physics, we have shown \[19,20\] that the typical consequence is an ordered “stripe crystal” or fluctuating “stripe liquid” phase. Within the stripe liquid phase, there is also the possibility of a “nematic stripe liquid” phase in which the stripes are positionally disordered, but are, on average, oriented along a particular crystallographic direction, thus spontaneous breaking the four-fold rotational symmetry of the crystal. The stripes are antiphase domain walls in the antiferromagnetic order, and the doped holes are concentrated in the domain walls, where the antiferromagnetic order vanishes.

IV. CONCERNING THE MICROSCOPIC ORIGIN OF THE STRIPES

It is necessary to distinguish the various microscopic routes to stripe phases, since they have rather different consequences \[17,21,22\]. In one mechanism, stripes (*i.e.* long period charge-density waves) arise from Fermi-surface nesting in a weakly incommensurate system \[24\]. So far as is known, in the Hartree-Fock approximation which captures the essence of the Fermi surface instability, the phase separated state \[17\] and stripes \[24,17\] give the best variational solutions of the two-dimensional Hubbard model at small values of doping.

The Hartree-Fock stripes are, in fact, extremely close analogues of the solitons in polyacetylene, in that they are a lattice of antiphase domain walls whose mean separation is determined self-consistently from the hole concentration so that the mid-gap bands are com-
pletely empty. It is, of course, a general feature of a Fermi-surface instability that the order develops in such a way as to open gaps on the Fermi surface. Moreover in the Hartree-Fock solution, the instability is spin-driven, in the sense that there is a single transition temperature below which the broken symmetry solution of the Hartree-Fock equations is stable, and that the magnitude of the spin-order parameter $m$ turns on with the usual mean-field exponent, $m \sim (T_c - T)^{1/2}$, while the charge modulation turns on more weakly, (i.e. $\sim m^2$).

In short, there are three clear features of stripes that arise from a Fermi surface instability: i) The transition is spin driven. ii) In the low temperature phase, there are gaps (or pseudogaps) on the Fermi surface. iii) The spacing between domain walls is equal to $1/x$, where $x$ is the hole concentration. (We have checked, by explicit calculation, that inclusion of long-range Coulomb interactions in the Hartree-Fock calculation has little effect on this result [21].) iv) Although it is not easy to quantify, the notion of a Fermi-surface instability requires that the high temperature phase should be a Fermi liquid, with quasiparticle scattering rates no greater than the ultimate low-temperature energy gap.

The situation is quite different if the stripes arise from Coulomb-frustrated phase separation: i) One typically expects the transition to be charge-driven [25, 23]. That is to say, local spin order between the anti-phase domain walls can only develop after the holes are expelled from these regions. In this case, general Landau-Ginzburg considerations [25], lead one to expect either a first order transition, in which spin and charge order turn on simultaneously, or a sequence of transitions, in which first the charge order and then the spin order appears as the temperature is lowered. ii) Since the stripe concentration is determined primarily by the competition between the Coulomb interaction and the local tendency to phase separation, we do not necessarily expect that the spacing between stripes should be a simple function of $x$ and, as a consequence, there is no reason to expect the Fermi energy to lie in a gap or pseudogap; in fact, the Fermi energy typically will lie in a region of large density of states [21]. iii) A high temperature Fermi liquid phase is not a prerequisite, since it is not an essential part of the physics of frustrated phase separation.

Although the formation of stripes is driven by frustrated phase separation, their con-
formation is influenced by other more subtle effects. i) As with any other charge-density wave system, commensurability energies are likely to be important. For instance, in the 214 family of superconductors (discussed below) either the stripe separation is nearly equal to 4 lattice spacings or the concentration of holes along a stripe is near to one per two sites. These two commensurabilities are compatible at \( x = 1/8 \); otherwise the system must choose which one (if either) to satisfy. Commensurability effects have been explored in some detail in doped \( \text{La}_2\text{NiO}_4 \) by Tranquada and co-workers [26]. Since systems of this sort can easily support a disorder line [2], commensurability effects can be important even in a stripe liquid phase. ii) The underlying crystalline lattice possesses, at best, fourfold rotational symmetry, not full rotational symmetry. This gives rise to a lattice anisotropy energy which strongly affects the ordering of stripe phases [20], and can also stabilize a nematic stripe-liquid phase. Moreover, the strength of the commensurability and anisotropy energies may be strongly influenced by structural phase transformations [27].

V. THE \( \text{La}_2\text{CuO}_4 \) (214) FAMILY

The “high temperature superconductors” are a group of materials which contain essentially equivalent \( \text{CuO}_2 \) planes separated by a variety of interstitial charge reservoir regions which are the source of the doping. It is generally believed that the basic physics is the same for all these materials, although subtle differences sometimes make it difficult to distinguish the essential and universal from the inessential or material dependent.

We choose to focus on the so-called 214 sub-family of these materials. Not only are they among the best studied but neutron scattering structure factors provide direct “photographic” evidence of the topological character of the doping process. In particular, we will contrast two slightly different materials of the family: \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) and \( \text{La}_{1.6-x}\text{Nd}_{0.4}\text{Sr}_x\text{CuO}_4 \). In both cases, the undoped system \( (x = 0) \) is an antiferromagnetic insulator and the concentration of doped holes in the \( \text{CuO}_2 \) planes is equal to the Sr concentration, \( x \). However, at the temperatures and dopant concentrations of interest to us here,
La$_{2-x}$Sr$_x$CuO$_4$ has an orthorhombic structure, whereas La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ undergoes a structural phase transition to a low temperature tetragonal (LTT) phase below about 70K. Above 70K, the electronic properties of the two materials are essentially indistinguishable for the same dopant concentration $x$ but the LTT phase supresses superconductivity at dopant concentrations $x < 20\%$ and, as has been recently discovered [23], stabilizes an ordered “striped” state, in which dopant-induced antiphase domain walls crystallize.

The Undoped State: The undoped state of all the high temperature superconductors is a quasi two-dimensional antiferromagnetic insulator. At all temperatures below 1000K, there are substantial antiferromagnetic correlations, although the system does not finally order into a Néel state until a temperature of the order of 400K. Since the low-energy charge excitations involve the movement of charge from copper to oxygen, the material is known as a charge-transfer insulator. However, in common with a Mott insulator, the gap in the charge excitation spectrum (roughly 2eV) is much greater than the scale of magnetic ordering [28].

The Doped Insulator: A breakthrough in understanding the properties of the doped insulating state was achieved recently through neutron scattering studies [23] of a crystal of La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ with $x = 0.12$. As the temperature is lowered, there is a succession of transitions to 1) the LTT phase, 2) a charged-ordered state (charge-stripes) and 3) at a slightly lower temperature, a period-doubling magnetically-ordered state. This is a photograph of an ordered stripe phase of the sort predicted above. The factor of two between the periods of the charge and spin orders implies that the charge is localized in magnetic antiphase domain walls, and the fact that the charge order appears first implies that the physics is driven by charge (i.e. frustrated phase separation), rather than by Fermi surface or Hartree-Fock physics. Moreover the charge density along the stripes corresponds to a half-filled band (one doped hole per unit cell containing two Cu ions), which is consistent with the mobility required by kinetic phase separation and commensurability with the underlying lattice, but half as large as the prediction of Hartree-Fock theory. Therefore, the origin of the stripe crystal phase of this material may be attributed uniquely to frustrated phase separation.
La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ with $x = 0.12$ is thought not to exhibit any bulk superconductivity. In a manner that we believe we understand well [25], the LTT phase stabilizes an ordered stripe phase and, the same time, suppresses superconductivity. That the ordered stripe phase is in direct competition with superconductivity already suggests that it is an extremely important piece of the physics. However, there is more direct evidence. La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ (with $x = 0.12$) has static magnetic order below about 50K, but La$_{2-x}$Sr$_x$CuO$_4$ (with $x = 0.15$) is magnetically disordered at all temperatures. Nevertheless the dynamical neutron scattering structure factors of both materials, measured at a frequency $\omega = 3$ meV and $T=40K$ [30] (which effectively take a snapshot of the magnetic structures of the systems [29]) are somewhat broadened versions of the elastic (Bragg) scattering observed in La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$. Thus, there can be no question that there exist substantial dynamic stripe fluctuations in the optimally superconducting samples of La$_{2-x}$Sr$_x$CuO$_4$. Moreover, the fact that these fluctuations appear at such low frequencies, implies that they are very nearly frozen, even in the superconducting material!

This evidence is merely the latest and most graphic demonstration of topological doping in the high temperature superconductors. It is a dramatic confirmation of our interpretation of other experiments, as discussed in our earlier reviews, which includes analogues of most of the properties of polyacetylene, discussed above. A noteworthy property of the lightly-doped superconducting materials (known in the field as “underdoped”) is the existence of a spin gap in the normal state, which we have associated with local pairing correlations without global phase coherence [32]. Recent photoemission experiments [31] appear to confirm this interpretation. The only known ways of realizing this situation are in highly anisotropic systems (e.g. quasi one-dimensional where the superconducting phase coherence is suppressed by thermal and quantum fluctuations) or in granular, spatially inhomogeneous, systems in which global superconductivity is suppressed by the small Josephson coupling between grains. To some extent, both of these features are present in the high temperature superconductors.

The Overdoped Metal: It is conventional to classify the high temperature superconduct-
tors as “optimally doped” (i.e. having the highest transition temperature in a given class of materials), “underdoped” (i.e. having a lower dopant concentration than optimal), and “overdoped” (i.e. having a larger than optimal dopant concentration). By now, the characteristics of the members of these three classes are sufficiently well known that it is possible to make an assignment to a given material, even if systematic studies of the transition temperature as a function of dopant concentration are unavailable. We have identified “underdoped” materials as doped insulators, in the sense of this article, and have suggested that “optimally doped” is simply a crossover between underdoped and overdoped. As in polyacetylene, the overdoped material appears to be more conventionally metallic. Certainly the conductivity at all temperatures is much greater than $\sigma_m$, and it is much more isotropic (i.e. three dimensional) than in under and optimally doped materials, although it still has a strange temperature dependence. Moreover, the magnetic properties appear to be those of a conventional metal. Thus, while it is not certain that the overdoped state can be classified as a Fermi liquid, it surely is a more conventional metallic state than at lower doping.

The essential features of topological doping in the 214 family of high temperature superconductors are summarized in Table II, which includes some additional properties discussed in our published papers.

**VI. OTHER CUPRATE SUPERCONDUCTORS**

The existence of charge-density wave fluctuations adds a new dimension to discussions of the physics of the high temperature superconductors which, almost from the outset, have been dominated by the interplay of antiferromagnetism and superconductivity. It is clear that the three phenomena are simply different manifestations of a common underlying physical theme, and that the best way to investigate any one of them is to find the material in which it shows up the most clearly. Nevertheless, although charge-density fluctuations are most clearly manifested in the 214 family, it is natural to ask how their effects might be
revealed in other materials. Evidently it is desirable to have a space-sensitive probe and, in the absence of suitable neutron or X-ray scattering data, the obvious technique is angle-resolved photoemission spectroscopy (ARPES), which, until recently, was most reliable for \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x} \). We have undertaken a detailed study of the implications of ordered and fluctuating charge stripes for the single-particle properties of high temperature superconductors \[21\], and have found that it is possible to understand the most striking features of the ARPES data on \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x} \), especially the shape of the Fermi surface and the existence of nearly dispersionless states in its neighborhood. The essential ingredient in this interpretation of the data is a background of slowly-fluctuating stripes whose dynamics is determined by collective effects (the competition between phase separation and the long-range Coulomb force), rather than the single-particle behavior.

Recently a detailed analysis of the ARPES experiments \[34\] has led to an understanding of the magnitude and temperature-dependence of the width \( \Gamma \) of the single-particle spectral functions, with two important consequences. First of all, in the normal state, \( \Gamma \) is too large to be consistent with any kind of quasiparticle picture; this observation strongly supports our analysis of the resistivity of the normal state \[14\], which was based on the violation of the Ioffe-Regel condition \[13\]. Secondly, it was found that \( \Gamma \) decreases rapidly as the temperature falls below \( T_c \), indicating that quasiparticles are resurrected in the superconducting state. In our picture, quasiparticle propagation is inhibited in the normal state by the charge inhomogeneity, and especially by the frustration of hole motion in the direction perpendicular to the stripes, but phase order restores coherent particle motion, even though the stripes persist in the superconducting state.

**VII. WHAT DOES THIS HAVE TO DO WITH HIGH TEMPERATURE SUPERCONDUCTIVITY?**

Our discussion has scarcely mentioned superconductivity which, after all, provoked the worldwide interest in the oxide superconductors. But, as might be expected, an apprecia-
tion of the electronic structure and the physics that gives rise to it also leads to a natural mechanism of high temperature superconductivity. The fundamental driving force is the frustration of the motion of holes in an antiferromagnet. This implies that when the holes on the stripes tunnel into the intervening region, which has a low charge density and strong antiferromagnetic correlations, they experience the very same effective attraction that would have caused them to coalesce (phase separate) in the absence of the longer range Coulomb interaction [35]. Moreover, the Coulomb force, which so effectively inhibits pairing with a short coherence length and yet is widely ignored in discussions of the mechanism of high temperature superconductivity, has been incorporated into the picture from the outset. In fact, the holes moving on a stripe form a quasi one-dimensional electron gas in an “active” environment with low-energy excitations in the spin (and possibly charge) degrees of freedom, which renormalize the kinetic energy of the holes and mediate effective interactions between them [25]. We have investigated this problem as a generalization of the standard theory of the one-dimensional electron gas, and have shown that it provides a possible microscopic explanation of the phenomenon of high temperature superconductivity [25]. Whatever the mechanism, it must survive (and even thrive) on significant charge-density wave (stripe) fluctuations, and account for their intimate competition with superconductivity. In this regard, we find the mechanism described above to be an attractive possibility.

Empirically and on general theoretical grounds [12,32], it is clear that the optimal place for high temperature superconductivity is in the crossover regime between the doped insulator and overdoped regimes. This suggests a general strategy for looking for superconductivity in other doped correlated insulators [12].

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### TABLE I. Topological Doping in Polyacetylene (CH \( x \))

| General Property               | Particular Manifestation                                                                 |
|--------------------------------|-----------------------------------------------------------------------------------------|
| Correlated insulator           | Commensurate (dimerized) CDW                                                            |
|                                | Spontaneously broken reflection                                                         |
|                                | and glide plane symmetry                                                                |
|                                | Charge gap                                                                             |
|                                | Spin gap                                                                               |
|                                | Single-particle gap                                                                     |
| Topological Doping             | Soliton liquid or glass                                                                  |
|                                | Rapid restoration of symmetry                                                           |
| Doped insulator for \( y < y_c \)| \( y_c \sim 1/ \) (soliton width)                                                       |
|                                | Spin gap survives doping                                                                |
|                                | Low-energy optical oscillator strength proportional to \( x \)                         |
|                                | Charge gap feature persists with reduced oscillator strength                             |
| Inhomogeneous on intermediate  | Transfer of oscillator strength to “mid-gap” states                                     |
| scales                         | Pinning of chemical potential in the gap                                               |
|                                | Conductivity \( \ll \sigma_m \)                                                        |
| “Overdoped” metallic state     | 3D metallic state                                                                      |
| for \( y > y_c \)              | Pauli spin susceptibility                                                               |
|                                | 3D Coherent quasiparticle propagation                                                  |
|                                | Metallic magnitude of the conductivity                                                 |
|                                | Density of states at \( E_F \) consistent with band theory                            |
| General Property | Particular Manifestation |
|------------------|--------------------------|
| **Correlated insulator** | Commensurate (Néel) SDW  
Spontaneously broken spin rotational  
and translational symmetry  
Charge gap  
Spin waves  
Single particle gap |
| **Topological doping** | Stripe liquid, glass, or crystal  
Rapid restoration of spin-rotational symmetry  
x_c \sim 1/ \text{(stripe width)}  
Spin gap appears at intermediate doping  
Low-energy optical oscillator strength proportional to x  
Charge gap feature persists with reduced oscillator strength  
Transfer of oscillator strength to “mid-gap” states  
Pinning of chemical potential in the gap  
Conductivity at high T < \sigma_m  
Ordered striped phase in LTT structure  
Macroscopic phase separation when dopants are mobile  
Fluctuating stripes observed in neutron scattering |
| **“Overdoped” metallic state**  
for \( x > x_c \) | 3D metallic state  
Destruction of spin gap  
3D Coherent quasiparticle propagation  
Metallic magnitude of the conductivity |
REFERENCES

[1] For the present purposes, it is not extremely important whether the interaction which produces the correlated insulating state is a direct electron-electron repulsion, as in the cuprate superconductors, or the electron-phonon interaction, as in polyacetylene. We can always view the system in a formalism in which we integrate out the phonons, and consider the resulting induced interaction; the only differences are that this induced interaction is attractive and retarded. Of course, for many purposes, this distinction is important but, for illustrating the nature and consequences of topological doping, it is not.

[2] For an excellent review, see V. L. Prokrovsky, A. L. Talapov, and P. Bak, in Solitons, eds. S. E. Trullinger, V. E. Zakharov, and V. L. Prokrovsky (North-Holland, Amsterdam, 1986) p. 73.

[3] An illuminating example, in which this evolution can be studied in detail, is presented in V. J. Emery, Phys. Rev. Lett. 65 1076 (1990), in which the properties of the one dimensional large $U$ copper-oxygen model are worked out as a function of doping concentration. Here, one can explicitly study the evolution from a doped insulator regime, in which the Drude weight is proportional to the density of holes relative to the half-filled band, to an overdoped regime, in which the Drude weight is proportional to the number of electrons.

[4] For a comprehensive review, see A. J. Heeger et al, Rev. Mod. Phys. 60, 781 (1989). Where statements are not otherwise attributed, they are discussed in this review with references to the original literature.

[5] In real samples there is always a small Curie-law susceptibility, which is now thought to be an effect of the finite chain lengths and a corresponding small concentration of neutral solitons in the ground state; this type of excitation would be absent in an ideal material.
[6] W-K. Wu, Phys. Rev. Lett. 61, 1119 (1988) pointed out that the two-photon resonance in the third-harmonic spectrum, which is proportional to the non-linear susceptibility, \( \chi^{(3)}(-3\omega, \omega, \omega, \omega) \), probes the neutral (i.e. dipole forbidden) excitations in the system. In the large \( U \) limit, one would thus find a resonance at low energy compared to the charge gap corresponding to magnon pair production. Wu computed \( \chi^{(3)}(-3\omega, \omega, \omega, \omega) \) explicitly for \( U = 0 \) (i.e. taking into account only electron-phonon interactions in the adiabatic approximation) where the spectrum is that of a one-dimensional semiconductor. These calculations were found to agree surprisingly well with the later experimental measurements of S. Fan et al., Phys. Rev. Lett. 62, 1492 (1989) using a free electron laser. This suggests that the spin gap and charge gap are approximately equal in undoped polyacetylene.

[7] See, for example, the recent work of Miyamae et al, Bull. Chem., Soc. Jap. 68, 1897 (1995). As in the high temperature superconductors, the Fermi energy is found to move rather little relative to the insulating gap features, but states move steadily into the gap upon doping. Unsurprisingly, no meaningful angle resolved photoemission data exist for polyacetylene.

[8] In a purely one-dimensional system with no disorder, the ground state symmetry would, indeed, be restored at vanishingly small dopant concentration. In the real material, disorder and interchain interactions complicate the theory, and the experimental situation is not completely resolved. However, it is clear that even at very small dopant concentrations, no static dimerization can be resolved in X-ray scattering.

[9] W. P. Su, J. R. Schrieffer, and A. J. Heeger, Phys. Rev. Lett. 42, 1698 (1979).

[10] C. Bourbonnais and L. Caron, Int. J. Mod. Phys. 7, 169 (1991).

[11] Were polyacetylene truly one-dimensional in the absence of disorder, the correct long-distance behavior would be given by a Tomonaga-Luttinger model for the charge degrees of freedom, with a spin gap due to the attractive interactions. All the soliton physics
would simply go into the value of the critical exponent which describes this state.
The possibility of a soliton liquid state for polyacetylene was suggested in W-P. Su, S. A. Kivelson, and J. R. Schrieffer, in *Physics in One Dimension*, ed. by T. Bernasconi and T. Schneider (Springer, Berlin, 1980), p. 201.

[12] S. A. Kivelson and V. J. Emery, Synth. Met. 65, 249 (1994).

[13] A. F. Ioffe and A. R. Regel, Semicond. 4, 237 (1960).

[14] V. J. Emery and S. A. Kivelson, Phys. Rev. Lett. 74, 3253 (1995).

[15] S. A. Kivelson and A. J. Heeger, Synth. Met. 17, 183 (1987).

[16] H. H. S. Javadi et al, Phys. Rev. B 43, 2183 (1991).

[17] For a review of the theoretical and experimental evidence for frustrated phase separation in the cuprate superconductors, including a comparison between the stripe phases produced by frustrated phase separation and Hartree-Fock or other variational treatments, see S. A. Kivelson and V. J. Emery, in *Proceedings of ”Strongly Correlated Electronic Materials: The Los Alamos Symposium 1993”*, ed. by K. S. Bedell, et al (Addison Wesley, Redwood City, 1994) p. 619. Other aspects of the problem, especially the implications of frustrated phase separation for the charge and spin dynamics, are reviewed in V. J. Emery and S. A. Kivelson, Physica C 209 594 (1993).

[18] More recent discussions of the theory of topological doping appear in a series of conference proceedings, especially V. J. Emery and S. A. Kivelson, Physica C 235-240 189 (1994), and V. J. Emery and S. A. Kivelson, Proc. of the First US-Polish Conference on High Temperature Superconductivity, Wroclaw, Poland, September, 1995, to be published.

[19] U. Löw et al Phys. Rev. Lett. 72, 1918 (1994).

[20] L. Chayes et al, Physica A, in press.
[21] M. I. Salkola, V. J. Emery and S. A. Kivelson, Proc. of the Third International Conf. on Phase Separation in High T_c Superconductors, Erice, July, 1995 (in press) and submitted to Physical Review Letters.

[22] Although other work on this subject is reviewed in Ref. ([17]), the reader who is interested in a broader, more complete, and detailed discussion of some of these issues is referred to the proceedings of the three International Conferences on Phase Separation in High T_c Superconductors, which were published as: Phase Separation in Cuprate Superconductors, eds. K. A. Müller and G. Benedek (World Scientific Singapore, 1993); Proc. of the Second International Conf. on Phase Separation in Cuprate Superconductors, Cottbus, Germany, 1993; Proc. of the Third International Conf. on Phase Separation in High T_c Superconductors, Erice, July, 1995. In particular, for an alternative discussion of the physics of electronic phase separation in doped, Mott insulators, and for extended discussions of its consequences in the context of a large N theory, the reader is directed to the work of Di Castro and collaborators, of which a most recent (and important) reference is C. Castellani, C. DiCastro, and M. Grilli, Phys. Rev. Lett. 75, 4650 (1995).

[23] J. Tranquada et al, Nature 375, 561 (1995) and unpublished.

[24] See, for instance, J. Zaanen and O. Gunnarsson, Phys. Rev. B 40, 7391 (1989); H. J. Schulz, Phys. Rev. Lett. 64, 1445 (1990) and J. Phys. (Paris) 50, 2833 (1989).

[25] V. J. Emery, S. A. Kivelson, and O. Zachar, unpublished.

[26] See, for example, J. M. Tranquada, D. J. Buttrey, and D. E. Rice, Phys. Rev. Lett. 70 (1993) 445; V. Sachan, D. J. Buttrey, J. M. Tranquada, J. E. Lorenzo, and G. Shirane, Phys. Rev. B51, (1995) 12742; J. M. Tranquada, J. E. Lorenzo, D. J. Buttrey, and V. Sachan, Phys. Rev. B52 (1995) 3581.

[27] J. D. Axe et al., Phys. Rev. Lett. 62, 2751 (1989).

[28] For a comprehensive review of the properties of the antiferromagnetic insulating
state of the high temperature superconductors with special focus on La$_2$CuO$_4$, see S. Chakravarty, in *High Temperature Superconductivity* ed. by K. S. Bedell, *et al* (Addison Wesley, Redwood City, 1990) p. 136.

[29] Technically, we are discussing imaginary time dynamics, as the structure factor is a property of the thermal stationary state; however, thinking of the dynamic structure factor in this way is of considerable aid to intuition.

[30] B. Sternlieb and J. Tranquada, private communication.

[31] D. S. Marshall *et al.*, (Stanford University Preprint) submitted to Phys. Rev. Lett.

[32] V. J. Emery and S. A. Kivelson, *Nature* **374**, 434 (1995).

[33] H. Takagi *et al* Phys. Rev. Lett. **69**, 2975 (1992).

[34] J. C. Campuzano *et al*, preprint (Sissa listing: cond-mat/9602120).

[35] This attractive interaction can also be viewed as a different realization of the physical ideas discussed in the context of the “spin-bag” picture; see, J. R. Schrieffer, X-G. Wen, and S-C. Zhang, Physica **C162**, 300 (1989) and references therein.