Quantum Criticality As A Possible Theory For High Tc Superconductivity

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May 6, 2002

Abstract

Recent neutron scattering, nuclear magnetic rersonance, and scanning tunneling microscopy experiments have revealed the coexistence of charge and spin density waves and superconductivity in the cuprate superconductors and have yielded valuable new information on the interplay between these distinct orders. They suggest that the theory for a High Tc superconductor can perhaps be built out of a theory of competing ground states and quantum orders.

Trying to solve for the wave function of a system comprising of about 10^{23} particles using Schrodinger's wave equation can be an impossibly daunting task. But Landau had outlined a powerful strategy involving quasi particles which had its first triumph when it was succesfully used to give an essentially exact description of the low temperature properties of metals. At T=0, the system sits comfortably at its lowest possible energy state - the many body ground state. As T rises, the system has small excitations above its ground state and one can write a theory for the dynamics of these excitations, which are called 'quasiparticles', and go ahead to describe the low temperature physics of the system. Extensions of Landau's approach have been used to explain the low temperature properties of metals , the superfluid phases of He^4 and He^3, the superconductivity of metals as described by the Bardeen-Cooper-Schreifer theory and the Quantum Hall liquid state of electrons in 2 dimensions in a strong magnetic field, making it a very powerful tool for describing the non-zero temperature physics of systems. But no successful quasiparticle-like theory has emerged so far in the case of materials exhibiting High Tc superconductivity for much of the accessible temperature range. One may wonder, however, whether this is surprising since we still dont what the ground state of these materials looks like when its either normal or superconducting.

A lot of attention has been lavished on these transition metal compounds, among which the most important are the ceramics like $YBa_2Cu_3O_7$ (YBCO) and BSCCO. In recent years there has been a new approach for describing the properties of these materials focussing on the notion of competing ground states and competing order parameters.In this paper, I will review the work done by theorists and experimentalists which seem to add credibility to the theory that the ordinary superconductor is proximate in a phase diagram to a superconductor with co-existing spin/charge density wave order.

The key point in Landau's strategy was to properly identify the quantum 'coherence' or 'order' in the ground state of the system. As an example, take the case of free electrons in metals. The order in the many-electron ground state exists in the momentum distribution of the electrons - all wave vectors less than the fermi wave vector are occupied and the rest of the wave vectors are absolutely empty of electrons. In the superfluid state of liquid helium, the order in the ground state is the presence of the Bose Einstein condensate - the fact that the ground state is macroscopically occupied by the He atoms. One then identifies which elementary excitations perturb the order of the ground state in a fundamental way. These can be called 'quasiparticles' because they are seen to transport spin, charge, momentum and energy and their mutual collisions are described by a Boltzmann-like transport equation. In metals, the quasi particles are electrons and holes, in a semiconductor, they could be excitons which are electron-hole bound states, while in superfluid Helium, they are phonon and roton excitations. The nature of the quasi particles - ie, the nature of the excitations - is therefore specific to the symmetry of the ground state above which the excitations are taking place.

1 Competing Ground States

However we may have a system which is delicately poised between two or more distinct ground states with very different quantum ordering properties and low lying excitations. The energies of the states may be quite close to each other and so only at low temperatures would a particular state be chosen as the ground state. Which state is chosen as the ground state would depend on parameters appearing in the Hamiltonian. If the parameters are in a regime which favors a particular ground state over others, the system will choose it to be the ground state at zero temperature and Landau's quasi particle approach can be applied to describe the low temperature physics of the system as long as the temperature is low enough. The crucial point is that the nature and properties of these quasi particles will, in general, be very different from those of the quasiparticles of other ground states.

At slightly higher temperatures, one cannot ignore the competition between the different ground states and their respective quasiparticles and therefore the simple quasiparticle picture breaks down. The complex behavior which results wont be characteristic of any one of the possible ground states.
Lets look at the intricate temperature dependence of a system with two competing ground states. Lets imagine following the ground state of the hamiltonian as a function of a parameter g appearing in the Hamiltonian. If the two competing states have very distinct quantum order which precludes the possibility of continuously moving from one kind of quantum order to another, there must be a critical value $g = g_c$ where the ground state undergoes a quantum phase transition from one possible state for $g < g_c$ to the other for $g > g_c$. One now first develops a theory for the ground state for the quantum critical point precisely at $g = g_c$. This may in general be a difficult task but for 'second order' quantum transitions, the critical point has special symmetry properties which allow progress. Examples will be shown below. Then we move away from the critical point and map out the physics for non-zero $\mid g - g_c \mid$ and temperature. It is to be noted that often the point $g = g_c$ is not experimentally accessible. But even in such cases it is useful to work out the theory for the inacessible point $g = g_c$ and then use it as a point of departure to develop a systematic theory for accessible values of g.

Let us now show in some detail how this thing works using examples of increasing complexity and discuss how it bears up to experimental observations.

2 Ising Chain in a Transverse Field

This is the simplest model of a quantum phase transition. The model is described by the Hamiltonian ($J > 0$, $g > 0$)

$$H_I = -J\Sigma_j(\hat{\sigma}_j^x + \hat{\sigma}_j^z\hat{\sigma}_{j+1}^z) \tag{1}$$

Here, $\hat{\sigma}_j^{x,z}$ are Pauli matrices that measure the x,z components of the electron spin on a magnetic ion in an insulator. The ions reside on the sites j of a 1 D chain. Each site has two possible states $|\uparrow>_j$ and $|\downarrow>_j$ which are eigenstates of $\hat{\sigma}_j^z$ with eigenvalues +1 and -1 and thus identify the electron spin on site j as 'up' or 'down'.

The two terms in the Hamilonian give rise to two very different effects. Because of the presence of the second term, the system would like to have parallel spins for adjacent sites in order to lower its energy, while the first term in the Hamiltonian allows quantum tunneling between the $|\uparrow>_j$ and $|\downarrow>_j$ states with amplitude proportional to g.

For $g << 1$, we can neglect the quantum tunneling and the preferred ground state is the state with all spins either up or spins down. The order in this ground state is therefore the fact that all the spins are parallel. The quasiparticles are domain walls which disturb this order (see Fig 1). A quasiparticle state, $| Q_j >$ between sites j and $j+1$ has all spins up (down) at and to the left (right) of the site j ($j+1$). For $g=0$, every such spin configuration is an energy eigenstate and therefore dont evolve with time. For small and finite g, the first term in the hamiltonian becomes nonzero - though still small - and the domain walls become mobile and acquire zero point motion. We can develop a theory for the quantum kinetics of these particles, describing their collisions, lifetime and the relaxation of the magnetic order using Landau's general strategy involving quasiparticles.

In the opposite limit of $g >> 1$, we see from Eq 1 that the state which minimizes the energy is the one built out of eigenstates with eigenvalue +1. These are

$$|\rightarrow>_j = \frac{1}{2}(|\uparrow>_j + |\downarrow>_j)$$

i.e. the right pointing spin which is quantum mechanically just a linear superposition of up and down spins. The ground state therefore has all spins pointing to the right. It is evident that this state is very different from the $g=0$ ground state. This distinction also extends to the excited states which are going to be states in which an electron in a particular site j decides to flip spin from right to left, which therefore results in a small increment of energy of magnitude J, the smallest increment of energy possible. Quasiparticle states in this regime therefore corresponds to a single 'left pointing' spin in a background of 'right' spins (see Fig 1) instead of a domain wall. For $g=\infty$, these states are eigenstates of the hamiltonian and therefore stationary states but for $g<\infty$, the quasiparticles move around and scatter among themsleves, the dynamics of which can be described using a Landau theory of quasiparticles. This would describe the relaxation phenomenon at low T.

We now allow competition between the distinct orders at small and large g by considering values of g of order unity when the two terms of the hamiltonian acquire comparable strength. At T=0, it is known that there is a quantum phase transition between these states at $g=g_c=1$. It is to be emphasized that since the two orders are very distinct, there can be no gradual crossover from one kind of ground state to another. Instead there is a sharp critical point, a critical value of $g = g_c$ where the transition occurs. For $g < g_c$, the ground state is qualitatively similar to the g = 0 ground state, while a state like $g = \infty$ is favored for $g > g_c$. The ground state at $g = g_c$ is very special and cannot be characterized by a simple cartoon picture. Its fundamental property is scale invariance. The ground state correlation function (5)

$$< \hat{\sigma}_j^z, \hat{\sigma}_k^z > \sim \frac{1}{|j-k|^{\frac{1}{4}}}$$

Since this is a power law decay, the functional form of the correlation is only modified by an overall factor if we stretch the length scale at which we are observing the spins. Therefore the ground state wavefunction doesnt tell us anything about how far apart any pair of well-seperated spins are. Therefore there is nothing that sets the spatial length scale in this system. At $T > 0$, a new time scale does appear : $\frac{\hbar}{k_B T}$. It is a fundamental property of the quantum critical point that this time scale, which only involves the temperature and the fundamental constants of nature and *not* the coupling constant J, universally determines the relaxation rate for spin fluctuations. The zero-momentum dynamic response function

$$\chi(w) = \frac{i}{\hbar k} \int_0^\infty dt < \hat{\sigma}_j^z(t), \hat{\sigma}_k^z(0)] > e^{iwt}$$

Dimensional considerations following Eq 3 and the fact that the time scale is set by $\frac{\hbar}{k_B T}$ imply that for low temperatures

$$\chi(w) \sim T^{-\frac{7}{4}} \Phi_I(\hbar w / k_B T)$$

with Φ_I as a universal response function. The exact result for Φ_I is known and it is a universal function in the sense that if we add a small second neighbour coupling to H_I, the critical coupling g_c would change slightly but Φ would remain exactly the same. Φ_I can be replaced by the following approximation,

$$\Phi_I(\frac{\hbar w}{k_B T}) = A(1 - iw/\Gamma_r + ...)^{-1}$$

where A is a dimensionless prefactor and the relaxation rate is then given as $\Gamma_R = [2tan(\frac{\pi}{16})]k_B T/\hbar$. This is therefore the response of an overdamped oscillator with a relaxation rate a function of only the temperature. One can think in terms of a dense gas of $\mid Q >_j$ particles scattering off each other at a rate of order $k_B T/\hbar$. The strength of the underlying exchange interaction between the spins does not appear in the above.

For $d = 2$, the physics for the quantum Ising model is very similar. The response function $\chi(w)$ looks the same but the exponent of T is different. However for $d = 3$ (8), the kinetic theory of the analog of the $\mid Q_j >$ quasiparticles applies even at the critical point and their scattering crosssection is dependent on the exchange interaction.

3 Coupled Ladder Antiferromagnet

This model is indirectly related to microscopic models of High Tc superconductivity. Consider the antiferromagnet described by the Hamiltonian with $J > 0$ and $0 < g \leq 1$

$$\mathrm{H}_L = J_{i,j \in A} S_i.S_j + g J_{i,j \in B} S_i.S_j$$

where S_i are spin-1/2 operators on the sites of the coupled-ladder lattice with the A links forming the 'two leg ladders' and the B links coupling the ladders. Again, as we will see later, the two competing ground states have very distinct order and therefore there is a critical value of $g = g_c$ when there is a quantum phase transition from one state to another. g_c comes out to be ≈ 0.3.

For g close to unity, the ground state is the magnetically ordered Neel state as shown in Fig 2A. The mean moment in the sites has a staggered sublattice arrangement and therefore it is in this respect that it is different than the analogous ground state for H_I for small g. Also the nature of the quasiparticles are different. This is because H_L now has the continuous symmetry of arbitrary rotations in spin space, while H_I had a discrete spin inversion symmetry. Therefore the low lying quasiparticles correspond to a gradual precession in the orientation of the staggered magnetic order of the Neel state. Since the precession can be either clockwise or anticlockwise, each spin wave mode has a two fold degeneracy. All this is therefore within the spirit of the quasiparticle picture.

For small g, the second term in the Hamiltonian H_L becomes unimportant. Therefore the electrons in a ladder dont feel the presence of the electrons sitting on other ladders. Therefore the preferred ground state is the one in which electrons in two adjacent sites on a ladder pair up to form a singlet state, thereby minimising the energy. The average moment on each site is therefore zero because of the formation of the singlet bonds with $S = 0$. The ground state is therefore a quantum paramagnet. The interesting thing is that inorder to create quasiparticles one has to break the singlet bonds and replace them with a triplet and this requires a finite energy Δ. The motion of this broken bond will then correspond to a threefold degenerate quasiparticle state.

The degenerate spin wave quasiparticle state for large g as discussed previously was twofold degenerate. Therefore we see that the quasiparticle states for the two regimes are very different from each other.

For $g \leq g_c$, quantum criticality appears for $1 << k_BT << J$. In this regime, The relaxation rate is again proportional to $\frac{k_BT}{\hbar}$ and the dynamic spin response functions has a similar form as in earlier examples. If we describe the dynamics in the basis of the triplet quasiparticles, these results imply that the scattering crosssection is universally determined by the energy k_BT alone. As k_BT is lowered across Δ for $g < g_c$, the scattering cross section evolves as a function of the dimensionless ratio $\frac{\Delta}{k_BT}$ alone. As a result, transport coefficients like the spin conductance σ_s are determined just by the ration Δ/k_BT and the fundamental constants of nature.

$$\sigma_s = \frac{(g\mu_B)^2}{h}\Phi_\sigma(\frac{\Delta}{k_BT})$$

where g is the gyromagnetic ratio of the ions carrying the spin, μ_B is the Bohr magneton and Φ_σ is a universal function.

Although one cant take H_L as a literal model for the High T_c superconductors, many measurements of spin fluctuations carried out in the last decade display crossovers similar to those found near the quantum critical point in figure 3. This seems to hint that the high temperature superconductors are near a quantum critical point where the spin properties show a universal character closely related to that of H_L.

The evidence has appeared in the following experiments: (1) the dynamic spin structure factor measured in neutron scattering experiments at moderate temperatures have been seen to obey scaling forms similar to Eq 5.(9) (2) Low temperature neutron scattering measurements at higher carrier density show a resolution-limited peak above a finite energy gap (10). This is a signal of the long-lived triplet quasiparticle states like those found at low T for $g < g_c$ in H_L. It has been argued by Sachdev and Chubukov that such a peak is a generic property of the vicinity of a quantum critical point. Sachdev proposes that another test of quantum criticality in the spin fluctuations could be provided by measurements of the spin conductance and comparison with Eq 7, but it has still not been found feasible to carry out such experiments.

4 High Tc superconductors

In the cuprate superconductors, the electronic motion primarily occurs in the 2D CuO_2 layers. The Cu ions are located at the vertices of the squares and it is commonly believed that its only the dynamics of the 3d orbitals of the Cu thats relevent and the other orbitals are mainly inert, and one therefore has a tightbinding model of electrons with one orbital per site with coulomb interaction between electrons. If we make the electron density equal to one per site, then the ground state is known to be an insulator with Neel order and this corresponds to the state with $g = 1$ in Fig 2A, for $La_2Cu)_4$. We can change the electron density in the square lattice by changing the stochiometric ratio x in $La_{2-x}Sr_xCuO_4$ and this is achieved through doping. x here measures the density of holes with one electron per site. High Tc superconductivity is observed for x greater than about 0.5.There have been various proposals for the ground state of such a system. Author Sachdev advocates the use of the theory for quantum critical points separating distinct ground states, to develop a controlled expansion at intermediate coupling.

Inorder to identify possible groundstates, a minimal approach would be to assume that they characterized by any broken syymetries of the hamiltonian. The possible symmetries which could be broken are time reversal, the group of spin rotations, the space group of the square lattice and the electromagnetic gauge symmetry which is related to charge conservation. The possibilities are therefore rich and it is hoped that they will provide an explanation for all the experiments.

As an example the Neel state which has been discussed above can be one important state. Its known to be the ground state when $x = 0$. We can view it as a density wave of spin polarization wave vector $K = (\pi_{\overline{a,\frac{\pi}{a})}}$ with a as the lattice spacing. It has been observed by Y.S Lee *et al*, that at small $x \neq 0$ there are spin sdensity waves with a period incommensurate with the lattice and that they have a mean spin polarization at a wavevector K that varies continuously away from $(\pi_{\overline{a,\frac{\pi}{a}).}}$

Another relevant ground state is the superconducting ground state formed by the Bose condensation of Cooper pairs which leads to a breaking of the electromagnetic gauge symmetry. The pair wavefunction is known to have symmetry of the $d_{x^2-y^2}$ orbitalin the relative coordinate of the two electrons. There is also the question of whether the wave function also has an imaginary component with d_{xy} or possibly s symmetry. If so then this would break time reversal symmetry(13). If so then it has been argued that the quantum phase transition between two such superconductors could explain the quantum criticality, like the scaling form of Eq 5, observed in recent photoemission experiments (14).

Another state thats relevant is the one with Peierls order which is associated with broken transalational symmetries. A competitor state to Peierls order in the quantum paramagnet is the 'orbital antiferromagnet' which is a state that breaks time reversal symmetries and translational symmetries but not spin rotation symmetries. In this state there is a spontaneous flow of current clockwise or anticlockwise around each plaquette ofthe square in a checkerboard pattern. Ivanov et al proposed that closely related state os responsible for the psuedo gap phenomena in High Tc.

Another state could be a charge density wave. This has been observed by Howald et al (3), who used scanning tunneling microscopy (STM) to show the existence of static striped charge density of quasiparticle states in nearly optimally doped BSCCO in zero field.They observed charge density moulations The LDOS varied in stripes. They were able to obtain this by measuring the differential conductance ($\frac{dI}{dV}$) which is proportional to the LDOS(Fig 7).

5 Conclusion

Coexistence of Charge Density Waves or Spin Density Waves and superconductivity has been shown in the lower Tc materials or in the presence of magnetic fields or both and also recently by Howard et al in BSCCO in zero field. This suggests that the ordinary superconductor is proximate to a superconductor with coexisting spin/charge density wave order and quantum criticality can be exploited to build a theory that can succesfully describe these materials.

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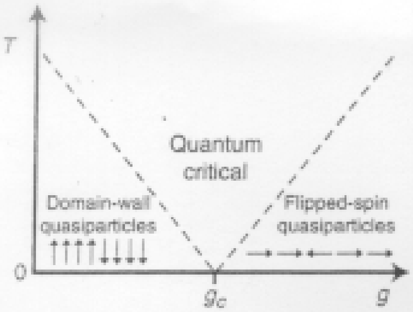

Fig. 1. Phase diagram of H_I. The quantum phase transition is at $g = g_c$, $T = 0$, and the dashed red line indicates a crossover. Quasiparticle dynamics applies in the blue shaded regions: for $g < g_c$, the quasiparticle states are like the $|Q_i\rangle$ states, whereas for $g > g_c$, they are like the very different $|\bar{Q}_i\rangle$ states. The quantum critical dynamics in the pink shaded region is characterized by Eq. 5.

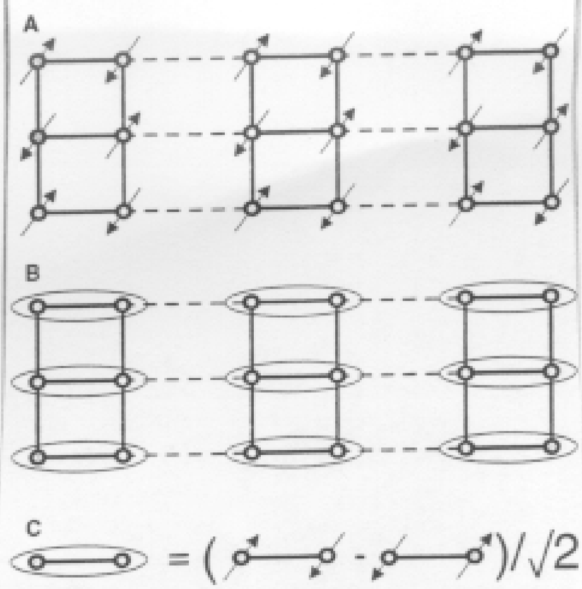

Fig2

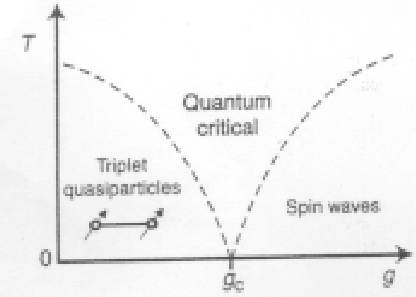

Fig. 3. Crossover phase diagram for H_L with the same conventions as Fig. 1. The ground state is a paramagnet (Fig. 2B) for $g < g_c$, and the energy cost to create a spin excitation, Δ, is finite for $g < g_c$ and vanishes as $\Delta \sim (g_c - g)^{z\nu}$, where $z\nu$ is a critical exponent. There is magnetic Néel order at $T = 0$ for $g > g_c$ (Fig. 2A), and the time-averaged moment on any site, N_0, vanishes as g approaches g_c from above. Quasiparticle-like dynamics applies in the blue-shaded regions. For $g < g_c$, in the cartoon picture of the ground state in Fig. 2B, the triplet quasiparticle corresponds to the motion of broken singlet bond in which Fig. 2C is replaced by one of $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, or $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$. For $g > g_c$, the quasiparticles are spin-waves representing slow, long-wavelength deformations of the ordered state in Fig. 2A.

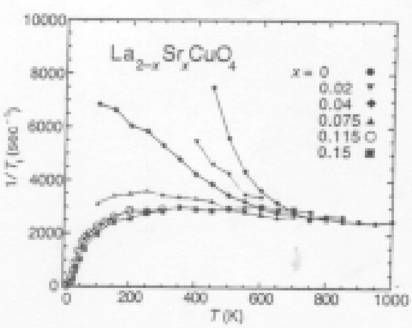

Fig. 4. Measurements (*21*) of the longitudinal nuclear spin relaxation ($1/T_1$) of ^{63}Cu nuclei in the high-temperature superconductor $La_{2-x}Sr_xCuO_4$ as a function of x and T. This quantity is a measure of the spectral density of electron spin fluctuations at very low energies. At small x, $1/T_1$ increases rapidly as T is lowered (red circles). This is also the behavior in the spin-wave regime of Fig. 3 ($g > g_c$): the energy of the dominant thermally excited spin-wave decreases rapidly as T decreases, and so the spin spectral density rises (*22*). In contrast, at large x, $1/T_1$ decreases as T is lowered (blue squares). This corresponds with the triplet quasiparticle regime of Fig. 3 ($g < g_c$): the low-energy spectral density is proportional to the density of thermally excited quasiparticles, and this becomes exponentially small as T is lowered. Finally, at intermediate T, $1/T_1$ is roughly temperature-independent for a wide range of T (orange triangles), and this is the predicted behavior (*18*, *23*) in the quantum critical regime of Fig. 3.

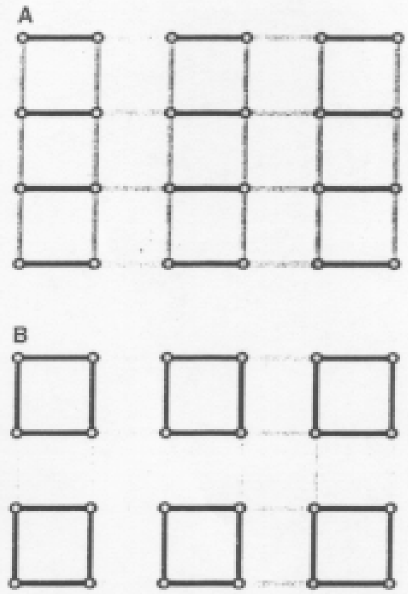

Fig. 5. Two examples (**A** and **B**) of square lattice ground state with Peierls order. All sites are equivalent, and distinct values of the energy and charge densities on the links are represented by distinct colors. These distinctions represent a spontaneous breaking of the symmetry of the square lattice space group. The spontaneous ordering appears because it optimizes the energy gained by resonance between different singlet bond pairings of near-neighbor spins. This figure should be contrasted with Fig. 2, where there is no spontaneous breaking of translational symmetry, and the distinction between the links is already present in the Hamiltonian Eq. 6.

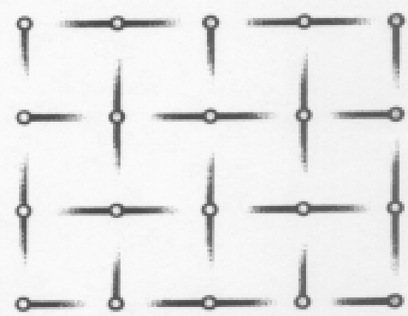

Fig. 6. The orbital antiferromagent. The gradient in the red shading represents the direction of spontaneous current flow on the links, which breaks time-reversal symmetry.

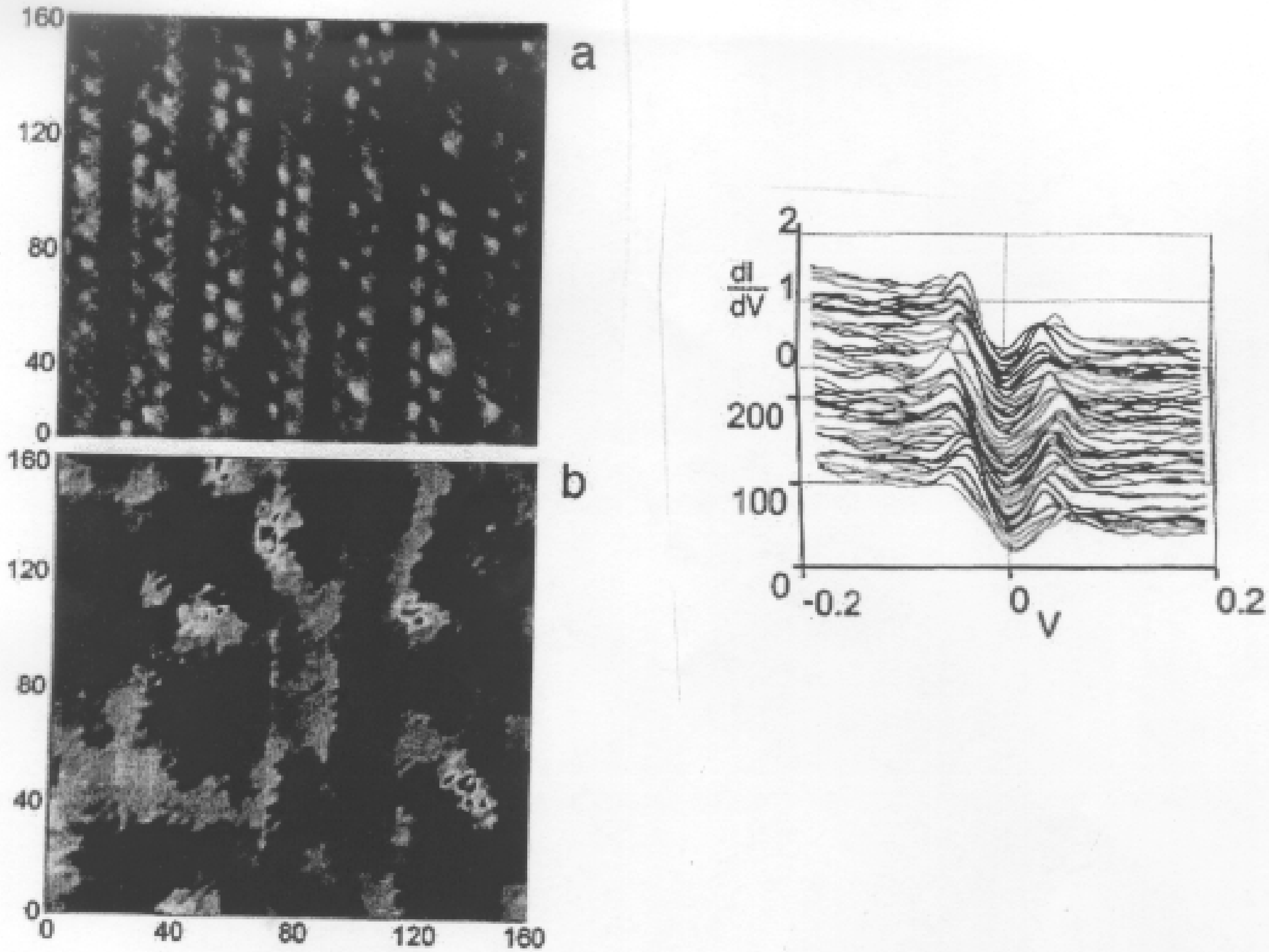

Figure 7 Topographic image, gap size map, and representative line scan of a slightly overdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ single crystal.

a, Constant current image (160 Å x 160 Å) of the cleaved BiO surface. The vertical streaks are the superstructural modulation. Also visible are the Bi atoms, as well as an irregular modulation that is probably due to variations in the LDOS[16], not actual height variation. **b,** The superconducting gap magnitude (Δ) over the same area, as measured by the voltage of the maximum in dI/dV. Color scale corresponds to 26 mV (blue) to 100 mV (red). **c,** Differential conductance as a function of voltage along the diagonal of **a** and **b**, from lower left to upper right.