Pseudogap in Cuprates or How to Almost Elude Bloch’s Theorem

C. M. Varma

Department of Physics, University of California, Riverside, CA.

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Abstract

Forward scattering of fermions due to disorder is shown to push states near the chemical potential to energies both above and below it. The magnitude and the energy scale of the resulting depletion of the density of states near the chemical potential is determined by the magnitude and correlation length of the disorder potential and the coupling at long wavelengths of the fermions to the order parameter. Scanning tunneling microscopy (STM) has revealed that the magnitude of the pseudogap in under-doped cuprates varies spatially and is correlated with disorder. The loop-current order, characterized by the anapole vector \( \Omega \), discovered in under-doped cuprates occurs in the same region of the temperature-doping plane as the pseudo gap observed in tunneling and ARPES experiments. Since translational symmetry remains unchanged in the pure limit, no gap occurs at the chemical potential, as required by Bloch’s theorem. On the other hand for disorder coupling linearly to the four possible orientations of \( \Omega \), as is consistent with distortions visible in STM, there can only be a finite temperature dependent static correlation length for the loop-current state below the ordering temperature of the pure problem. In this situation, forward scattering of fermions is shown to induce a pseudo-gap with the observed angular dependence. The peaks in the spectral function at the fermi-vectors of the pure problem are away from the chemical potential proportionally to the square of the average loop order parameter measurable by polarized neutron scattering. This result is compared with experiments. The density of states measured by STM and the observed changes in magnetic susceptibility and specific heat with temperature and very notably the apparent violations in particle sum-rule found in experiments also follow. Some predictions for further experiments are provided. Due to the finite correlation length there always exist low frequency excitations at long wavelength at all temperatures in the "ordered" phase. Such fluctuations motionally average over the shifts in frequencies of local probes such as NMR and muon resonance expected for a truly static order.

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I. INTRODUCTION

Imry and Ma [1] presented a simple physical argument to show that an Ising model with disorder which couples linearly to the order parameter has no long-range order down to zero temperature for arbitrarily small disorder in 2 or lower dimensions. Instead domains of order in different orientations form. The Imry-Ma argument generalizes to discrete models with more possible equivalent directions. A transverse field discrete model [2] also does not change the essential results. These works are concerned with insulators. The new question that is posed here is, suppose there is a model in the class of the random field Ising model in a metal which in the pure limit has a phase transition with lattice symmetry preserved so that in the ordered phase the single-particle spectra is of the usual form. What then is the spectra of one-particle excitations in the problem where the static correlations at temperatures below the ordering temperature of the pure system are affected by quenched random fields leading to formation of domains of the ordered phase.

In a disordered situation, there is a large density of static fluctuations of the order parameter below the ordering temperature of the pure problem. I show below that a reduction in the spectral weight at the chemical potential and around $k$ where the usual fermi-surface is expected follows if there is a singularity, or a large low frequency spectral weight, in the fluctuation spectra around momenta $q = 0$, and provided fermions scattering off such fluctuations have finite coupling to it. This is the only way to get around Bloch’s or Floquet’s theorem for electronic structure in periodic systems that gaps (other than those due to superconductivity or due to some unknown state which also generates new quantum numbers) occur only at Brillouin-zone boundaries, not at arbitrary chemical potential. Recall for example [3] that the exchange self-energy due to unscreened Coulomb interaction ($\propto 1/q^2$) leads to the density of states near the chemical potential $N(E) \to 0$ as $\log^{-1} |E - E_f|$ in $d = 3$ and as $1/|E - E_f|$ in $d = 2$.

This basic idea is applied to the ”pseudo-gap ” phenomena observed in under-doped cuprates. A large anisotropic reduction in the single-particle spectral weight measured in Angle-Resolved Photoemission (ARPES) experiments [4], [5] at the chemical potential, over a wide range of doping $x$, occurs in all cuprates starting at temperatures $T$ below about $T^*(x)$, below which they also show changes in transport and thermodynamic properties from those above [6], [7], [8]. This is one of the many astonishing features of the universal
phenomenology of the cuprates.

The pseudo-gap was first discovered through Knight-shift or magnetic susceptibility experiments [9] and confirmed by Scanning tunneling microscopy [10][12]. It has been the *siren-song* in the high $T_c$ problem. Since tunneling and ARPES experiments have revealed it to be a reduction in the single-particle density of states, the idea that the pseudo-gap is some kind of "spin-gap", meaning a reduction in the magnetic susceptibility through particle-hole correlations, as in the Resonant Valence Bond type of ideas [13] is untenable. The anisotropy of the reduction in the single-particle density of states can in turn easily seduce one to various other untenable directions. The reduction is maximum close the ($\pi$, 0) and equivalent directions and minimum in the ($\pm \pi/4$, $\pm \pi/4$) directions. This is what would be expected for a spin-density wave order of the same (or nearly the same) $Q$ vectors as the insulating AFM phase of the cuprates. This is indeed what is found in well defined calculations on the Hubbard model [14], [15]. But there is no sign of AFM order or even large AFM correlation lengths [16] at $T \lesssim T^*(x)$ for which the phenomena is observed. Similarly, no charge density wave formation of any sort is observed at $T \lesssim T^*(x)$. For some cuprates charge density modulations that occur [19], [17], [18] in some range of $x$ at lower temperatures have neither the symmetry nor the amplitude to compare with measured single-particle spectra or with thermodynamic experiments. They also appear to be stronger or only exist when a sufficiently strong magnetic field is applied and therefore not an issue for consideration of the pseudo-gap. The anisotropy of the pseudo-gap is also similar to the anisotropy in the density of states of the d-wave superconductivity in the cuprates below temperatures $T_c$, which are over most of the region of $x$ well below $T^*(x)$. So, one might think that long superconducting correlations of amplitude or phase might be responsible for the pseudo-gap [20][23]. But there is evidence of measurable superconducting correlations only in regions of at most $\pm 20$ K above $T_c(x)$, i.e. far below $T^*(x)$ for most range of $x$ for which pseudogap is observed.

Based on mean-field calculations on a three-orbital model for cuprates, it was suggested that $T^*(x)$ is actually a line of transitions below which a novel state emerges and that this line terminates at a quantum-critical point within the dome of superconductivity [24], [25]. On variants of the basic model, such states have recently been shown to be the ground state in similar range of doping through variational Monte-Carlo calculations in asymptotically large lattices and exact diagonalization in clusters of 24 sites [26]. Extensive experiments
in a number of families of cuprates have revealed an order consistent with such a proposed state in under-doped compounds setting in at a temperature consistent with \( T^*(x) \). This state breaks time-reversal symmetry through generation of two current loops in each unit-cell of opposite chirality (Anapole Order), while preserving translational symmetry. Thermodynamic evidence of a change of symmetry at a temperature consistent with \( T^*(x) \) has also been presented \[31\] \[32\]. Signatures of time-reversal breaking accompanying this transition are observed in a number of cuprate families through Kerr effect \[33\]. On one sample of Bi2201 \[34\], ARPES, Kerr effect and time-resolved reflectivity measurements have all been performed consistent with symmetry breaking and growth of an order below \( T^* \).

The magnitude of the principal order parameter in this state measured by polarized neutron scattering is large, as much as 0.2\( \mu_B \) per loop or a staggered order of \( O(0.4)\mu_B \) in each unit-cell \[28\] at low temperatures. Since the only order ever observed at \( T^*(x) \) is the proposed order, it is natural to seek to understand the pseudogap phenomena in terms of the properties of fermions in such a state. But since translational symmetry is not broken, no gap at the chemical potential can occur for such a state in the pure limit. In the fluctuation regime of the loop order transition, forward scattering does indeed lead to pseudo-gap behavior \[25\] but not in the ordered phase.

There is however one important fact which makes the fluctuation to the loop order state persist for \( T \lesssim T^*(x) \). The order parameter of the loop ordered state is a discrete order parameter (with 4 possible directions in a unit-cell) in an extremely anisotropic problem which may be regarded as two dimensional. For any disorder coupling linearly to discrete order parameter in \( d = 2 \), there is no long-range order even at \( T = 0 \) \[1\]. In effect, the fluctuations in the vicinity of the phase transition in the pure limit are frozen (with important temperature dependent modifications and slow fluctuations as a function of time) down to \( T = 0 \). I show that in this situation for fermions which have finite coupling constant to the fluctuations in the \( q \rightarrow 0 \) limit, anisotropic reductions of the density of states must occur for temperatures below the putative loop current order in the pure problem. There is never a true gap at the chemical potential but a change in the form of the spectral function, which is compatible with the experimental results. The fact that different cuprate compounds and even different samples of the same compound show differences in details of the change in transport and thermodynamics and indeed in the value of \( T^*(x) \) suggests that disorder might play a crucial role. In one family of cuprates, Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\) (Bi2212) in
which scanning tunneling microscopy (STM) measurements [11], [12] has been very successful, vivid evidence of disorder and its correlation with the local pseudo-gap has been presented. Various other experimental tools reveal considerable disorder in essentially all the cuprates [35]. The importance of defects to the properties of cuprates has been variously emphasized [36]. As discussed below, the nature of the disorder induced in the CuO$_2$ layers deduced by STM measurements is consistent with that which couples linearly to the loop current order parameter.

The problem posed for the single-particle spectra in the presence of local disorder favoring one of the four directions of order is illustrated in Fig. 1. Such a problem is of interest more generally than in the cuprates. Domain of a given order is surrounded by domains of a different order by a complicated boundary. The characteristic size of the domains is the correlation length determined by the disorder. The fermions have wave-functions inside a domain which are nearly the eigenstates of the Hamiltonian for that domain but scatter to the eigenstates for the Hamiltonian of the adjoining domain due to static fluctuations whose correlation function is calculated using the structure factor of the domains and with matrix elements derived from the microscopic Hamiltonian. The global wave-functions are the average over domains of sums of wave-functions in different domains which go from one domain to another continuously, assuming no localization.
Although neutron scattering presents clear evidence of a change of symmetry in going across the pseudo-gap boundary and thermodynamic signatures of the change in symmetry consistent with it are observed, there is an important class of measurements using local probes such as muon resonance, as well as Nuclear Quadrupole Resonance and Nuclear Magnetic Resonance, which do not observe the magnetic fields expected for long-range static order \[37\], \[38\], \[39\]. The time-scale of these experiments is typically 5 orders of magnitude finer than the resolution of the ”elastic” neutron diffraction experiments. The dynamics of the glassy phases such as in Fig. [1] is such that the expected shifts in the resonance lines are motionally narrowed \[40\] over alternate directions of the local magnetic field.

This paper is organized as follows. In the next section, I discuss the symmetry of random fields due to local strains which couple to the loop-current order parameter for the cuprates. I also provide a summary of what is understood about the static structure factor \(S(q)\) and the inverse correlation length \(\kappa\) of the random field discrete models, as these are necessary inputs to the calculation of the single-particle spectra. Sec. III presents the principal new theoretical calculations of the paper - that of the single-particle spectral function. The calculation of the matrix elements for the coupling of the fermions to the fluctuations is presented in the Appendix. In Sec. IV, a comparison of the spectral function and results following from it are compared with ARPES, STM and thermodynamic and transport experiments. I also present the characteristic scale of low energy fluctuations in the model and compare them to the time-scales in neutron diffraction on the one hand and the local probes, such as NMR and muon-resonance in the other. A discussion of the validity of the calculations presented here may also be found there. The concluding Sec. V contains a few predictions for further experiments.

II. CORRELATIONS IN THE RANDOM FIELD DISCRETE MODELS

A. Coupling of Defects to the Loop-Current Order Parameters

The observed order parameter in the under-doped cuprates may be specified by the magnitude and direction of the anapole order, specified in each cell \(i\) by the polar-time-reversal odd vector

\[
\Omega_i = \int_{\text{cell}-i} d^2r \ (L(\mathbf{r}) \times \hat{r}).
\]
Here \( \mathbf{L}(\mathbf{r}) \) is the magnetic moment distribution due to two orbital current loops formed between the O-ions and the Cu-ions in each cell; the four possible directions of \( \mathbf{\Omega}_i \) are shown in Fig. \([2]\).

Each of the four \( \mathbf{\Omega} \) breaks time-reversal and inversion but they break reflection symmetry in different ways. Non-magnetic disorder in the form of local lattice distortions can only couple quadratically to the order parameter. It might then appear that the random-field model of disorder of the Imry-Ma type is inapplicable. But this is not true. To see this, let us denote the four vectors in Fig.\([2]\) by \( \mathbf{\Omega}_{x'} = \pm|\mathbf{\Omega}_{x'}|; \mathbf{\Omega}_{y'} = \pm|\mathbf{\Omega}_{y'}| \). The pure limit interactions are such that any (and only) one of the four is stable in the thermodynamic limit. This is exactly as say in the pure four state ferromagnetic clock model. The coupling of lattice distortion \( \mathbf{u}_i \) at a cell \( i \) to the possible local order parameters in the cell was derived in Ref. \([32]\). The relevant distortion is of \( B_{2g} \) symmetry, i.e. transforming as \( (x'^2 - y'^2) \) which corresponds to the local monoclinic distortion of the unit-cell. It appears in the Hamiltonian coupling to the order parameter as

\[
\sum_i \mathbf{u}_i(B_{2g})(|\mathbf{\Omega}_{i,x'}|^2 - |\mathbf{\Omega}_{i,y'}|^2).
\] (2)

The sign of \( \mathbf{u}_i(B_{2g}) \) is assumed randomly distributed over \( i \) where its magnitude is non-zero. Quite clearly, given the pure Hamiltonian and the form of disorder \([2]\), there is no question of using the Imry-Ma argument to form domains between regions of \( |\mathbf{\Omega}_{x'}| \) and \( -|\mathbf{\Omega}_{x'}| \) or domains between regions of \( |\mathbf{\Omega}_{y'}| \) and \( -|\mathbf{\Omega}_{y'}| \). \([2]\) does provide a “random” temperature model which affects the temperature where local order parameters of the favored local symmetry forms and its magnitude at lower temperatures. But consider the possibility of domains between regions of order of \( |\mathbf{\Omega}_{x'}| \) and \( |\mathbf{\Omega}_{y'}| \). For this purpose, it is clearer to write \([2]\) as

\[
\sum_i \mathbf{u}_i(B_{2g})(|\mathbf{\Omega}_{i,x'}| - \mathbf{\Omega}_{i,y'})(|\mathbf{\Omega}_{i,x'}| + \mathbf{\Omega}_{i,y'}).
\] (3)

The second term in the product is constant. So the sign of \( \mathbf{u}_i(B_{2g}) \) determines whether \( |\mathbf{\Omega}_{i,x'}| \) or \( |\mathbf{\Omega}_{i,y'}| \) is favored locally, just as the random-field problem. This leads to the Imry-Ma type problem. One then concludes that domains must form between states of \( |\mathbf{\Omega}_{x'}| \) and \( |\mathbf{\Omega}_{y'}| \) of a characteristic size as in random-field problem in \( d \lesssim 2 \). Given that such domains must form and given the form of the pure free-energy which favors (through the fourth-order terms in the possible order parameters) only one of the four order parameters, any domain in the disordered problem can be of \( \pm|\mathbf{\Omega}_{x'}| \) or \( \pm|\mathbf{\Omega}_{y'}| \) only with equal probability. The difference
from the case of a four state model with disorder favoring one or the other states linearly is that in the latter case, domain of a given state has boundaries to domains of the three other states, while in the present case, it has linear boundaries to only two other states; the third state can occur only touch at corners in the limit $T \to 0$. At finite temperature entropy will force a finite boundary between such domains also. Here I do not consider the details of this issue as it is not crucial to the principles in the calculation of the single-particle self-energy.

Most of the defects in well prepared cuprates are the dopants which are usually in between the layers and not uniformly distributed. The elastic and electronic perturbations due to such distant defects have low enough symmetry that they couple linearly to the order parameter for loop-current order in the manner specified above. In particular local monoclinic distortions consistent with $B_{2g}$ symmetry have been identified on the surface through STM measurements [11], [12]. The effect of these defects is to change the local energies of the O and Cu orbitals and to change the transfer integral between a given Cu and its O neighbors or between two O neighbors. In considering disorder, one should note that carefully prepared samples of cuprates have very low impurity resistivity. In fact, for Bi2212, where extensive ARPES results are available, single-particle elastic scattering rate [41] is more than an order of magnitude large than what one deduces from residual resistivity. This is consistent with primarily having off-planar defects which can cause only small angle scattering on the fermi-surface [42]. Direct demonstration of the correlation of the variation in the pseudo-gap magnitude and such disorder has been obtained in STM measurements [11], [12]. A correlation length in the pseudo-gap magnitude of about 15-20 unit-cells is inferred from the real space maps at the surface.

B. Static Structure factor of the Random-Field Discrete Models

In the next section, the self-energy of fermions due to static disorder is calculated using the classic result [43] that it can be related to the static structure factor. Approximate theory of the static structure factor in a random field problem was also given long ago, by Lacouer-Gayet and Toulouse [44] and by various others using more sophisticated methods [47]. A simple version of the calculation for the static structure factor $S(q)$ including the region below the critical point has been given by Halperin and Varma [45] and by Vilfan and Cowley [46]; the latter also provide a self-consistent determination of the inverse correlation
length $\kappa$ which is a crucial parameter in the calculations. They also give a summary of the experimental evidence for the effects of random fields on antiferromagnets, both in two and three dimensions. The results we need for the present paper are summarized here. The static Structure factor consists of two parts, one directly due to independent disorder fields and the other due to the re-orientation effect on the induced random fields by the background random field:

$$S(q) \approx S_e(q) + S_c(q),$$

$$S_e(q) = \frac{T}{J} \left( \frac{<\Omega(T) >^2}{q^2 + \kappa^2} \right), \quad S_c(q) = < h^2 > \left( \frac{<\Omega(T) >^2}{q^2 + \kappa^2} \right)^2.$$  

The first average is over the local order parameter $\Omega$ is the thermal average for fixed disorder and the second is the disorder average. $J$ is the near neighbor interaction of the pure model, $< h^2 >$ is the dimensionless mean-square random field on the cells defined as

$$< h^2 >= c <\Omega >^2,$$  

where $c$ is a concentration of defective cells. $\kappa$ is the inverse of the correlation-length of disorder. Vilfan and Cowley have derived through a simple self-consistency argument that for $d = 2$, $\kappa$ is given by

$$t\kappa^2 + \kappa_0^2 = 2\pi^2 \kappa^2 (\kappa^2 - \kappa_0^2), \quad \kappa_0 = \frac{1}{2\pi^{3/2}} \frac{< h^2 >^{1/2} J}{T^*};$$

$$t = - < \Omega^2 (T) > / \Omega^2 (0) = (T - T^*) / T^*.$$  

Here $T^*$ is the ordering temperature for the pure problem, i.e. for $< h^2 >= 0$. In that case $\kappa \to 0$ as $T^*$ is approached from above. With finite $< h^2 >$, $\kappa$ does not $\to 0$ at any
III. SINGLE-PARTICLE SPECTRAL FUNCTION

I calculate here the single-particle spectral function due to the frozen fluctuations of the loop-current order parameter. The contribution of the inelastic scattering is unimportant compared to these. The single-particle self-energy due to such fluctuations can be calculated using the structure factor of the static fluctuations [43], given by Eqs. (4):

$$\Sigma(k, \omega) = \sum_q |M(k, q)|^2 G(k - q, \omega) S(q).$$  \hspace{1cm} (9)

$M(k, q)$ is the matrix element for scattering of fermions of momentum $k$ through $q$ by the static fluctuations at the boundary between the domains of Fig. 1. $G(k, \omega)$ is the single-particle Green’s function. As discussed near the end, given at $S(q)$, Eq. (9) is exact to $O(1/N)$, where $N$ is the number of domains. Other approximations in the evaluation of (9) are also discussed below.
A. Limit of Infinite correlation Lengths

Before presenting the calculations with finite size for the domains, I will show the plausibility of the idea of pseudo-gaps through singular forward scattering in the limit $\kappa^{-1} \to \infty$. In that case, because $\gamma^2$ defined below is finite, we may properly approximate \[1\] the q-dependence in the structure factor in the second term in \[4\], which will be found to be the important term, by

$$C\left(\frac{1}{\kappa^2 + q^2}\right)^2 \to (2\pi)^2 C \gamma^2 \delta^2(q); \quad \gamma^2 = \int \left(\frac{1}{\kappa^2 + q^2}\right)^2 \frac{d^2q}{2\pi^2}.$$ \[10\]

Then \[9\] gives that $\Sigma(k,\omega) \to \gamma^2 C|\mathcal{M}(k,0)|^2 G(k,\omega)$. Inserting this in the expression for the self-consistent Green’s function $G(k,\omega)$, we see that in this limit, there exists a well-defined gap at the chemical potential over energies $\pm \sqrt{C\gamma^2 |\mathcal{M}(k,0)|^2}$. For finite $\kappa$ one may expect that the gap is replaced by a diminution of the density of states whose value and angular form depends on the matrix elements and the spectral function in the pure limit. The calculations in the rest of this section carry out this program.

B. Calculations for the Disordered Loop-Current Problem

The Hamiltonian $H_0^\alpha$, the ground state, and the one-particle excited states and energies for each of the order parameters $\Omega_\alpha$ in the pure limit are known. In Fig.\[1\], space is divided into different regions, a particular $H_0^\alpha$ reigns inside $\mathcal{R}_\alpha$. The ground state of $H_0^\alpha$ is orthogonal to those of $H_0^\beta$ in the thermodynamic limit; their overlap is of order the inverse of the area of a domains in the situation in Fig. \[1\] which may be taken to be zero. In such a situation, the global ground-state and the wave-functions of excitations should be calculated such that they correspond to those of $H_0^\alpha$ inside each $\mathcal{R}_\alpha$ and transform continuously to those of $H_0^\beta$ on entering $\mathcal{R}_\beta$. I employ the average $t$-matrix approximation in the theory of random systems \[49\] that any given region is imbedded in an equal mixture of other regions. The self-energy for the states of a given domain $\alpha$ due to scattering at the boundary to states of the other domains $\beta \neq \alpha$ is calculated. The matrix elements $M_{\alpha,\beta}(k,q)$ are to be evaluated at the boundary $\ell(\alpha - \beta)$. One then has

$$\Sigma_\alpha(k,\omega) \approx \sum_{q,\beta \neq \alpha} |M_{\alpha,\beta}(k,q)\ell(\alpha - \beta)|^2 G_\beta(k - q,\omega) S(q).$$ \[11\]
From the $\Sigma(k, \omega)$ and $G_\alpha(k, \omega)$ thus obtained, $\Sigma(k, \omega)$ is obtained by averaging over the four $\alpha$'s. As a first step, one may use $G^0_\alpha(k, \omega)$, the Green’s function corresponding to $H^0_\alpha$.

It is important to note that for a given $k$, the eigenvalues (and eigen-vectors) for $H^0_\alpha$ are different for different $\alpha$. The anapole vectors $\Omega_\alpha \equiv (\Omega_x, \Omega_y) = |\Omega|(\pm 1, \pm 1)$ break inversion symmetry (in addition to time-reversal) such that the conduction band states (which alone we will be interested in) have in the simplest approximation the eigenvalues

$$e^0(k, \Omega_\alpha) \approx t pd \sqrt{\sin^2(k_xa/2 + \Omega_x) + \sin^2(k_ya/2 + \Omega_y)}$$

$$\approx t pd \sqrt{\sin^2(k_xa/2) + \sin^2(k_ya/2) + \frac{\Omega_x \sin(k_xa) + \Omega_y \sin(k_ya)}{\sin^2(k_xa/2) + \sin^2(k_ya/2)}} \tag{12}$$

for $\Omega_x, \Omega_y << 1$. The four set of states for different $\alpha$ are degenerate in the direction $(0, \pi)$ and equivalents and maximally displaced in energy from each other in the directions $(\pi, \pi)$ and equivalents. It then follows that the self-energy $\Sigma_{\alpha, \beta}(k, \omega)$ are maximal in the directions $(0, \pi)$ and minimal for the directions $(\pi, \pi)$. As shown below, this will give the angular dependence of the pseudo-gap and the so-called "fermi-arc" phenomena.

The matrix elements are calculated in the Appendix. It is shown there that they are finite for momentum transfer $q \to 0$. Since $\kappa$ is much less than $k_F$, dropping the $q$ dependence of $M$ in the calculation of the self-energy is a good approximation.

It is easy to calculate the imaginary part of the self-energy without paying detailed attention to the shape of the boundary $\ell(\alpha - \beta)$, which is justified for large domains.

$$Im\Sigma_{\alpha, \beta}(k, \omega) = Im\Sigma_{e, \alpha, \beta}(k, \omega) + Im\Sigma_{c, \alpha, \beta}(k, \omega). \tag{14}$$

$\Sigma_e$ is the contribution due to $S_e$ and $\Sigma_c$ due to $S_c$. The retarded part $Im\Sigma_{eR}$ is first found,

$$Im\Sigma_{eR, \alpha, \beta}(k, \omega) = Im\Sigma_{e, \alpha, \beta} \frac{2\pi \kappa v_F}{a} \frac{1}{\sqrt{(\omega - \xi^0(k, \beta))^2 + (2\pi \kappa v_F/a)^2}} \tag{15}$$

$$Im\Sigma_{e, \alpha, \beta} \equiv -\frac{2}{\pi} \ll \Omega(T) \gg \left( \frac{|M_{\alpha, \beta}(k)|^2}{2\pi \kappa v_F/a} \right) \frac{T}{J}. \tag{16}$$

$\xi^0(k, \alpha) \equiv e^0(k, \Omega_\alpha) - \mu$ are measured from the chemical potential or equivalently from $e^0(k_F(\alpha))$. $Im\Sigma_{e0}$ is the value of $Im\Sigma_e(k, \omega)$ at the fermi-surface and for $\omega = 0$. The real
part of the self-energy is obtained by the Kramers-Kronig transformation:

\[ Re\Sigma_{c,\alpha}(\mathbf{k}, \omega) = Im\Sigma_{c0}(\mathbf{k}_f, 0) \left( \frac{2\pi v_F k/a}{\sqrt{(\omega - \xi^0(\mathbf{k}, \beta))^2 + (2\pi v_F k/a)^2}} \right) \]

\[
\times \log \left| \frac{(2\pi v_F k/a)^2 + (\omega - \xi^0(\mathbf{k}, \beta))^2 + \sqrt{(2\pi v_F k/a)^2 + \xi^0(\mathbf{k}, \beta)^2}}{\omega_c(\omega - \xi^0(\mathbf{k}, \beta) + \sqrt{(2\pi v_F k/a)^2 + (\xi^0(\mathbf{k}, \beta) - \omega)^2})} \right| - \frac{2\pi v_F k/a}{\sqrt{(\omega + \xi^0(\mathbf{k}, \beta))^2 + (2\pi v_F k/a)^2}}

\times \log \left| \frac{(2\pi v_F k/a)^2 + (\omega + \xi^0(\mathbf{k}, \beta))^2 + \sqrt{(2\pi v_F k/a)^2 + \xi^0(\mathbf{k}, \beta)^2}}{\omega_c(\omega + \xi^0(\mathbf{k}, \beta) + \sqrt{(2\pi v_F k/a)^2 + (\xi^0(\mathbf{k}, \beta) + \omega)^2})} \right| .
\]

\( \omega_c \) is an upper cut-off in the energy, which may be taken to be \( \infty \) safely.

Looking at the relation between \( S_c(q) \) and \( S_c(q) \), \( \Sigma_c \) is found from \( \Sigma_e \) by

\[ \Sigma_{eR}(\mathbf{k}, \omega) = -\frac{J}{\hbar^2} \frac{\langle\langle \Omega(T) \rangle\rangle}{\langle\langle T \rangle\rangle} \frac{\partial}{\partial(k^2)} \Sigma_{eR}(\mathbf{k}, \omega). \]  

(18)

Let us first compare the relative magnitude of \( \Sigma_e \) and \( \Sigma_c \) to decide which is more important for the range of parameters of interest. For \( \kappa(T) \approx \kappa_0 \) and at typical energies of \( O(2\pi \kappa v_F / a) \), we obtain that a lower estimate on the ratio \( \Sigma_e / \Sigma_c \) is \( (J/T) \langle\langle \Omega(T) \rangle\rangle / \langle\langle \kappa^2 \rangle\rangle = 4\pi^3 \ll \langle\langle \Omega(T) \rangle\rangle / T \approx 4\pi^3 \ll \langle\langle \Omega(T) \rangle\rangle / T \). As mentioned already, typically, \( \langle\langle \Omega(T) \rangle\rangle / T \) is of \( O(4\pi 10^{-2}) \) at low temperatures, (measured in units of \( \mu_B^2 \)). So, except for \( T \) close to \( T^* \), \( \Sigma_e \) is more important than \( \Sigma_c \) and this alone will be considered henceforth, especially as for the same magnitude, \( \Sigma_e \) produces sharper features in the spectral function than \( \Sigma_c \).

I show the imaginary and real part of the self-energy for the directions near \( (\pi, 0) \) and equivalent, where the bare energies for different \( \Omega_\alpha \) are nearly the same, in Fig. [4]. Included is a background large-angle impurity scattering rate \( i \tau^{-1/2} \) added to the imaginary part.

The spectral function is calculated using the approximations described above,

\[ A(\mathbf{k}, \omega) = -\frac{1}{\pi} ImG_R(\mathbf{k}, \omega) \approx -\frac{1}{4\pi} \sum_\alpha Im \frac{1}{\omega - \xi^0(\mathbf{k}, \alpha) - \Sigma_{\alpha R}(\mathbf{k}, \omega)}. \]  

(19)

The results for \( \xi(\mathbf{k}, \alpha) = 0 \) in (or close to) the \( (\pi, 0) \) directions are shown in Figs. [5] for various values of the pre-factor of the self-energy \( Im \Sigma(\mathbf{k}_F, 0) \). In Fig. [6] the sensitivity of the spectral function to the width parameter \( (2\pi \kappa v_F / a) \) is exhibited.

The results for \( \xi(\mathbf{k}, \alpha) = 0 \) in the \( (\pi, \pi) \)-directions are shown in Figs. [7]. As explained above the contributions of the spectral function for different \( \Omega_\alpha \) have been summed after the self-energy for each of them to scatter to the others in the adjoining spatial regions is
Figure 4: The Imaginary and the Real part of the normalized Self-energy $Im\Sigma_{\epsilon}(1)$, in the $(\pi, 0)$-direction at the "Fermi-vector" as a function of energy normalized with respect to the width parameter $(2\pi \kappa v_F/a)$.

summed. One of the curves is drawn with the matrix element for scattering set to zero representing the spectral function without loop order and the other two are for increasing magnitude of loop-order. To see the passage from the $(\pi, \pi)$ direction to $(\pi, 0)$ direction, the spectral function is plotted for the same three coupling constants and values of $\Omega_{\alpha}$ at the angle bisecting $(\pi, \pi)$ direction to $(\pi, 0)$ directions, in Fig. (8).

C. Qualitative features of the Results

Before comparing with experiments let us discuss the properties expected of the spectral function. An inspection of Eq. (19) together with the self-energy in Fig. (4) leads to the conclusions that:

(i) The principal peaks in the spectral weight for $\mathbf{k} = \mathbf{k}_F$ and in the anti-nodal direction, may be estimated in the limit of very long correlation length $a/(2\pi \kappa)$ from the real and imaginary part of the self-energy given above and taking $|M(\mathbf{k})|$ from the Appendix. Such an estimate gives that it is moved from the chemical potential near the $(\pi, 0)$ and equivalent directions by

$$G \approx \pm <\langle \Omega(T) \rangle^2> \left( \frac{V_{pd}^2}{4\pi v_F/a} \right).$$

(20)

This estimate is true provided $|G|$ is much larger than about $(\pi v_F/a)\kappa$. In this, the dilute impurity limit, the gap is independent of $c$ and varies as the square of the impurity averaged order parameter.
Figure 5: The single-particle spectral function at the fermi-vector near the $(\pi,0)$ direction as a function of energy in units of the width parameter $2\pi \kappa v_F(\theta)/a$. The successive curves are for the coefficient $\text{Im } \Sigma_e(k_F,0) = 0, 0.25, 0.5, 1, 2$ in units of $(2\pi \kappa v_F/a)$. This coefficient defined through Eq. 18 depends on the order parameter and the Matrix elements, which increase on decreasing temperature. An impurity scattering contribution to the imaginary part of the self-energy $(2\tau)^{-1} = (2\pi \kappa v_F/a)$ has also been used in the calculations. The hump at $\omega = 0$ for large order parameter disappears for larger impurity scattering.

(ii) The temperature dependence of the position of the peaks is expected to be similar to that of the square of the measurable order parameter $\langle \Delta(0) \rangle^2$. There is a weak dependence of the *average gap* on the impurity concentration in the approximate theory presented here. But the *local gap* is proportional to the local impurity density (and the strength of their potential favoring the order parameter).

(iii) The angle dependence of the characteristic peak position at a given angle, provided the condition for the peak in relation to the width is satisfied, is largest in the $(\pi,0)$ directions in which the energy differences in $\epsilon(k,\Omega_\alpha)$ are 0 and least in the $(\pi,\pi)$ directions where they are maximum.

(iv) For $|\omega - G| >> |\xi(k)|$ the spectral function is unaffected and returns to its values for $T >> T^*(x)$.

(v) There is always finite weight in the spectral weight at the chemical potential ($\omega = 0$) at $\xi(k) = 0$, but which is reduced to $\text{Im } \Sigma^{-1}(0,k_F)$ with a width which is proportional to
Figure 6: The single-particle spectral function at the fermi-vector as a function of energy in units of a background scattering rate $\tau^{-1}$ for various values of the normalized width parameter $2\pi\kappa v_F(\theta)/\tau/a$. The successive curves are for $(2\pi\kappa v_F/a) = 0.5, 1, 2$ in units of $\tau^{-1}$. $\text{Im}\Sigma(0, k_F) = 1$ for all the curves.

Figure 7: The single-particle spectral function at the fermi-vector in the $(\pi, \pi)$ direction as a function of energy in units of a background scattering rate $\tau^{-1}$ in the $(\pi, \pi)$-directions for no loop current order and for increasing loop-current order, with $\text{Im} \Sigma(e, k_F, 0) = 0, 1, 2$ in units of $(2\pi\kappa v_F/a)$. The differences of energies for different $\Omega_0$ are correspondingly changed in each curve.
revealed in Eqs. (21,24) is that the imaginary part is a homogeneous function of \( \omega \) due to the usual impurity contribution and inelastic and temperature dependent relaxation in Fig. (5). Whether the peak occurs or not depends on details such as the scattering rate inverse of its height. For large value of the pseudo-gap, a weak peak is displayed at \( \omega < 0 \) well below the chemical potential, \( \omega << 0 \) (or well above) decays very slowly as \( \log |\xi(\mathbf{k})/\omega_c| \) for positive \( \omega = \xi(\mathbf{k}) \). The almost homogeneous dependence of the spectral function on \( (\omega - \epsilon_\mathbf{k}) \) may be tested experimentally by ARPES but it should be remembered that inelastic scattering at finite temperatures and frequencies above \( T^*(x) \) must revert it to the marginal fermi-liquid form and that is almost purely \( \omega \)-dependent, as is indeed observed \([55][56]\).

(vi) An interesting general aspect of the self-energy from the forward scattering process revealed in Eqs. \([14][17]\) is that the imaginary part is a homogeneous function of \( (\omega - \xi(\mathbf{k})) \), so that as a function of this quantity it is important throughout the band. The real part well below the chemical potential, \( \omega << 0 \) (or well above) decays very slowly as \( \log |\xi(\mathbf{k})/\omega_c| \) for positive \( \omega = \xi(\mathbf{k}) \). The almost homogeneous dependence of the spectral function on \( (\omega - \epsilon_\mathbf{k}) \) may be tested experimentally by ARPES but it should be remembered that inelastic scattering at finite temperatures and frequencies above \( T^*(x) \) must revert it to the marginal fermi-liquid form and that is almost purely \( \omega \)-dependent, as is indeed observed \([55][56]\).

(vii) The spectral function at \( \mathbf{k}_F \) as a function of frequency displays particle-hole symmetry. For any finite \( \pm(\epsilon_\mathbf{k} - \xi(\mathbf{k}_F)) \) the value of the spectral function at \( \omega = 0 \) is identical.
but there is no reason that it has particle-hole symmetry in detail, i.e. the spectral weight at $\pm \omega$ (or at $\pm (\omega - \xi(k))$ are in general different.

Each of these points is discussed in relation to the experiments below.

IV. COMPARISONS WITH EXPERIMENTS

Let us now compare features of the derived pseudo-gap first to the ARPES experiments because the most detailed information about the pseudo-gap is obtainable in principle from ARPES. In doing so, one notes that there are no detailed analysis of the line-shapes observed in the experiments or extracted self-energies from which quantitative features of the data may be compared in detail with the calculations. Indeed, most of the data is only analyzed to get the peak position as a function of angle on the fermi-surface and the temperature. I suggest that the self-energy below $T^*(x)$ be deduced from experiments and compared with the expressions and calculations give here to test their validity, However several general qualitative and some quantitative features may already be compared.

Temperature and Angular Dependence of the Pseudo-gap - “The Fermi-Arc”: In Fig. (5), the spectral function is plotted for several values of $Im \Sigma(k_F, 0)$ in the $(\pi, \pi)$ direction. The curves can be interpreted as the spectral function as a function of temperature. The value of the characteristic $\Omega$ for the peak in the spectral function is given by Eq. (20); the position of the peaks in Fig. (5) corresponds well with it. Consider the temperature dependence: the result derived here, point (ii) after Eq.(19), is that the scale of the pseudo gap increases as the square of the impurity averaged order parameter $<\Omega(T)>^2$ if the temperature dependence of $\kappa$, which only very weakly determines the pseudo-gap is ignored. $<\Omega(T)>^2$ can be obtained from the polarized neutron scattering intensity, for which the results are available for $YBa_2Cu_3O_{6+x}$ [27] and for $HgBa_2CuO_{4+x}$ [28] while the information about the pseudo-gap is obtained in $Bi(2201)$ and $Bi(2212)$. Within the (rather large) error bars in the experimental results, the normalized Intensity of neutron scattering vs. the normalized temperature $T/T^*(x)$ of all the four measured samples for different $x$ in the latter and all the six measured samples in the former fall on top of each other. In Fig. (9), the experimental data, taken from Ref. (34) for the temperature dependence of the deviation of the peak in the spectral function from the chemical potential at $k = k_F$ in two different directions is plotted in normalized units as a function of $T/T^*$, where $T^*$ is
Figure 9: The data for the movement of the position of the peak in the spectral function for Bi2201 as a function of temperature, Fig.(S1-F) from Ref(34) from above $T^*$ to $T_c$ is plotted in a normalized to its value at $T_c$ as a function of $T/T^*$. The measured magnetic Bragg peak intensity at (101) measured by polarized neutrons in Ref (28) in $HgBa_2CuO_{4+x}$ from above $T^*$ to near $T_c$ is similarly normalized and plotted as a function of $T/T^*$. The ratio $T_c/T^*$ for these two compounds is the same to within about 10%. $T^*$ in both sets of data also have an uncertainty of about 10% determined only to an accuracy of about ±10K. On the same plot, the normalized square of the order parameter, measured by neutron scattering for $HgBa_2CuO_{4+x}$ is plotted. Within the error bars of both the set of measurements, the expectations of the theory are borne out.

The effect of the correlations is felt at an angle $\hat{k}_F$ only when $G(T, \hat{k}_F)$ is comparable or larger than the characteristic width $(2\pi v_F/a)\kappa(T)$. This is clearly in evidence in Figs. (5) and (6). This automatically produces the phenomena termed ”Fermi-arcs”, which is simply the result that the spectral function as a function of angle $\hat{k}_F$ from the nodal direction has a peak at the chemical potential for any $k$ only over some angles near the nodal direction which decreases as temperature decreases. On comparing Figs. (5), (7) and (8) for the $(\pi,0)$, $(\pi,\pi)$ and the direction at an angle bisecting them for the same values of $|\Omega|$, one finds that over this range, the gap is larger for the first than the third and non-existent for the second. As temperature decreases below $T^*$ and $\Omega$ increases, the pseudo-gap appears
first in the \((\pi,0)\) directions and progressively moves towards the \((\pi,\pi)\) directions. This naturally simulates the appearance of a Fermi-arc.

**Characteristic Magnitude of Pseudo-Gap:** The average gap, estimated in Eq. 20 depends only weakly on the disorder. Its value may then be estimated from the magnitude of the order parameter and from the electronic energy parameters \(V_{pd}\) and \(2\pi v_F/\alpha\) which are of similar magnitudes, about 1 eV. This then gives the average gap to be about \(2 \times 10^{-2} eV\), which is a reasonable experimental scale.

While as noted, the average pseudo-gap depends very weakly on the average impurity concentrations of the kind which locally favors one of the orientations of the order, locally the structure factor depends linearly on the impurity concentration and its relevant potential. Also, there is the effect of impurities which couples to the magnitude of loop-order. So, one should expect local gaps to be larger in the neighbor-hood of impurities. This has been observed in STM measurements [11], which shows larger gaps in the vicinity of identifiably impurities with the correlation length of the gap-map similar to that of the distribution of impurities.

**Density of States:** Scanning Tunneling Spectroscopy (STM) measures the angle-integrated density of states as a function of energy \(N(\omega)\) multiplied by tunneling matrix elements which in general are functions of angle for which no precise information is possible. With this reservation STM provides very accurate density of states both below and above the chemical potential as well as its variation from one region to another on unit-cell size or better length scale. A feature found in these experiments both above and below \(T^*(x)\) is a decrease in the background density of states from below to above the chemical potential. Since, it is quantitatively similar above and below \(T^*(x)\), it cannot have to do with the physics of the pseudo-gap. Over the range \(-100\) meV to \(+100\) meV, the decrease in density of states is about 25% of the density of states at the chemical potential. The simplest reason for the variation of the background density of states must be sought in the band-structure before any more sophisticated explanation are invoked. For tight-binding one-electron models which fit the experimentally determined fermi-surface for a Bi2212 sample with 16% doping, which is in the pseudo-gapped region for which STM and ARPES results are available, the density of states has been calculated by Norman [59] and shows variation similar to the background variation in the experiments. I plot in Fig. 10, the calculated density of states with such a background variation showing the pseudo-gap, which is about the scale
Figure 10: The density of states $N(\omega)$, normalized to its constant assumed value without the pseudo gap, is shown as a function of energy $\omega$ in units of the width parameter $2\pi v_F(\theta)/a$. Impurity scattering rate is taken as 1 and $\text{Im}\Sigma^{(1)}(\hat{k}_F, 0) = 1$ in units of the width parameter.

of the depression of density of states at $\omega = 0$ relative to the background which is observed with the pre-factor in self-energy indicated.

Thermodynamic and Transport Properties - The apparent Anomaly in the particle number:
It has been extensively shown \cite{60} that a model density of states similar to that measured by STM may be used to fit the specific heat and the magnetic susceptibility. This shows that these thermodynamic quantities reflect one-particle properties and given that the correct form of the density of states is obtained, these then follow.

A remarkable feature noted in the specific heat results and the c-axis optical sum-rule \cite{6}, \cite{67}, \cite{68} needs closer attention. Over the range of measurements, which extends from low temperatures to just above $T^*(x)$ the entropy is not conserved compared to samples without a pseudo-gap (taking fully into account the change in particle density). The same anomaly is found in the deduced c-axis optical spectral weight where sum-rules are apparently not satisfied when integrating up to energies up to an order of magnitude larger than the pseudo-gap energy scale, obtained for example, STM measurements. (It is harder to deduce this from a-b plane conductivity, firstly because unlike c-axis conductivity, it is dominated by
the region of states near the node due to their higher velocity [68] and also because it cannot be measured as accurately as the c-axis conductivity.) Indeed STM measurements directly show a diminution in density of states at low energies without a the bump in the density of states at larger energy needed to conserve the particle number when integrating it over a few times the gap energy. Similar aspects are visible in the calculated density of states in Fig. [10]. This is quite unlike what is seen by STM in the extra change in the density of states below $T_c$, where the d-wave BCS singularity at $\pm \Delta_0$ and the satisfaction of the sum-rule within $\omega \approx 4\Delta$, are found.

In the calculations presented here, and noted in point (vi) above, this feature is traced to the fact that forward scattering gives a self-energy which is (almost) homogeneous in $(\omega - \epsilon_k)$. This leads to anomalies in the spectral function tied to $\epsilon_k$ irrespective of the value of $\epsilon_k$ within the band. This is to be contrasted with $\omega$ dependent but $\xi(k)$ independent features of the marginal fermi-liquid form [61] and for heavy-fermions [62], [63], where the anomalous features are tied to the chemical potential. Forward scattering singularities imply that in measuring physical quantities, for instance the entropy or the optical spectral weight, one must integrate over temperatures or frequencies over the scale of the band-width to conserve the necessary weight in the pseudo-gap region. There should be anomalies at band-edges but these may be wiped out by additional sources of line-width, either intrinsic or inherent in the experimental tool employed.

*Low energy transport measurements:* For frequencies and temperatures below the pseudo-gap scale $G$, there is a finite density of states at the chemical potential. The singularities responsible for the marginal fermi-liquid anomalies in the quantum-critical region are also removed in the low-energy spectra of the loop-ordered state. So if one confines experiments to low energy and temperature compared to $G$ for $T$, deceptively simple normal fermi-liquid behavior is to be expected. This has been well documented in various experiments [64], [65]. Theoretical calculations for transport properties in the pseudo-gap regime using the remnant ”Fermi-Arc” in agreement with experiments have been presented [66].

*Particle-hole assymmetry:* Finally we note that the spectra is not particle-hole symmetric *in detail* even when we assume a constant normal density of states over the pseudo-region of energies. Evidence for this is presented in the calculated density of states, Fig. [10]. Similar asymmetry is calculated when only a range of $\epsilon_k$ on either side of the normal $k_F$ is integrated over or if the spectral function is compared for $\pm |k - k_F|$. The diminution in spectral
weight above the chemical potential is smaller than that below in such measurements. This asymmetry was first observed in Ref. [54]. In the calculations here, the asymmetry comes about from the analytic properties of the real part of the self-energy for forward scattering singularity, which insist that it be zero in the limit $\omega \to -\infty$ from negative values, in the limit $\omega \to +\infty$ from positive values, be zero at $\omega = 0$ and have features at $\omega = \xi(k)$.

**Frequency Dependent Susceptibility: Effects on Local Probes:**

It is known from experiments in random-field Antiferromagnets that time-dependent fluctuations in such problems are very complicated [70], [71], [47], similar to that in spin-glasses. Experiments with different time-scales have given different results [69]. Specifically in relation to the dichotomy in the results from "elastic" neutron scattering and NMR probes in cuprates mentioned in the Sec. I, there are instances such as in UPt$_3$, where neutron scattering found long-range order [72] but NMR did not find an onset of static fields [73] below the AFM transition. There are two distinct aspects of the time-dependence. One is the complicated problem of the dynamics of the domain walls [47] which also leads to hysteretic phenomena. These are in general very slow phenomena and not of our concern for the present problem. The other is that of the characteristic scale of fluctuations of lengths smaller and up to order of their finite size. Such fluctuations at low temperature are dominated by quantum fluctuations.

Then derivation of the static structure factor [44–47], summarized in Sec. II, assumes that the dynamic fluctuations are of the Orenstein-Zernike form

$$\chi_c(q, \omega) = \frac{\langle\langle \Omega(T) \rangle^2 \rangle_{\eta \Omega}}{i\omega + J(q^2 + \kappa^2)}.$$  \hfill (21)

At long wavelengths, $q \lesssim \kappa$, the characteristic frequency of oscillations never truly go to 0 at any temperature because $\kappa(T)$ never approaches 0. For larger $q$, the dynamics well below $T^*$ must revert to that of the pure system, i.e. finite energy oscillations between different possible configurations of the order parameter. These have been observed [52] and extensively investigated theoretically [53]. Eq. (21) says that there must exist low frequency excitations with a characteristic frequency width of order

$$\Delta \omega \approx J\kappa^2(T).$$  \hfill (22)

The lower limit to the correlation length $\xi = (2\pi\kappa)^{-1}a$ through neutron scattering measurements in the crystal studied by neutron scattering is about 25$a$. With the characteristic
nearest neighbor or zone boundary energy scale $J/(a/(2\pi))^2 \approx 500$ Kelvin, i.e. $10^{13}sec^{-1}$ this gives $\Delta \omega$ less than about $10^{10}sec^{-1}$. This is much smaller than the characteristic resolution of the neutron scattering experiments which for ”quasi-elastic peaks” integrate over energies of $O(1meV) \approx 10^{11}sec^{-1}$, while it is much above the typical NMR shifts expected which are $O(10^9)sec^{-1}$. Static fields in different directions and with varying magnitudes are then motionally averaged [40] due to the fluctuations at frequencies much larger than the NMR or $\mu$SR shifts or expected in the pure model. Motional averaging occurs if the fluctuation frequency between alternate configurations, $\Delta \omega$ is much larger than the energy splitting $\delta \nu$ between alternate configurations or the frequencies over which they are distributed. Only the un-split line can then be seen. The contribution to the line-width of this process is $\approx (\delta \nu)^2(\Delta \omega)^{-1}$. For $\Delta \omega \approx 10^{10}secs^{-1}$ and $\delta \nu \approx 10^5secs^{-1}$, this is $\approx 1sec^{-1}$. If there are independent sources of line-width much larger than this, say direct nuclear relaxation through conduction electrons or dipolar interactions, then this line width is unobservable in $T_1^{-1}$ measurements. For NMR relaxation in $YBa_2Cu_3O_{6.63}$, the nuclear relaxation rate [74] of $^{17}O$ at the chain sites at 200 K is about 40 sec$^{-1}$. The NQR experiment [38] on $^{137}$Ba shows a relaxation rate [38] of about 3 X $10^3secs^{-1}$. In experiments with muons, the muon lifetime itself is only 2 $\mu$secs. So motional narrowing leaves in every case an unshifted line with no traces left of the shift or the motionally averaged relaxation rate. However, if there are nuclei with relaxation rate much slower than a few secs$^{-1}$, one should observe a change of relaxation rate due to the motional narrowing discussed here.

One can also ask, what would the correlation length have to be in order to see line-splittings and shifts similar to static long-range order, i.e. when is the characteristic scale of fluctuations smaller than $10^5sec^{-1}$. The answer from the above estimates is $\xi \gtrsim 10^4 a$, i.e. O(4 micron).

These consideration would resolve the apparent conflict between the observed order in neutron scattering and in low frequency local experiments. There are some special aspects of the NQR experiments [38], which will be discussed in a separate paper [75]. The test of this idea is further experiments. It is advanced here because of the high quality of both the NMR and the $\mu$SR experiments on the one hand and the neutron scattering experiments on the other. Some evidence of new relaxation rates setting below the pseudo-gap temperature has been obtained in pump-probe spectroscopy [78]. There also appear to be some abnormal low frequency relaxational processes [76] and low frequency microwave absorption up to the
range of about 10 GHz \[77\] in under-doped cuprates, which appear to disappear for dopings without a pseudo-gap. These need further investigation in light of the results presented here.

Validity of the Calculations:

The calculations for the single-particle spectral function reported in this paper are very simple - just the leading perturbation calculation due to the structure factor. But because of the formation of the pseudo gap, they are reliable for energies below its magnitude. Let us examine the corrections to such calculations. The vertex corrections to the current vertex \( \delta \Lambda(k, \omega, q, \nu) \) and to the density vertex \( \delta \Lambda_0(k, \omega, q, \nu) \) with \( q, \nu \) the momentum and energy transfer for \( \omega \) at the chemical potential and at \( k = k_F \) respectively are fixed by the Ward identities which relate them to derivative of the self-energy with respect to \( k \) at \( \omega = 0 \) and derivatives with respect to \( \omega \) at \( k = k_F \). From Eq. (18) and equations which it draws on, one finds that such derivatives are always proportional to \( (\omega - v_F (k - k_F)) / \kappa^2 \) as long as \( \kappa \) is finite. So for forward scattering processes of the kind considered for the pseudo-gap, both the vertex corrections are irrelevant. Paradoxically, the frozen fluctuations which lead to a pseudo-gap are less disruptive very near the chemical potential than even the scattering leading to Landau parameters.

One may consider repeated self-energy insertions in the calculation, for example by self-consistent Born approximation. This amounts to the Coherent Potential Approximation in the theory for random electronic structures. The Coherent Potential approximation is exact in the \( 1/N \rightarrow 0 \) limit where \( N \) is the number of distinct domains \( N. N = 4 \) in our case. Since the self-energy due to forward scattering depends only on the local angular density of states, this can be easily carried out. A first iteration produces essentially no change in the finite spectral weight at \( \omega \approx 0 \). These results imply that for energies below the peak of the spectral functions, i.e. well in the pseudo-gap region of the spectral function, the results obtained here are robust. This does not imply however that the detailed line shape, especially near the region of the peaks in the spectral function may not be changed from that given in the simple calculations.

V. CONCLUDING REMARKS

Previous and present work are based on three guiding principles: (1) A three orbital model is essential \[79\] in the metallic state induced by doping charge transfer insulators \[80\].
Properties of the Strange Metal phase including its instability to Superconductivity are governed by the hypothesized quantum-critical fluctuations with $\omega/T$ scaling and negligible momentum dependence. The quantum-critical fluctuations are the fluctuations of a time-reversal and inversion breaking phase which occupies the region of the phase diagram below $T^*(x)$. For a theory based on these guiding principles to be credible, all universal properties of the metallic and superconducting state of all the cuprates must follow from it and it should have verifiable and unique predictions. In the present paper, the principal lacunae in the development so far, that of the pseudo-gap in the under-doped cuprates, is corrected through forward scattering among domains of the loop order phase. There is no doubt through STM measurements that there are domains formed below $T^*$ and of the size assumed and with inversion breaking. But that technique is insensitive to the time-reversal breaking feature of loop order revealed by polarized neutron scattering, which averages over domains. Measuring time-reversal breaking on the scale of domain size does not appear possible by present day techniques but may be possible in the future. Some further predictions are made here.

The most important suggestion for the experiments is a detailed investigation of the $(\omega, k)$-dependence of the self-energy to test whether it is consistent in detail with the form derived in Sec. (IV) here. In particular the predicted $(\omega - \xi(k))$ dependence is rather unique to forward scattering. These can be deduced by quantitative measurements using the ARPES technique. Another direct prediction for experiment is unfortunately difficult to carry out. This is that the line-shape in Magnetic Bragg scattering should have a large anomalous contribution of Lorentzian squared form, given in Eq. (4). Such a structure factor is observed in random-field Antiferromagnets. These are difficult in the case of $q = 0$ transitions such as loop order, because the magnetic scattering, which is a small fraction of the usual lattice Bragg scattering, must occur atop some of the lattice Bragg peaks for magnetic patterns because there is no change in the translational symmetry. Another prediction is to control the magnitude of the defects or at least those coupling linearly to the loop-current order parameter and study if the changes in thermodynamic and transport properties due to the change in the magnitude of the pseudo-gap calculated here. An easily testable experimental proposal is the measurements of the slow time-dependence of the magnetic correlations and the electronic properties to which they couple. This may be done by pump-probe techniques or low frequency microwave absorption measurements or...
through the techniques of spin-echoes.

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Appendix: Matrix Elements for One-particle Scattering due to Domains

In Fig. (1), space is divided into different regions, inside each which, a particular $H(\Omega_s) = H_{\Omega_s,\Omega_y}$ reigns. Let this region of space be denoted by $\mathcal{R}_\alpha$. The ground-state fermion wave-function and the wave-functions of excitations calculated in one region must transform into states of the other regions continuously through matrix elements for scattering between them evaluated at the boundary. The Hamiltonian for Fermions in the region $\mathcal{R}_\alpha$ is

$$H_{\Omega_s,\Omega_y}^0 = K_0 + h_{\Omega_s,\Omega_y},$$

(23)

where $K_0$ is the Kinetic energy in the non-interacting problem, which is the same for all regions and $h_{\Omega_s,\Omega_y}$ is the effective Fermion Hamiltonian generated by the ordering field $(\Omega_s, \Omega_y)$ in that region. $h_{\Omega_s,\Omega_y}$ has been derived in the simplest approximation to be

$$h_{\Omega_s,\Omega_y} = (V_{pd}/16) \sum_{k,q} i \left( \langle \Omega_{x,q} \rangle c_{xk} p_{k+qx}^+ d_k + \langle \Omega_{y,q} \rangle c_{yk} p_{k+qy}^+ d_k \right) + H.C.$$  

(24)

$\Omega_{q,x,y}$ is the collective variable which condenses in the pure system at $q = 0$, i.e. $<\Omega_{x,y}>$ is the order parameter inducing an extra kinetic energy. In the pure limit, there are then four distinct possible Hamiltonians globally.

In the situation depicted in Fig. (1), there is a packet of $q$ of typical size (and shape in a more detailed theory) given by $\kappa$ in which the "almost-condensation" occurs in the
region $R_{(x,y)}$. For $\kappa a << 1$, the one-particle states may be constructed starting from the states of $H(\Omega_x, \Omega_y)$ in the region $R_{(x,y)}$. These states transform to states of the neighboring $R(\Omega'_x, \Omega'_y)$ through scattering by the perturbation Hamiltonian $H'(R_{(x,y)}, R_{(x',y')})$ at the boundary between the two regions. The perturbation is the difference

$$H'(R_{(x,y)}, R_{(x',y')}) = h_{\Omega'_x, \Omega'_y} - h_{\Omega_x, \Omega_y}.$$  \hfill (25)

The unperturbed conduction band states, in the simplest representation in the chosen gauge are

$$c^+_k,\Omega_x,\Omega_y = d^+_k/\sqrt{2} + i \left( s_{xk}\Omega x^+ + s'_{yk}\Omega y^+ \right) / \sqrt{2(s^2_{xk}\Omega_x + s^2_{yk}\Omega_y)}. \hfill (26)

s_{xk}\Omega_x \equiv \sin(k_x a/2 + \Omega_x) \approx (\sin(k_x a/2) + \Omega_x \cos(k_x a/2)); s'_{yk}\Omega_y \equiv \sin(k_y a/2 - \Omega_y) \approx (\sin(k_y a/2) - \Omega_y \cos(k_y a/2));$$

etc. Note that the sign difference of the $\Omega$ dependent term between $s$ and $s'$ needed for the closed loop formation of fluxes, as depicted in Fig. (2).

The mixing matrix element to be integrated over the boundary between the regions $R(\Omega'_x, \Omega'_y)$ and $R(\Omega_x', \Omega_y')$ are to first and second order in the $\Omega$’s,

$$<k + q,\Omega'_x,\Omega'_y|H'(R_{(x,y)}, R_{(x',y')})|k, \Omega_x, \Omega_y> = (V_{pd}/16) \left( \sin(k_x a)(\Omega_x - \Omega'_x) + \sin(k_y a)(\Omega_y - \Omega'_y) \right) + \frac{c^2_{xk} s^2_{yk}(\Omega'_x - \Omega_x^2) + c^2_{yk} s^2_{xk}(\Omega'_y - \Omega_y^2)}{s^2_{xk} + s^2_{yk}}.$$  \hfill (27)

Here $s_{xk} \equiv \sin(k_x a/2), s_{yk} \equiv \sqrt{s^2_{xk} + s^2_{yk}}$. Such matrix elements are to be taken at all the boundaries depicted in Fig. (1) through out the solid. This really implies integration over the angle between the normal to the boundary and the direction of the velocity operator of the conduction electrons at $k_F$. Consider the leading term in Eq. (27). Integrated over all such angles, it is clearly zero for any two given $\Omega_\alpha$. But the boundary is only over finite angular regions, where it is in general non-zero. Considering average over all such regions, the matrix element becomes independent of the direction of $k_F$. The only important thing is its magnitude, of $O(V_{pd}|\Omega|/4)$. More appropriately, one should introduce a probability distribution for the domain boundary between any two given $\Omega_\alpha$. But it does not add anything to the properties at the level calculated. The next order term specifically depends on the difference in the magnitudes $\Omega^2_\alpha$. It also after integration over the boundaries is angle independent and is an order of magnitude smaller for typical $|\Omega|$.

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