How Much Phase Coherence Does a Pseudogap Need?

Paul E. Lammert
Department of Physics, The Pennsylvania State University, University Park, PA 16802

Daniel S. Rokhsar
Department of Physics, University of California, Berkeley, CA 94720,
and the DOE Joint Genome Institute, Walnut Creek, CA 94598
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It has been suggested that the “pseudogap” regime in cuprate superconductors, extending up to hundreds of degrees into the normal phase, reflects an incoherent d-wave pairing, with local superconducting order coherent over a finite length scale $\xi$, insufficient to establish superconductivity. We calculate the single-particle spectral density in such a state from a minimal phenomenological disordered BCS model. When the phase-coherence length exceeds the Cooper pair size, a clear pseudogap appears. The pseudogap regime, however, is found only over a relatively narrow range of phase stiffnesses, hence is not expected to extend more than about 20% above $T_c$.

It is widely believed that the peculiar normal pseudogap regime in underdoped cuprate superconductors (see refs. 1, 2 for recent reviews), holds keys to unraveling the entire problem of cuprate superconductivity. In this regime, between the superconducting transition temperature $T_c$, and $T_s$, possibly hundreds of degrees higher, spectral density near the putative Fermi surface is suppressed – in contrast with the familiar behavior of BCS superconductors. Evidence of this phenomenon is consistently observed most clearly in angle-resolved photoemission (ARPES)3, 4 but also in $c$-axis tunneling, magnetic susceptibility, heat capacity, Raman scattering, neutron scattering, and NMR measurements. The variation of the pseudogap with momentum, strongest near the $(\pi,0)$ directions and weak or nonexistent near $(\pi,\pi)$, mirrors that of the full $d_{x^2−y^2}$ superconducting gap.

One potential explanation of this behavior, as suggested by Kivelson and Emery5, is that local superconducting correlations (Cooper pairing) set in at $T_s$, but that long-range phase coherence is not established until the temperature drops below $T_c$. The plausibility of the idea derives from the facts that phase fluctuations generally play a larger role in lower- (here two) dimensional systems, and the superfluid density in the cuprates is very low, making the order parameter phase “floppy.” The notion is analogous to a magnetic material in which local moments form far above the temperature at which they become ordered. Nevertheless, this is not quite the same thing as pre-formed pairs.

Several previous calculations have investigated this idea6, 7, 8, 9. With the exception of reference 8, which studies effects of uniform superflow fluctuations, these are essentially diagrammatic approaches, with the attendant need for various sorts of truncations or resummations. The purpose of the present work is to get a better understanding of the possibilities and limitations of the incoherent pairing scenario in a BCS-like framework with as few additional uncontrolled approximations or dubious assumptions as possible. We do that by investigating a minimal phenomenological model permitting essentially exact (albeit numerical and statistical) solution. This model has the following ingredients.

(1) Electrons propagate according to a tight-binding model in the presence of a disordered pair order parameter with local $d_{x^2−y^2}$ symmetry:

$$H[\Delta] = - \sum_{ij} T_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \sum_{ij} \left( \Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + \text{h.c.} \right).$$  (1)

The chemical potential has been included in the hopping matrix $T_{ij} \equiv t_{ij} + \mu \delta_{ij}$. We take the ratio of next-nearest-neighbor hopping ($t'$) to nearest-neighbor...
(t) to be $t'/t = -0.35^{10}$, and the chemical potential
$\mu = -1.1076t$, corresponding to a doping of $x = 0.15$. We
estimate $t \approx 1/5$ eV, roughly 1/4 of the observed
bandwidth.

(2) The complex pair field $\Delta_{ij} = \Delta_{ji}$ couples to singlet
pairs spanning nearest-neighbor sites $i$ and $j$. In a $d_{x^2-y^2}$
superconductor, the (spatially uniform) pair field $\Delta_{ij}$ is
$\Delta_0$ on horizontal bonds, and $-\Delta_0$ on vertical bonds.

(3) In a traditional BCS approach, the gap parameter
$\Delta_0$ is computed self-consistently taking into account the
underlying pairing interaction. In our phenomenological
approach, this linkage is decoupled. Instead, the pair
field $\Delta_{ij} = \Delta_0 e^{i\theta_{ij}}$ in eq. (1) is treated as a quenched
random variable, chosen from a thermal ensemble. We
assume that $|\Delta_{ij}|$, the magnitude of the pairing correla-
tions is a fixed (large) energy scale $\Delta_0$ equal to the full
gap below $T_c$, but that the phase suffers thermal fluctua-
tions determined by the classical XY model

$$\beta H_{XY} = 1.12 K \sum_{\langle ij, ik \rangle} \cos(\theta_{ij} - \theta_{ik}).$$  \hspace{1cm} (2)

The sum runs over all pairs of nearest-neighbor links, i.e.,
links $ij$ and $ik$ related to each other by a $90^\circ$ rotation
about a common site $i$. The centers of these links form
a square lattice, canted at $45^\circ$ to the lattice of tight-
binding sites. The factor of 1.12 in eq. (2) means that
$K$ is measured in units of the critical coupling, i.e., the
Kosterlitz-Thouless-Berezinskii (KTB) transition occurs
at $K = 1^{11}$. One may think of the Hamiltonian of Eq.
(2) as arising from the Hamiltonian

$$\mathcal{H}_{pair} = g \sum_{ij} \Delta_{ij}^* \Delta_{ik},$$  \hspace{1cm} (3)

which describes the pivoting$^{13}$ of a Cooper pair from a
nearest-neighbor link $ik$ to a perpendicular link $ij$ (see
inset of Fig. 2). Positive $g$ encourages local d-wave order.

Assumptions 1–3 above specify our model. In con-
trast to BCS theory, a distinction is drawn between
the local pairing strength $\Delta_0$ and the phase stiffness
$K$; we take them as independent phenomenological
parameters. A genuinely two-dimensional system of this
sort develops only algebraic order for $K > 1$. In a
real material, coupling between planes causes crossover
to three-dimensional behavior and true long-range
order. For $K < 1$, there is no superconductivity, but local
superconductor-like correlations. The primary questions are:
for what range of phase stiffness $K$ does the local
pairing manifests itself above the KTB transition, and,
to how high a temperature is the picture able to hold
together?

**Methods.** Given a pair field $\Delta_{ij}$, we solve numerically
for the ground state and quasiparticles by a suitable
Bogoliubov transformation:

$$\Gamma_m = \begin{pmatrix} \gamma_1^\alpha \gamma_1^\beta \\ \gamma_2^\alpha \gamma_2^\beta \end{pmatrix}_m = \begin{pmatrix} U & V \\ -V^* & U^* \end{pmatrix}_{mi} \begin{pmatrix} c_i^\dagger \\ c_i \end{pmatrix}_j,$$  \hspace{1cm} (4)

where the index $i$ labelling lattice sites is summed over on the
right-hand side. Since the $\Gamma$ operators destroy quasi-
particles, we have the Bogoliubov-de Gennes equation

$$\begin{pmatrix} -T & \Delta^* \\ \Delta & T \end{pmatrix} \begin{pmatrix} U_m^T \\ V_m \end{pmatrix} = -E_m \begin{pmatrix} U_m^T \\ V_m \end{pmatrix},$$  \hspace{1cm} (5)

where $U_m^T$ and $V_m^T$ are column vectors to be determined.

With Bogoliubov quasiparticle states in hand, we
calculate the experimentally relevant particle and hole
spectral densities $A^+(\omega) \equiv \langle c(k)\delta(H - \omega)c(k)^\dagger \rangle$ and $A^-(\omega) \equiv \langle c(k)\delta(H - \omega)c(k)^\dagger \rangle$. Since the basic assump-
tion is that the crucial thermal effects are fluctua-
tions of the order parameter phase, we compute the
quenched average spectral densities at zero “quasiparticle
temperature”$^{14}$ over the distribution of $\{\Delta_{ij}\}$:

$$A_0^+(\omega) = \sum_m |U_{mk}|^2 \delta(\omega - E_m),$$

$$A_0^-(\omega) = \sum_m |V_{mk}|^2 \delta(\omega - E_m).$$  \hspace{1cm} (6)

Representative full spectral densities $A_0(k,\omega)$ [equal
to $A_0^+(k, -\omega)$ for $\omega < 0$ and to $A_0^-(k, \omega)$ for $\omega > 0$
over a range of $K$ are displayed in Figures 2 and 3 for
a point near the Fermi surface in the $(\pi, 0)$ direction
with $\Delta_0/t = 0.05$ and 0.15, respectively. Results for a
Fermi surface point much closer to the $(\pi, \pi)$ (nodal) di-
rection is shown in Figure 4. These plots are the result of
Monte Carlo sampling of the pairing field ensemble.

**FIG. 2:** Upper right-hand quadrant of the Brillouin zone grid
used for numerical computation. The heavy solid curve in-
cludes a pair hopping event.

(0,0) (0,π)

(π,0) (π,π)
for a 48 × 48 site lattice, with averaging over three to five disorder realizations and crystallographically equivalent k points. In each figure, the inner dashed lines indicate plus or minus the tight-binding energy \( \epsilon(k) \), and the outer dashed lines are the quasiparticle energies \( \epsilon(k) = \pm \sqrt{\epsilon(k)^2 + \Delta_0(k)^2} \) for a perfectly ordered pairing field with the specified \( \Delta_0 \) (i.e., \( K = \infty \)).

What do these results tell us? First, the single-particle spectral function exhibits a pseudogap even for fairly short-ranged phase coherence. Roughly speaking, the phase correlation length, \( \xi \), is the distance over which Cooper pairs propagate coherently, or the characteristic vortex-antivortex separation. The figures show a pseudogap developing by about \( \xi = 15a \) for \( \Delta_0 = 0.05t \). For this pairing magnitude, the Cooper pair size, estimated according to \( \xi_0 = \hbar v_F/\Delta_0(k) \), is of order 8a. (For this estimate, we use Fermi velocity \( v_F \) and full gap at the Fermi surface near the (π, 0) direction. Other choices give an estimate a few times larger.)

Second, the onset of the pseudogap with \( K \) is relatively rapid near the KTB critical point. The (π, 0) gap achieves nearly half its full value by the KTB transition, continuing to increase slowly with increasing \( K \). The variation of the pseudogap along the Fermi surface closely resembles the pure \( d_{x^2-y^2} \) form. If we invert the usual BCS relationship between energy gap and pairing amplitude, using the peak position of the spectral density as a surrogate for the BCS quasiparticle energy, we can extract an effective “gap parameter” \( \Delta_{\text{eff}}(k) \equiv \sqrt{E_{\text{peak}}(k)^2 - \epsilon(k)^2} \). At \( K = 0.9 \), and for both \( \Delta_0/t = 0.05 \) and \( \Delta_0/t = 0.10 \), the ratio \( \Delta_{\text{eff}}/\Delta_0(k) \) of effective gap to full gap is between 0.41 and 0.63 everywhere on the Fermi surface (with most points being close to 0.5).

Third, spectral peaks are broad with widths roughly linear in the pairing magnitude \( \Delta_0 \). As shown in Figure 3, this broadening can wash out the clear pseudogap, though it does not affect the shift of the peaks. The widths do not monotonically decrease as \( K \) is increased, but are greatest near \( K = 1 \).

Fourth, although the pseudogap appears at a modest phase correlation length (comparable to a few Cooper pair radii), the most natural interpretation of this in terms of temperature is quite discouraging if the aim is to explain experimentally observed pseudogaps. As stressed earlier, \( K \) is a phenomenological parameter, but it should probably be close to \(|\Delta_0|^2 n_s^0/m_0 \), where \( n_s^0 \) is the bare superfluid density. In that case, \( K \) is roughly proportional to \( 1/T \), and our results imply \( T_s/T_c \lesssim 1.2 \). The collapse of the pseudogap in our model corresponds to \( \xi \sim \xi_0 = \hbar v_F/\Delta_0 \), the Cooper pair size. If a pseudogap is to be maintained to high temperature, something must halt the decrease of \( \xi \) at that point. In other words, the order parameter phase must remain stiff at wavelengths comparable to \( \xi_0 \). This issue is not addressed by our phenomenological model.

It is interesting to see how well the numerical results can be reproduced by a standard diagrammatic approximation, using a self-consistent Green function. This approximation is similar to that used by Kwon and
Dorsey, and is represented by

\[
\begin{pmatrix}
\cdots
\end{pmatrix}^{-1} = \begin{pmatrix}
\cdots
\end{pmatrix}^{-1} + \begin{pmatrix}
\cdots
\end{pmatrix}
\]

Equivalently, the self-energy is given by

\[
\Sigma_G(k, \omega) = \int \langle |\Delta(q)|^2 \rangle G(-\omega, q - k) \, d^2 q. \tag{7}
\]

We solve this iteratively, including \(\langle |\Delta(0)|^2 \rangle\) only in the final iteration. For \(K < 1\), the pair field correlator is accurately approximated by \(\langle |\Delta(q)|^2 \rangle - 1 \propto \left[\xi^{-2} + 2 \sum_{e} (1 - \cos(q \cdot e))\right]\), with a proportionality constant fixed by the sum rule \(\sum |\Delta(q)|^2 = 2N\Delta_0^2\) (\(N\) is the number of sites in the lattice). Spectral densities calculated via this method (Fig. 5) also show the development of a pseudogap at values of \(K\) in close agreement with the exact results. However, the peaks are narrower, by a factor of as much as two.

In summary, we have shown, using a simple phenomenological model, that a single-particle pseudogap, per se, is natural in the presence of order parameter phase fluctuations. In this context, it is unclear what mechanism could maintain short range phase stiffness up to the experimentally observed \(T^*\). On the other hand, recent microwave conductivity measurements suggest that the bare superfluid density vanishes at a temperature comparable to the most natural pseudogap collapse temperature found here, about 20% above \(T_c\). This is also consistent with other previous theoretical findings.

\[\begin{align*}
\Delta_0 &= 0.05 t, \quad ka = (\pi, 0.125 \pi) \\
\xi &= 60 \\
\xi &= 40 \\
\xi &= 20 \\
\xi &= 15 \\
\xi &= 7
\end{align*}\]

FIG. 5: Spectral density at \((3, 23)\frac{\pi}{24}\) for \(\Delta_0 = 0.05t\) and several values of the phase correlation length \(\xi\) (lattice-spacing units), calculated by the self-consistent Green function method.

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* Electronic address: lammert@phys.psu.edu

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