On the origin of the Fermi arc phenomenon in the underdoped cuprates: signature of KT-type superconducting transition

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Abstract

The origin of the Fermi arc phenomenon in the pseudogap phase of the underdoped cuprates is studied in the thermal phase fluctuation scenario. An \( XY \)-type lattice model with a built in \( d \)-wave structure is introduced to describe the phase fluctuation effect in the cuprates. A sharp ridge-like structure in the spectral function \( A(k, \omega = 0) \) is found to emerge abruptly above the Kosterlitz–Thouless (KT) transition temperature (\( T_{KT} \)) on the underlying Fermi surface. This ridge-like structure in \( A(k, \omega = 0) \) bears a close resemblance to the observed Fermi arc phenomenon in its temperature dependence and shape in the momentum space. These results provide yet more strong evidence for the KT transition nature of the superconducting transition in the underdoped cuprates.

The origin of the pseudogap phenomenon in the underdoped cuprates is among the most hotly debated issues in high-\( T_c \) physics. The existing theories on the pseudogap fall into two categories: while it is taken by many as the evidence for the existence of preformed Cooper pairs and strong phase fluctuation in the normal state [1–4], some people believe that it should be attributed to an as yet unidentified order [5–8]. One puzzle about the pseudogap is its momentum and temperature dependence. While early experiments suggested that the pseudogap may inherit the \( d \)-wave structure of the superconducting gap, more detailed angle resolved photoemission spectroscopy (ARPES) measurements show that this is not the case [9–11]. Below \( T^* \), the pseudogap is first seen in a small momentum region around the antinodal point \((\pi, 0)\). The gapped region enlarges with decreasing temperature until the whole Fermi surface (except the nodal points) is gapped below \( T_c \). The gradual development of the pseudogap on the Fermi surface leaves the system with a finite segment of ungapped Fermi surface which is dubbed the Fermi arc in the literature. The length of the Fermi arc increases with temperature and is reported to have a jump at \( T_c \): the Fermi arc emerges abruptly at \( T_c \).

The Fermi surface, by its very definition as an equal-energy contour at the chemical potential, is always closed for any well defined quasiparticle dispersion. It is proposed that the Fermi arc is just a half of a closed pocket-like small Fermi surface whose other half is too weak to be detected by ARPES [12]. Such a scenario is widely adopted in the second kind of theory for the pseudogap (related to an unidentified order). In this paper, we try to understand the Fermi arc phenomenon in the framework of the phase fluctuation scenario. In this scenario, the Fermi arc is not a genuine Fermi surface in the momentum space across which a finite jump of the occupation number occurs, but a phase fluctuation induced pile up of the spectral weight on the Fermi energy in a \( d \)-wave paired state.

The effect of the phase fluctuation on the electronic spectral function have been studied by many authors [13–21]. However, most of these studies are limited to the semiclassical treatment of the phase fluctuation. At the semiclassical level, the phase fluctuation is modeled by a uniform supercurrent with a phenomenological distribution of velocity. The Doppler effect of the quasiparticle moving in such a uniform supercurrent background then causes a shift of the electronic spectral function in both momentum and energy. More specifically, when the center of mass momentum of the moving Cooper pairs is \( 2q \), the electron pairing then happens between momentum \( q + k \) and \( q - k \), and the excitation energy becomes \( E_k - \mathbf{v}_k \cdot \mathbf{q} \) to the first order in \( q \). The net effect of the supercurrent on the electron spectral function is to shift it by

\( T_{KT} \) physics.
In a recent study \[17\], it was found that in a d-wave superconductor the Doppler effect of the fluctuating supercurrent will cause a pile up of the spectral weight exactly at the Fermi energy on the underlying Fermi surface, no matter what the detailed distribution of the fluctuating supercurrent is. The pile up of the spectral weight results in an inverse square root singularity at the Fermi energy in the electronic spectral function, resembling a quasiparticle peak. The key point for this to happen is that in a d-wave superconductor, the quasiparticle has linear dispersion around the gap node.

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The semiclassical approach, though intuitively attractive, has limited value in giving quantitative estimates of the phase fluctuation effect. To simulate the actual temperature dependence of the phase fluctuation effect, one must go beyond the long wavelength limit and take into account the singular effect of the vortex excitation on the quasiparticle motion. Even for the simulation of the phase fluctuation involved in the far field region of the vortex, the semiclassical approach fails to provide a quantitative measure of its strength.

In this work, we try to go beyond the semiclassical limit by simulating the effect of thermal phase fluctuation in d-wave superconductors with a lattice model. For this purpose, an XY-type lattice model with a built-in d-wave character is introduced to describe the phase degree of freedoms, which are coupled to the quasiparticles through the standard pairing Hamiltonian. We have performed Monte Carlo simulation of the phase fluctuation and calculated the electron spectral function \( A(k, \omega) \) on a 64 \( \times \) 64 lattice with the help of a special cutoff strategy. A Fermi arc structure is found to emerge abruptly above the KT transition temperature of the XY model. The Fermi arc so obtained bears a close resemblance to that observed in the underdoped cuprates in its temperature dependence and shape in the momentum space.

The phase degree of freedom is described by the following XY-type lattice model

\[
H_{\text{phase}} = J \sum_{\langle \alpha, \beta \rangle} \cos(\theta_\alpha - \theta_\beta),
\]

in which \( \theta_\alpha \) is the phase variable defined on the bonds of a square lattice on which the electrons reside. The center of these bonds forms another square lattice (see figure 1) and the sum in equation (1) is over neighboring sites of this latter square lattice. The coupling constant \( J \) is set to be positive so that a d-wave-like phase structure is favored at low temperatures in this model and a phase shift of \( \pi \) is preferred between the phase variables on neighboring bonds. Here the phase variables live on the link and can be understood as the Hubbard–Stratonovich field in the path integral representation of some microscopic model \[14\], rather than the phase of some coarse grained superconducting order parameter.

In principle, the energetics of the phase degree of freedom should be determined by the dynamics of the electron system itself. Here we have treated it as a separated degree of freedom governed by a coupling constant \( J \). Except for being simpler to simulate, such a model has the advantage that it takes into account the fact that in the underdoped cuprates the spin pairing and phase coherence are controlled by two separate energy scales \[1, 5\]. In a doped Mott insulator, such a separation of the energy scales is a naturally expected fact. We note the strong electron correlation effect is indispensable for a consistent description of the phase fluctuation effect in the underdoped cuprates and it is the Mott physics that is responsible for the reduction of the phase rigidity of the system in this regime. If we neglect the strong correlation effect in our description of the pseudogap phase, as it is assumed in the BCS–BEC (Bardeen–Cooper–Schrieffer to Bose–Einstein condensation) crossover scenario, then the phase rigidity of the system can be reduced only at the price of an increased pairing gap (inversely proportional to each other in the BCS–BEC crossover scenario), which will eventually cause instability of the nodal d-wave pairing pattern against some fully gapped pairing pattern of mixed symmetry \[15\]. However, the pairing gap of the cuprates is observed to be finite throughout the phase diagram and the nodal d-wave pairing pattern is found to be robust.

The electron degree of freedom is described by the standard pairing model \( H_{\text{pair}} = H_i + H_\Delta \), in which \( H_i \) and \( H_\Delta \) are given by

\[
H_i = -t \sum_{\langle i, j \rangle, \sigma} (\hat{c}_{i, \sigma}^\dagger \hat{c}_{j, \sigma} + \text{h.c.})
- t' \sum_{\langle\langle i, j \rangle\rangle, \sigma} (\hat{c}_{i, \sigma}^\dagger \hat{c}_{j, \sigma} + \text{h.c.}) - \mu N
- \mu N\]

\[
H_\Delta = \sum_{\langle i, j \rangle} \Delta e^{i \hat{\theta}_{ij}} (\hat{c}_{i, \uparrow}^\dagger \hat{c}_{j, \downarrow} + \hat{c}_{i, \downarrow}^\dagger \hat{c}_{j, \uparrow} + \text{h.c.})
\]

Figure 1. The lattice on which model equation (1) is defined. The electrons reside on the square lattice made of the solid lines. The phase variables resides on the bonds of this square lattice which are indicated by the gray dots. These gray dots form another square lattice.
in which \( t \) and \( t' \) are the hopping integrals between neighboring and next neighboring sites. The next neighboring hopping \( t' \) is introduced to model the curvature of the real Fermi surface. \( \hat{N} \) is the electron number operator, \( \Delta \) denotes the magnitude of the pairing potential and is kept as a constant in the whole simulation. \( \theta_{0} \) is the phase variable on the bond between site \( i \) and \( j \).

The phenomenological description presented above can actually be understood as a low energy effective theory of the \( t-J \) model. Equation (2) can be taken as the effective Hamiltonian of the Fermionic spinon in the slave boson mean field theory of the \( t-J \) model. The parameters \( t, t', \) and \( \Delta \) in equation (2) are related to the bare parameters of the \( t-J \) model as follows: \( t = \hbar t_{0}x + \frac{\Delta}{\Delta_{1}}x, \) \( t' = \hbar t'_{0}x, \) and \( \Delta = \frac{\Delta}{\Delta_{1}}\Delta', \) where \( \hbar t_{0} \) and \( \hbar t'_{0} \) are the bare hoping integrals between neighboring and next neighboring sites in the \( t-J \) model, \( J_{ex} \) denotes the spin superexchange interaction between neighboring sites. \( \chi \) and \( \Delta' \) are the mean field order parameters. \( x \) is the density of doped holes. Beyond the mean field theory, there exist both the phase fluctuation mode and the gauge fluctuation mode at low energy. If we neglect the gauge fluctuation, which is gapped when the bosonic holon tends to condense, the effective action for the phase degree of freedom just takes the form of equation (1), in which the phase stiffness parameter \( J \) is estimated to be \( J \propto t \times t' \) [5].

The phase stiffness parameter \( J \) decreases with doping \( x \) as a result of the electron correlation effect. However, the gap parameter \( \Delta \) is found to show the opposite trend [5]. Thus, at sufficiently low doping, the gap energy scale will be much larger than that of the phase coherence. In such a case, we can neglect the temperature dependence of the gap amplitude at the temperature scale below \( K_{B}T_{phase} \propto J \). The fluctuation of the gap amplitude becomes important only at a much larger temperature scale \( K_{B}T_{amp} \propto \Delta \). Thus, the pseudogap phase of the underdoped cuprates can be divided into two regions. In the high temperature region between \( T_{phase} \) and \( T_{amp} \), fluctuation of both the phase and the amplitude of the pairing gap are important. In particular, the pseudogap phenomena will be eliminated below \( T_{amp} \). However, in the lower temperature region between \( T_{g} \) and \( T_{phase} \), only the fluctuation of phase is important and a description of the phase degree of freedom in terms of equation (1) becomes feasible. It is reasonable to identify this lower temperature region with the Nernst region, in which a well defined vortex is believed to exist [4].

In this paper, we will focus on the physics below \( T_{phase} \) and neglect the temperature dependence of \( \Delta \). Thus the temperature evolution is totally determined by the value of \( J \), which will be set as the unit for temperature. Changing \( \Delta \) then amounts simply to a rescaling of the energy in the electronic spectral function. Thus we will not specify the value of \( \Delta/J \) in our simulation. In a real system, this ratio can take any value greater than one in the underdoped regime. To model the Fermi surface and gap function of the real system, we have used \( t'/t = -0.3 \) and \( \Delta/j = 0.1 \).

The simulation of phase fluctuation effect with lattice models like equation (2) has been done in many previous studies. However, most of these studies are limited to spectral features at the energy scale of order \( \Delta \) (or the pseudogap around the antinode region) [14–16, 18]. To simulate the spectral feature right at the Fermi energy, the Fermi arc, one should use a lattice of sufficiently large size to accommodate the momentums on the Fermi surface. In our simulation, we have used a lattice with \( 64 \times 64 \) sites. We first generate a thermal phase fluctuation configuration from the distribution \( \rho = \exp(-H_{phase}/k_{B}T) \). We then diagonalize the pairing Hamiltonian equation (2) and calculate the electronic spectral function with this configuration. To recover the translational invariance, we average the electron spectral function over all configurations that are related to the given one by spatial translation. The electronic spectral function so calculated is given by

\[
A(k, \omega) = \sum_{\eta} |u_{\eta}^{\dagger}(\omega - E^{\eta})|^{2},
\]

in which \( u_{\eta}^{\dagger} = \sum_{n} u_{\eta}^{\dagger} e^{iR_{n}k} \). \( u_{\eta}^{\dagger} \) denotes the eigenvectors of the following Bogoliubov–de Gennes (BdG) equation with eigenvalue \( E^{\eta} \):

\[
\left( H_{t,i,j} H_{\Delta,i,j} \right) \left( u_{\eta}^{\dagger} \right) = E^{\eta} \left( u_{\eta}^{\dagger} \right),
\]

in which \( H_{t,i,j} = -t\delta_{i,j}R_{k} - t'\delta_{i,j}R_{k} - \mu \delta_{i,j} \) and \( H_{\Delta,i,j} = \Delta_{0}e^{iR_{k}R_{k}} \delta_{i,j}R_{k} \) are the matrix elements of \( H_{t} \) and \( H_{\Delta} \). Here the sum over repeated indices is assumed and \( R_{k} \) denotes the neighboring and next neighboring vector on the square lattice. Finally, we average the electron spectral function over all kinds of thermal fluctuations

\[
\frac{\langle A(k, \omega) \rangle}{\sum_{e^{iR_{k}k}} e^{-iR_{k}kT_{phase}/k_{B}T}} A(k, \omega) = \frac{\sum_{e^{iR_{k}k}} e^{-iR_{k}kT_{phase}/k_{B}T} A(k, \omega)}{\sum_{e^{iR_{k}k}} e^{-iR_{k}kT_{phase}/k_{B}T}}.
\]

To resolve the Fermi surface on a finite momentum mesh, we have to study a lattice of a large enough size. However, the diagonalization of the BdG Hamiltonian on a large lattice is quite time consuming. To solve this problem, we have adopted the following cutoff strategy. First, we Fourier transform (by FFT algorithm) the BdG Hamiltonian into momentum space. The transformed Hamiltonian reads

\[
\left( \xi_{k} \delta_{k,k'} \quad \Delta_{k,k'} \right) \left( \begin{array}{c} u_{k}^{\dagger} \\ u_{k'}^{\dagger} \end{array} \right) = E^{\eta} \left( \begin{array}{c} u_{k}^{\dagger} \\ u_{k'}^{\dagger} \end{array} \right),
\]

in which \( \xi_{k} = -2t(\cos k_{x} + \cos k_{y}) - 4't\cos k_{x} \cos k_{y} - \mu \), \( \Delta_{k,k'} = 1/N \sum_{i,j} \Delta_{0} e^{iR_{k}R_{k}}-\mu k_{k'} \). To simulate the Fermi arc phenomena, we only need to calculate the electron spectral function right on the Fermi energy, \( A(k, \omega = 0) \). Obviously, those momentums for which \( |\xi_{k}| \gg \Delta \) are not expected to contribute significantly to \( A(k, \omega = 0) \). For this reason, we set a cutoff energy \( E_{C} \) and neglect all momentums for which \( |\xi_{k}| > E_{C} \). We then diagonalize the truncated BdG Hamiltonian below the cutoff energy and calculate the electron spectral function on the Fermi energy. The convergence of such a cutoff strategy can be easily checked by varying the cutoff energy \( E_{C} \). In real simulation, we find \( E_{C} = 5\Delta \) is large enough for convergence.

In our simulation, 1000 statistically independent phase fluctuation configurations had been used to calculate \( A(k, \omega) \). The strength of the phase fluctuation can be monitored by the correlation function of the phase variables. In figure 2,
we plot the correlation \( C(T) = \langle \cos(\theta_\alpha - \theta_\alpha') \rangle \) between the phase variables on the most distant bonds of the \( 64 \times 64 \) lattice as a function of temperature. For an infinite system, such a correlation should be zero at a finite temperature as required by the Wagner–Mermin theorem. The abrupt drop of the correlation function at \( k_B T / J \sim 1 \) signifies the KT transition of this finite system. This temperature is slightly above the KT transition temperature for the infinite system \( (k_B T \sim 0.8923J) \) \([22, 23]\).

Figure 3 shows the results of \( A(k, \omega = 0) \) calculated at \( k_B T = 0.5J, 1J, 1.2J, 1.3J \) and \( 1.4J \). Below the KT transition temperature \( (T_{KT}) \), the phase fluctuation effect is almost totally quenched and \( A(k, \omega = 0) \) is composed of four sharp peaks at the four nodal points. Right above the KT transition temperature, a ridge-like structure in \( A(k, \omega = 0) \) emerges on the underlying Fermi surface\(^1\). The intensity of this ridge-like structure increases rapidly in a small temperature region between \( k_B T = J \) and \( 1.1J \) and then switches to a more modest temperature dependence. In figure 4, we present the integration of the electron spectral function at the Fermi energy \( W(\omega = 0, T) = \int dk A(k, \omega = 0) \) (the density of state at the Fermi energy) as a function of temperature.

\(^1\) The strong oscillation of the electron spectral function on the Fermi surface in figure 3 is not due to statistical error. The oscillation has a fixed pattern and is caused by the finite lattice size effect. On a finite lattice, the momentum mesh in the Brillouin zone is not dense enough to resolve all the momentum on the Fermi surface and as a result some Fermi surface momenta are missed (or approximated by nearby momenta).
but the density of state at the Fermi energy) as a function of temperature. The quenching of the phase fluctuation effect below $T_{KT}$ and the abrupt emergence of the ridge-like structure above it can be clearly seen in this figure.

The temperature dependence and the shape in momentum space of the ridge-like structure found in this work bear a close resemblance to the Fermi arc phenomenon observed in experiments [10]. In [10], a length of the Fermi arc has been defined by choosing a certain threshold on the measured spectral intensity. The arc length so defined is found to show a jump at the superconducting transition temperature and then to increase linearly with temperature. In principle, the same can be done in our theory. However, the ridge-like structure emerges simultaneously on the whole Fermi surface, although with strong anisotropy in intensity. Thus the arc length defined will be sensitive to the intensity threshold chosen. Despite this uncertainty, it is clear from an inspection of figures 3 and 4 that the arc length predicted by our theory should follow the trends of the experimental observations.

These agreements strongly suggest that the phase fluctuation is at the origin of the Fermi arc phenomenon. The abruptness of the emergence of the Fermi arc at the transition point, which according to our theory is caused by the proliferation of the vortex excitation, provides yet more strong evidence for the KT transition nature of the superconducting transition in the underdoped cuprates. In the literature, the Fermi arc is also interpreted in many other scenarios. The uniqueness of the phase fluctuation scenario lies in the fact that it predicts a real arc structure exactly on the underlying Fermi surface of the normal state as a result of the specific way that the phase fluctuation couples to the quasiparticles, rather than some small Fermi pocket whose other half should then be argued to be unobservable as a result of its weak intensity, or some smeared-out spectral intensity around the Fermi surface. It also provides a natural understanding for the dramatic temperature evolution of the Fermi arc near the superconducting transition temperature. However, a large Fermi surface is obviously at odds with the observation of quantum oscillation in underdoped cuprates [12], which indicates the existence of a small closed Fermi surface. We believe that such a small Fermi pocket is induced by symmetry breaking of some intrinsic or extrinsic origin.

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