Phase fluctuations of $s$-wave superconductors on a lattice

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Based on an attractive $U$ Hubbard model on a lattice with up to second neighbor hopping we derive an effective Hamiltonian for phase fluctuations. The superconducting gap is assumed to have $s$-wave symmetry. The effective Hamiltonian we finally arrive at is of the extended XY type. While it correctly reduces to a simple XY in the continuum limit, in the general case, it contains higher neighbor interaction in spin space. An important feature of our Hamiltonian is that it gives a much larger fluctuation region between the Berezinskii-Kosterlitz-Thouless transition temperature identified with $T_c$ for superconducting and the mean field transition temperature identified with the pseudogap temperature.

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I. INTRODUCTION

The origin of the pseudogap phenomena in high-$T_c$ superconductors is one of the most challenging questions in the theory of superconductivity but there is no consensus on the correct theoretical approach to be taken to describe such phenomena. What is generally accepted is that the pseudogap is a manifestation of strong correlation effects which become progressively more important as the doping is reduced into the underdoped regime and the Hubbard Mott insulating state is approached. Roughly speaking, theories of the pseudogap state can be divided into two classes.

One is based on the idea of a precursor state to superconductivity. In this scenario the Cooper pairs are performed below the pseudogap temperature ($T^*$) assumed larger than the superconducting transition temperature ($T_c$) but there is no phase coherence in the temperature range between $T_c$ and $T^*$. The phase fluctuations destroy phase coherence and consequently the superfluid stiffness is zero in this temperature regime. Therefore, this picture envisions that the two gaps ($s$-wave and pseudogap) have the same origin. The precursor state idea is based on the results of angle resolved photoemission spectroscopy (ARPES) experiments which show a smooth evolution of the pseudogap into the superconducting gap as temperature is reduced. This is also consistent with tunneling results of Renner et al. who found a smooth evolution of tunneling characteristics as a function of temperature showing the gap filling but not closing as one goes through the superconducting transition temperature. On the other hand data by Krasnov et al. on intrinsic mesa junctions show a separate superconducting peak and a pseudogap hump. These data do not favor a pre-formed pair interpretation although superconducting and pseudogap both appear pinned to the Fermi energy. A different precursor scheme includes in the calculations finite momentum pairs which exist at any finite temperature below $T^*$ but do not contribute to the superfluid density made up of zero momentum Cooper pairs. Above $T_c$ there remain no zero momentum pairs and therefore no superfluid density. This approach constitutes a natural extension of BCS theory to the strong coupling regime and has many features that agree with experiments on the cuprates. For example pseudogap effects become more prominent as the doping is reduced into the underdoped regime of the phase diagram.

A second class of theories assumes that there is a second order parameter which competes with the superconducting gap and that the microscopic origin of the pseudogap associated with this second order parameter is different from that of the superconducting gap. The competition between the two gaps manifests itself most importantly in the underdoped regime and so in this doping regime the two gaps co-exist. As the doping is increased towards optimum and into the overdoped regime the second order parameter is weakened and could even vanish in the overdoped case. This feature is quite different from the precursor scenario. A recent theoretical approach based on this line of thought has assumed that the pseudogap has a $d$-wave charge density wave order, the so-called $d_{x^2-y^2}$-density wave (DDW). An experimentally observed phase diagram for the high-$T_c$ cuprates is consistent with this competing gap picture. However, a more recent theoretical work implies that the DDW model may not be consistent with tunneling experiments. Transport properties of the DDW state may also be used to test this picture.

In this paper we deal only with the phase fluctuation picture. CuO$_2$ planes play a crucial role in high-$T_c$ superconductivity and interlayer coupling is weak. Here it is assumed that the two-dimensional nature of the cuprates is an important feature of these compounds. For simplicity, however, we will consider only $s$-wave pairing on a lattice so that strictly speaking our work will not apply to high-$T_c$ cuprates which are known to have $d$-wave symmetry. In this sense the present work is a first essential step in a realistic treatment of the cuprates.

Noting that spontaneous breaking of continuous symmetry is impossible in 2D one may conceive that the superconducting transition, at least in underdoped cuprates, is not of the BCS kind but is rather related to the Berezinskii-Kosterlitz-Thouless (BKT) transition.
which is found in two-dimensional systems. Of course, in reality, the coupling between CuO$_2$ planes must be important right at $T_c$, since the transition must be three-dimensional with true off-diagonal long range order.

The two-dimensional XY model on a square lattice is an example of the BKT transition. This model describes a system of spins $S_i$ constrained to rotate on the lattice, where $i$ indicates the site. The Hamiltonian of the model can be written in the form $-J \sum_{<ij>} S_i \cdot S_j$, where $J > 0$ and $<ij>$ means a sum over nearest neighbor pairs. It has been proposed that the BKT transition is associated with unbound vortex-antivortex pairs. The mean-square distance $\langle r^2 \rangle$ between a vortex and an antivortex is

$$\langle r^2 \rangle = \frac{\pi J/T - 1}{\pi J/T - 2}.$$  
(1)

As temperature approaches the BKT transition temperature $T_{BKT} = \pi J/2$, $\langle r^2 \rangle$ diverges and the pairs become unbound.

In a theoretical approach to the precursor scenario, Cooper pairs are formed at the mean-field temperature ($T_{MF}$), which is identified as $T^*$. The phase fluctuations destroy the long range order until the phases are locked in at the BKT transition temperature $T_{BKT}$, which is $T_c$. Consequently, the effective Hamiltonian for phase fluctuations is mapped into a XY model Hamiltonian. In order to consider phase fluctuations of the superconducting order parameter, one has to go beyond mean-field BCS theory. This can be implemented by using the well-established path-integral formalism for fermionic fields. The effective phase Hamiltonian for an $s$-wave superconductor can be described by $H_{XY} = J_{XY} \int d\theta (\nabla \theta)^2$, where $\theta$ represents phase fluctuations. To obtain a lattice version of the XY Hamiltonian on a lattice, which will be derived and studied in detail in this paper.

The paper is organized as follows: In Section II, we introduce the path integral approach and derive the effective action for phase fluctuations. We apply the Hubbard-Stratonovich transformation to integrate out the fermionic degrees of freedom. We also consider a case where the phase is treated in the continuum limit while the fermions still remain on a lattice. This serves as a bridge to the continuum limit. We show in section III that the effective Hamiltonian is not of the usual XY type. There are extra terms which do not belong to the usual XY Hamiltonian. It is shown how the new more complex Hamiltonian reduces to the XY model in the continuum limit. In this section we also explain how a periodic boundary condition applied to the lattice leads directly to a simple expression for the effective Hamiltonian for phase fluctuations. In Section IV, we show that the effective Hamiltonian turns out to be of an extended XY type and investigate the effects of the extra terms. When we include next-nearest neighbor hopping in the electronic energy dispersion (Section V), we find that the extended nature of the Hamiltonian is preserved and the correction to the usual XY model becomes even more essential. We also explain a qualitative relation between the physics of the BCS-Bose Einstein (BE) crossover and the BKT transition temperature. Section VI contains discussions and conclusions.

II. FORMALISM

We begin with a 2D attractive Hubbard model on a square lattice in its simplest form conceivable, namely

$$H = -t \sum_{<ij>\sigma} C_{i\sigma}^+ C_{j\sigma} - \mu \sum_i n_{i\sigma} - U \sum_i n_{i\uparrow} n_{i\downarrow},$$  
(2)

where $C_{i\sigma}$ is a fermion field with a spin $\sigma$, $\mu$ is a chemical potential, $U(>0)$ is the pairing interaction, $n_{i\sigma} = C_{i\sigma}^+ C_{i\sigma}$, and $t$ describes nearest neighbor hopping. To start we consider only the nearest neighbor hopping for algebraic simplicity; however, later we will include the next nearest neighbor hopping. The symbol $<ij>$ means a sum carried out over nearest neighbor pairs as mentioned earlier. When we need a double summation over $i$ and $j$, the usual notation $\sum_{i,j}$ will be used. We will set the lattice constant $a = 1$ and also use units such that $\hbar = k_B = 1$. The partition function ($Z$) of this model in the path-integral formalism is written as

$$Z = \int DC^+ DC \exp[-S],$$  
(3)

where the action $S = \int d\tau \{ \sum_i C_{i\sigma}^+ \partial_\tau C_{i\sigma} + \mathcal{H} \}$ and the range for the integral over the imaginary time $\tau$ in the action is from $0$ to $1/T$.

Defining spinors $\Psi_i$ for the fields $C_{i\uparrow}$ and $C_{i\downarrow}^+$ such that $\Psi_i^+ = (C_{i\uparrow}^+ C_{i\downarrow})$, the action $S$ becomes

$$S = \int d\tau \left\{ \sum_i \Psi_i^+ \left[ \tilde{\tau}_0 \partial_\tau - \tilde{\tau}_3 \mu \right] \Psi_i - t \sum_{<ij>} \Psi_i^+ \tilde{\tau}_0 \Psi_j - U \sum_i \sum_{<ij>} \Psi_i^+ \tilde{\tau}_+ \Psi_j \Psi_i \Psi_j^+ \tilde{\tau}_- \Psi_i \right\},$$  
(4)

where $\tilde{\tau}_\alpha$ ($\alpha = 0, 1, 2, 3$) are Pauli matrices and $\tilde{\tau}_\pm = (\tilde{\tau}_1 \pm i \tilde{\tau}_2)/2$. The standard manipulations to derive the
effective action for phase fluctuations includes: i) the Hubbard-Stratonovich transformation\(^{12}\) to deal with the four-fermion-field term and ii) a gauge transformation to avoid violating the Mermin-Wagner theorem.\(^{12}\) In order to use the Hubbard-Stratonovich transformation, one needs to introduce a complex auxiliary field \(\phi_i\) and the partition function \(Z\) becomes a function of \(\Psi\) and \(\phi_i\):

\[
Z = \int \mathcal{D}\Psi^* \mathcal{D}\Psi \mathcal{D}\phi^* \mathcal{D}\phi \exp[-S],
\]

where

\[
S = \int dt \left\{ \frac{1}{U} \sum_i |\phi_i|^2 + \sum_i \chi_i \left[ \bar{\theta}_0 \partial_t - \bar{\gamma}_3 \mu \right] \psi_i - t \sum_{i,j>\text{<}} \bar{\psi}_i \bar{\gamma}_3 \psi_j - \sum_i \left[ \phi_i \bar{\psi}_i \bar{\gamma}_3 \psi_i + h.c. \right] \right\}.
\]

Note that if we require the equation for \(\phi_i\) to have \(\delta S[\phi, \phi^*]/\delta \phi_i = 0\), the solution of this equation is \(\phi_i = UC_i \bar{C}_i\). Consequently, \(\phi_i\) can be identified as the order parameter.

Parameterizing the auxiliary field \(\phi_j = \Delta \bar{C} e^{i\theta_j}\) and making a gauge transformation \(\Psi_j = \exp[i\bar{\gamma}_3 \theta_j/2] \chi_i\), where \(\chi_i\) is a spinor for neutral fermions, one can show that

\[
S = \int dt \left\{ \frac{1}{U} \sum_i |\phi_i|^2 + \sum_{i,j} \chi_i \left[ \bar{\theta}_0 \partial_t + \bar{\gamma}_3 \left( \partial_t \theta_j - \bar{\gamma}_3 \mu - \bar{\gamma}_1 \Delta \right) \right] \delta_{i,j} \chi_j 
+ \sum_{i,j} \chi_i \left[ -t \bar{\gamma}_3 \sum_\delta \delta_{i,j+\delta} e^{-i\gamma_3 \theta_{j,i}} / 2 \right] \chi_j \right\}.
\]

where \(\theta_{i,j} = \theta_i - \theta_j\) is a phase difference between sites \(i\) and \(j\), \(\delta = \pm \hat{x}, \pm \hat{y}\) for a square lattice. Note that if we equate \(\phi_j = UC_i \bar{C}_j\) and \(\phi_j = \Delta \bar{C} e^{i\theta_j/2}\), then we know that the phase part of \(C_{ij}\) is \(\exp[i\theta_j/2]\). This means that the gauge transformation\(^{21,22}\) splits the charged fermion field \(C_{ij}\) into a charge boson field \(\exp[i\theta_j/2]\) and a neutral fermion field \(\chi_j\), which obeys a Grassmann algebra.

After integrating out fermion fields, we obtain \(Z = \int \mathcal{D}\phi^* \mathcal{D}\phi \exp[-S_{\text{eff}}]\), where the effective action is

\[
S_{\text{eff}} = \int dt \sum_i \frac{1}{U} |\phi_i|^2 - \text{Tr} \ln[G^{-1}].
\]

Here, \(\text{Tr}\) means the trace over the functional space, depending on the representation, and on the spin space. We will use a symbol \(\text{tr}\) for a trace over spin space only. In the real (lattice) space, the Green function can be represented as

\[
G^{-1}(i, j) = G_0^{-1}(i, j) - \Sigma(i, j),
\]

where

\[
G_0^{-1}(i, j) = (-\bar{\gamma}_0 \partial_t + \bar{\gamma}_3 \mu + \bar{\gamma}_2 \Delta) \delta_{i,j} + t \bar{\gamma}_3 \sum_\delta \delta_{i,j+\delta}
\]

and the self energy has the form

\[
\Sigma(i, j) = \frac{i}{2} \bar{\gamma}_3 (\partial_t \theta_j) \delta_{i,j} + ut \bar{\gamma}_3 \sum_\delta \delta_{i,j+\delta} \sin \left( \frac{\theta_{i,j}}{2} \right) + t \bar{\gamma}_3 \sum_\delta \delta_{i,j+\delta} \left[ 1 - \cos \left( \frac{\theta_{i,j}}{2} \right) \right].
\]

In the expression for \(G_0^{-1}(i, j)\) the bulk value of \(\Delta\) is used. This means we consider only fluctuations of the phase and assume no fluctuation in the magnitude of the gap. Magnitude fluctuation will also change the self energy \(\Sigma\). However, in this paper we concentrate on the effects of phase fluctuations. For simplicity we also consider only the static case (\(\partial_t \theta_i = 0\)); therefore, we are not concerned with the Landau damping effects which are related to the scattering of the thermally excited quasiparticles with the excitations of the phase field. However, if
one is interested in dynamics associated with the phase fluctuations, then the Landau effects have to be taken into account.\textsuperscript{23} Before going further we would like to see what happens if the phase is treated in the continuum limit while the fermions are kept on a lattice. Let us consider \( \sum_{i,j} \chi_i^+ \Sigma(i,j) \chi_j \) in the static case. Since we consider the continuum limit for the phase, we change the phase difference to the phase derivative as follows:

\[
\sum_{i,j} \chi_i^+ \tilde{\tau}_0 it \sum_{\delta} \delta_j, i+\delta \sin(\theta_{i,j}/2) \chi_j \approx \frac{1}{2} \tilde{\tau}_0 it \sum_{i,\delta} \chi_i^+ \theta_{i, i+\delta} \chi_{i+\delta} .
\]

Since \( \theta_{i, i+\delta} = \theta_i - \theta_{i+\delta} \approx -\delta \cdot \nabla \theta - \frac{1}{2} (\delta \cdot \nabla)^2 \theta , \)

The fermions are on the lattice so we need to use Bloch state to expand \( \chi_i = \sum_k e^{i k \cdot r_i} \chi_k \). Now we have for example

\[
\sum_{i,\delta} \chi_i^+ (\delta \cdot \nabla \theta) \chi_{i+\delta} = 2i \sum_k \chi_k^+ [(\partial_x \theta) \sin(k_x) + (\partial_y \theta) \sin(k_y)] \chi_k .
\]

Note that \( \sum_{\delta} (\delta \cdot \nabla \theta) \cos(\mathbf{k} \cdot \delta) = 0 \) because of symmetry. We also have

\[
\sum_{i,\delta} \chi_i^+ \frac{1}{2} (\delta \cdot \nabla)^2 \theta \chi_{i+\delta} = \sum_k \chi_k^+ \left[ (\partial_x^2 \theta) \cos(k_x) + (\partial_y^2 \theta) \cos(k_y) \right] \chi_k .
\]

We therefore obtain

\[
\sum_{i,j} \chi_i^+ \tilde{\tau}_0 it \sum_{\delta} \delta_j, i+\delta \sin(\theta_{i,j}/2) \chi_j \\
\approx \tilde{\tau}_0 \sum_k \chi_k^+ \left\{ -\frac{1}{2} it \left[ (\partial_x^2 \theta) \cos(k_x) + (\partial_y^2 \theta) \cos(k_y) \right] \\
+ t [ (\partial_x \theta) \sin(k_x) + (\partial_y \theta) \sin(k_y) ] \right\} \chi_k .
\]

Similarly, one can show that

\[
\sum_{i,j} \chi_i^+ \tilde{\tau}_3 it \sum_{\delta} \delta_j, i+\delta [1 - \cos(\theta_{i,j}/2)] \chi_j \\
\approx \frac{1}{4} t \tilde{\tau}_3 \sum_k \chi_k^+ \left[ (\partial_x \theta)^2 \cos(k_x) + (\partial_y \theta)^2 \cos(k_y) \right] \chi_k .
\]

Consequently, when the phase is taken in the continuum limit while the fermions are still on the lattice, the self energy in the momentum space is

\[
\Sigma = \tilde{\tau}_0 \left\{ -\frac{1}{2} it \left[ (\partial_x^2 \theta) \cos(k_x) + (\partial_y^2 \theta) \cos(k_y) \right] + t [ (\partial_x \theta) \sin(k_x) + (\partial_y \theta) \sin(k_y) ] \right\} \\
+ \frac{1}{4} t \tilde{\tau}_3 \left[ (\partial_x \theta)^2 \cos(k_x) + (\partial_y \theta)^2 \cos(k_y) \right] ,
\]

which is the same as the self energy of Ref.\textsuperscript{23}

\[III. EFFECTIVE ACTION\]

In this section we concentrate on the effective action for phase fluctuations. By virtue of the gauge transformation used, the formalism associated with the derivation of the desired action has become quite simple because the self-energy that we have obtained in the previous section depends only on the phase of the order parameter.
The effective action $S_{eff}$ can be separated into the mean-field part ($S^{(0)}$) and the phase fluctuation part ($S_\theta$) as follows:

$$S_{eff} = \int d\tau \sum_i \frac{1}{U} |\phi_i|^2 - \text{Tr} \ln[G^{-1}]$$

$$= S^{(0)} - \text{Tr} \ln [1 - G_0 \Sigma]$$

$$= S^{(0)} + S_\theta,$$  \hspace{1cm} (19)

where

$$S^{(0)} = \int d\tau \sum_i \frac{1}{U} |\Delta|^2 - \text{Tr} \ln [G_0^{-1}] ,$$  \hspace{1cm} (20)

and

$$S_\theta = \text{Tr} \sum_{n=1}^\infty \frac{1}{n} [G_0 \Sigma]^n .$$  \hspace{1cm} (21)

In the saddle-point approximation $\frac{\partial}{\partial \Delta} \frac{\partial S^{(0)}}{\partial \Delta} = 0$ reduces to the BCS mean-field gap equation:

$$\Delta = \sum_k \frac{\Delta}{E_k} \tanh \left( \frac{E_k}{2T} \right)$$  \hspace{1cm} (22)

and $-(T/V) \frac{\partial S^{(0)}}{\partial \mu}$, where $V$ is a volume of the system, gives an equation for the filling factor:

$$n = 1 - \sum_k \frac{\xi_k}{E_k} \tanh \left( \frac{E_k}{2T} \right) ,$$  \hspace{1cm} (23)

where $E_k = \sqrt{\xi_k^2 + \Delta^2}$ with $\xi_k = -2t [\cos(k_x) + \cos(k_y)] - \mu$. In the calculation of the effective phase-only action $S_\theta$, we assumed that the phase fluctuations are small so that it is sufficient to consider only the first and the second trace in the expansion for $S_\theta$; in other words, $S_\theta \approx S^{(1)} + S^{(2)}$, where

$$S^{(1)} = \text{Tr} [G_0 \Sigma]$$  \hspace{1cm} (24)

and

$$S^{(2)} = \frac{1}{2} \text{Tr} [G_0 \Sigma G_0 \Sigma] .$$  \hspace{1cm} (25)

At finite temperature we obtain an extended XY model Hamiltonian which includes not only the nearest neighbor spin-spin interaction but also the next nearest neighbor and third neighbor interaction. This constitutes an extension of the usual XY Hamilton ($H_{XY}$), which contains only nearest neighbor interactions. Inclusion of the next nearest neighbor hopping in the electron energy dispersion makes the extended feature of the effective Hamiltonian even more robust. In this case the effective Hamiltonian manifests this extended property even at zero temperature. This will be discussed in section V.

The easiest way to calculate $S_\theta$ is in the momentum representation for $G_0$ and $\Sigma$. For simplicity, we will use a four vector notation: $K = (k, \omega_n)$, $\sum_K = T \sum \omega_n \sum_k$, where $\omega_n$ is a fermionic Matsubara frequency, and $\int dX_i = \int d\tau \sum_i$ with the sum over the lattice sites. It can be shown that

$$\langle K | G | K' \rangle = \delta(K - K') G(K')$$

and

$$\langle K' | \Sigma | K \rangle = \hat{\tau}_0 \hat{\Sigma}^{(0)}(K' - K, k) + \hat{\tau}_3 \hat{\Sigma}^{(3)}(K' - K, k),$$

where

$$\hat{\Sigma}^{(0)}(K' - K, k) = it \int dX_i e^{-i(K' - K)X_i} \sum_{\delta} e^{i k \cdot \delta} \sin \left( \frac{\theta_{i,i+\delta}}{2} \right) ,$$  \hspace{1cm} (26)

and

$$\hat{\Sigma}^{(3)}(K' - K, k) = t \int dX_i e^{-i(K' - K)X_i} \sum_{\delta} e^{i k \cdot \delta} \left[ 1 - \cos \left( \frac{\theta_{i,j+\delta}}{2} \right) \right] .$$  \hspace{1cm} (27)

Since $S^{(1)} = \text{tr} \sum_{K,K'} \langle K | G_0 | K' \rangle \langle K' | \Sigma | K \rangle$, we obtain

$$S^{(1)} = t \sum_K \text{tr} [G(K) \hat{\tau}_3 e^{i \eta \omega_n \hat{\tau}_3}] \cos(k_x) \int d\tau \sum_{<ij>} \left[ 1 - \cos \left( \frac{\theta_{i,j}}{2} \right) \right] ,$$  \hspace{1cm} (28)

where $\eta \to 0^+$ is a convergence factor which originates from $G(0, \tau - \tau^+)$. Note that $\Sigma^{(0)}$ makes no contribution to $S^{(1)}$. Since $S^{(1)}$ include the phase difference between the nearest neighbor sites, the first non-trivial term is $\theta_{i,j}^2$. We obtain immediately the action of the usual XY model; however, a $\theta_{i,j}^2$ term will also appear in $S^{(2)}$. Moreover, the phase difference between the next nearest neighbor sites is also obtained from the second
trace. As we will see later Section V, if we include the next nearest neighbor hopping, then even $S^{(1)}$ contains the phase difference between next nearest neighbor sites.

The second trace can also be calculated in a similar manner even though it is more complicated:

\[
S^{(2)} = \frac{1}{2} \sum_{K,K'} \text{tr} \left[ G(K) \hat{\Sigma}(K - K', k) G(K') \hat{\Sigma}(K' - K, k) \right],
\]

where $\hat{\Sigma} = \hat{\tau}_0 \hat{\Sigma}^{(0)} + \hat{\tau}_3 \hat{\Sigma}^{(3)}$. After some manipulation, one can arrive at

\[
S^{(2)} = \frac{1}{2} \sum_{K,K'} \text{tr} \left[ G(K) G(K') \right] \hat{\Sigma}^{(0)} (K - K', k') \hat{\Sigma}^{(0)} (K' - K, k)
+ \frac{1}{2} \sum_{K,K'} \text{tr} \left[ G(K) \hat{\tau}_3 G(K') \hat{\tau}_3 \right] \hat{\Sigma}^{(3)} (K - K', k') \hat{\Sigma}^{(3)} (K' - K, k).
\]

It can be shown that the mixed terms do not contribute to $S^{(2)}$ in our consideration which deals only with a local effective action. In order to calculate $S^{(2)}$ we need further manipulations. Define $A_{\delta}(X_i) = \sin(\theta_{i,i+\delta}/2)$ and express it in terms of its momentum counterpart as follows: $A_{\delta}(X_i) = \sum_{q} \hat{A}_{\delta}(Q) \exp[iQX_i]$, where $Q$ is a four vector $(q, \Omega_m)$ with a bosonic Matsubara frequency $\Omega_m$. Then, for example, one can show for the first term of $S^{(2)}$ that

\[
\sum_{K,K'} \text{tr} \left[ G(K) G(K') \right] \hat{\Sigma}^{(0)} (K - K', k') \hat{\Sigma}^{(0)} (K' - K, k)
= (it)^2 \sum_{\delta,\delta'} \sum_{Q} \hat{A}_{\delta}(Q) \hat{A}_{\delta'}(-Q) e^{-iq\delta} \sum_{K} \text{tr} \left[ G(K) G(K - Q) \right] e^{iQ(k+\delta')}. \quad (31)
\]

See Appendix A for a detailed derivation. A similar expression can be obtained for the second term. Since, as we mentioned earlier, we are concerned only with the local effective action for the phase only and since we wish to see if the equivalence between the phase-only Hamiltonian and the usual $H_{XY}$, which is found in the continuum limit, still holds on a lattice, we expand $S^{(2)}$ about $Q = 0$ and keep the leading order. Here we would like to explain that in contrast with the continuum limit this procedure requires a periodic lattice. In the continuum limit $\hat{A}_{\delta}(Q) \hat{A}_{\delta'}(-Q) \sim q^2 \theta_{-Q};$ therefore, we can put $Q = 0$ for $\text{tr} \left[ G(K) G(K - Q) \right]$. However, this is not the case on the lattice because $\hat{A}_{\delta}(X_i)$ does not deal with the phase derivative but rather it deals with the phase difference. One might expand $\hat{A}_{\delta}(Q)$ and $\text{tr} \left[ G(K) G(K - Q) \right]$ in terms of $Q$ and, then, regroup terms of the same order of $Q$. If we do so however, we cannot transform back to the lattice space with a function of the phase difference $2\pi$. Instead of doing so, we see under what condition we may simply put $Q = 0$ for $\text{tr} \left[ G(K) G(K - Q) \right]$ and neglect corrections. What we found is a periodic boundary condition for the phase $\theta_i$. If the size of the 2D lattice is $L \times L$, then $\theta(\mathbf{r}_i + L) = \theta(\mathbf{r}_i)$. See Appendix B for details.

Now, it can be shown that

\[
S^{(2)} = \frac{1}{2} \sum_{\delta,\delta'} \sum_{K} \text{tr} \left[ G(K) G(K') \right] e^{iQ(\delta - \delta')} \int dX_i \sin \left( \frac{\theta_{i,i+\delta}}{2} \right) \sin \left( \frac{\theta_{i,i+\delta'}}{2} \right)
+ \frac{1}{2} \sum_{\delta,\delta'} \sum_{K} \text{tr} \left[ G(K) \hat{\tau}_3 G(K') \hat{\tau}_3 \right] e^{iQ(\delta - \delta')}
\times \int dX_i \left[ 1 - \cos \left( \frac{\theta_{i,i+\delta}}{2} \right) \right] \left[ 1 - \cos \left( \frac{\theta_{i,i+\delta'}}{2} \right) \right]. \quad (32)
\]

In order to compare the effective Hamiltonian with the $H_{XY}$, we need to expand $S^{(2)}$ in terms of the phase
differences while keeping terms up to $\theta_{i,j}^2$. Since the first non-trivial term for the second term is $\theta_{i,j}^2$, we will ignore it in the effective Hamiltonian. Using symmetry properties for $G(K)$ such as remaining the same with respect to the exchange of $k_x$ and $k_y$, we obtain the effective local Hamiltonian: $\mathcal{H}_\theta = \langle \theta | M | \theta \rangle$, where $\langle \theta \rangle = (\theta_{i,i+\hat{x}}, \theta_{i,i-\hat{x}}, \theta_{i,i+\hat{y}}, \theta_{i,i-\hat{y}})$ and

$$\hat{M} = \begin{pmatrix} \alpha & \beta & \gamma & \gamma \\ \beta & \alpha & \gamma & \gamma \\ \gamma & \gamma & \alpha & \beta \\ \gamma & \gamma & \beta & \alpha \end{pmatrix}$$

with components as follow:

$$\alpha = \frac{1}{8} \sum_K \text{tr} [G(K) \hat{\tau}_3 e^{i\eta_{\alpha}}] \cos(k_x) + \frac{1}{8} t^2 \sum_K \text{tr} [G(K)G(K)]$$

$$\beta = \frac{1}{8} t^2 \sum_K \text{tr} [G(K)G(K)] \cos(2k_x)$$

and

$$\gamma = \frac{1}{8} t^2 \sum_K \text{tr} [G(K)G(K)] \cos(k_x) \cos(k_y).$$

As one can see, the $4 \times 4$ matrix $\hat{M}$ is not diagonal. This means that the effective Hamiltonian $\mathcal{H}_\theta$ is not equivalent to the usual $H_{XY}$, which would be pure-diagonal. Not only do we have terms like $\theta_{i,j}^2$ and $\theta_{i,j}^4$, but we also have terms of the form $\theta_{i,i+\hat{x}} \theta_{i,i-\hat{x}}$. See Appendix A. We will investigate effects of these off-diagonal terms in the next section.

It is worthwhile making sure our new result for $\mathcal{H}_\theta$ reduces to the well known XY-type Hamiltonian in the continuum limit. For this purpose, we need to recover the explicit dependence on the lattice constant $a$ in the expression for $\mathcal{H}_\theta$ which we have set equal to 1. This will allow us to track orders of $a$ and take the limit $a \to 0$. In this case the phase difference becomes a derivative of the phase $(\nabla \theta)$ while $a^2 \to \frac{m}{\hbar^2}$, where $m$ is an effective mass of the electron. It is straightforward to show that, in the continuum limit with $\xi = \frac{\hbar^2}{2m} - \mu$, $\mathcal{H}_\theta \to H^{(1)}_\theta + H^{(2)}_\theta$, where

$$H^{(1)}_\theta = \frac{1}{8m} \sum_K \text{tr} [G(K) \hat{\tau}_3 e^{i\eta_{\alpha}}] \int d\theta (\nabla \theta)^2,$$

and

$$H^{(2)}_\theta = \frac{1}{16m^2} \sum_K \text{tr} [G(K)G(K)] k^2 \int d\theta (\nabla \theta)^2.$$

See Appendix C for details. Consequently, the effective Hamiltonian $\mathcal{H}_\theta$ we have derived does reduce to the well-known XY-type expression, $H_{XY} = J_{XY} \int d\theta (\nabla \theta)^2$.

### IV. OFF-DIAGONAL TERMS

Let us now consider effects of the off-diagonal terms in $\mathcal{H}_\theta$. At $T = 0$, $\mathcal{H}_\theta$ again becomes equivalent to the XY-type Hamiltonian because the off-diagonal terms of $\hat{M}$, namely $\beta$ and $\gamma$ vanish. However, at finite temperature they are finite so that $\mathcal{H}_\theta$ is no longer of the usual XY type; that is

$$\mathcal{H}_\theta = \alpha \sum_{<ij>} \theta_{i,j}^2 + 2\beta \sum_{i} (\theta_{i,i+\hat{x}} \theta_{i,i-\hat{x}} + \theta_{i,i+\hat{y}} \theta_{i,i-\hat{y}})$$

$$+ 2\gamma \sum_{i} (\theta_{i,i+\hat{x}} + \theta_{i,i-\hat{x}}) (\theta_{i,i+\hat{y}} + \theta_{i,i-\hat{y}}).$$

Since the phase fluctuation between two sites is small by assumption, one can make the approximation that $\theta_{i,i+\hat{x}} \approx \sin(\theta_{i,i+\hat{x}})$. Introducing a 2D classical spin $S_i = (\cos(\theta_i), \sin(\theta_i))$ at a site $i$, it can be shown, within the approximation we have made, that, for example, $\theta_{i,i+\hat{x}} \theta_{i,i-\hat{x}} \approx (S_i \times S_{i+\hat{x}}) \cdot (S_i \times S_{i-\hat{x}})$. It can be seen that a spin at the site $i + \hat{x}$ couples to a spin at $i - \hat{x}$, which is the next nearest neighbor spin-spin in-

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**FIG. 1**: Geometrical illustrations of induced interactions for spin pairs. $\delta$ is a vector to the nearest neighbor site. $\delta_2$ is to the next nearest neighbor site and so forth.
teraction. The only assumption we make is that terms higher than $\theta_{ij}^2$ for a given $(i,j)$ are negligible. This does not mean, however, that only the nearest neighbor phase differences are important. Following the procedure we described in Appendix D, one can show that the second term of $\mathcal{H}_0$, which is proportional to $\beta$, becomes $\beta \sum_{<ij>} \theta_{ij}^2 + \beta \sum_{<ij>} S_i \cdot S_j$ up to a constant, where the symbol $<ij>$ indicates a sum over the next-next nearest neighbors. Similarly, the third term of $\mathcal{H}_0$ proportional to $\gamma$ turns out to be $2\gamma \sum_{<ij>} \theta_{ij}^2 + 2\gamma \sum_{<ij>} S_i \cdot S_j$, where $<ij>$ means a sum over the next nearest pairs.

Since $\theta_{ij}^2$ can also be represented in terms of $S_i \cdot S_j$, the effective Hamiltonian $\mathcal{H}_0$ can be written as

$$\mathcal{H}_0 = -J_1 \sum_{<ij>} S_i \cdot S_j + J_2 \sum_{<ij>} S_i \cdot S_j + J_3 \sum_{<ij>} S_i \cdot S_j,$$

where $J_1 = 2(\alpha + \beta + 2\gamma)$, $J_2 = 2\gamma$, and $J_3 = \beta$. It is clear that this Hamiltonian is not of the usual XY type but instead of an extended XY type. A geometrical explanation for the appearance of the next nearest neighbor and the next-next nearest neighbor term in Eq. (39) is illustrated in Fig. 1(a). Indeed, these terms come from the second trace proportional to $t''$, which has a factor $\Sigma^{(0)} \Sigma^{(0)}$. Each self-energy $\Sigma^{(0)}$ picks up $\delta = \pm \hat{x}, \pm \hat{y}$, and the second trace gives terms with resulting vectors $\delta + \delta' = \delta_2$ or $\delta_3$, where $\delta_2 = \pm \hat{x} \pm \hat{y}$ and $\delta_3 \pm 2\hat{x}, \pm 2\hat{y}$. This geometrical picture also works when we include the next nearest neighbor hopping ($t''$) in the electron dispersion curves.

The physics of $\mathcal{H}_0$ depends on the relative magnitudes of coefficients $J_1$, $J_2$, and $J_3$ in Eq. (39) as well as their relative signs. For example, if $\beta$ is negative, and $\alpha$ and $\gamma$ are both positive so that $J_1 > 2J_2$, $\mathcal{H}_0$ describe a non-frustrated XY model, and its critical behavior can be understood in terms of the usual XY Hamiltonian with an effective coupling constant $J_{eff} = (J_1 - 2J_2)$. However, this does not mean that in this case $\mathcal{H}_0$ is equivalent to $-J_{eff} \sum_{<ij>} S_i \cdot S_j$ because the local behavior of these two Hamiltonians is different. In general, however, as long as $J_1$ is dominant, the large length scale behavior is of the usual XY type. To calculate $J_1$, $J_2$, and $J_3$, we need to know how $\Delta$ and $\mu$ change with increasing temperature. We choose the pairing interaction $U = 1.4t$ and the filling factor $n = 0.9$ and self-consistently solve Eqs. (29) and (30) to determine $\Delta(T)$ and $\mu(T)$ as functions of $T$. In Fig. 2 we plot $J_{eff}$ vs $T$ scaled by $T_{MF}$ for $t'' = 0$. The value of the BKT transition temperature ($T_BKT$) is indicated by an arrow. As one can see, in this case $T_BKT/T_{MF} \approx 0.73$. If $n$ gets closer to 1 as well as $U$ becomes smaller; namely, $n \approx 1$ and $U < t$, $T_BKT/T_{MF} \approx 1$ as we verified numerically.
and the Green function

\[ G_0^{-1}(i, j) = (-\hat{\tau}_{0}\partial_{\tau} + \hat{\tau}_{3}\mu + \hat{\tau}_{2}\Delta)\delta_{i,j} + \hat{\tau}_{3} \left[ t \sum_{\delta} \delta_{j,i+\delta} + t' \sum_{\delta_{2}} \delta_{j,i+\delta_{2}} \right] \]  

(42)

with the self energies

\[ \Sigma^{(0)}(i, j) = it \sum_{\delta} \delta_{j,i+\delta} \sin \left( \frac{\theta_{i,j}}{2} \right) + it' \sum_{\delta_{2}} \delta_{j,i+\delta_{2}} \sin \left( \frac{\theta_{i,j}}{2} \right), \]  

(43)

and

\[ \Sigma^{(3)}(i, j) = t \sum_{\delta} \delta_{j,i+\delta} \left[ 1 - \cos \left( \frac{\theta_{i,j}}{2} \right) \right] + it' \sum_{\delta_{2}} \delta_{j,i+\delta_{2}} \left[ 1 - \cos \left( \frac{\theta_{i,j}}{2} \right) \right]. \]  

(44)

We obtain the effective Hamiltonian including the next nearest neighbor hopping contribution:

\[ \mathcal{H}_{\theta} = -J_1 \sum_{<ij>} S_i \cdot S_j + J_2 \sum_{<ij>} S_i \cdot S_j + J_3 \sum_{<ij>\neq 0} S_i \cdot S_j + J_4 \sum_{<ij>\neq 0} S_i \cdot S_j + J_5 \sum_{<ij>\neq 0} S_i \cdot S_j, \]  

(45)

where \( \sum_{<ij>\neq 4\delta} \) means \( \sum_{i,\delta\neq 4\delta} \). Figs. (1b) and (c) show geometrical descriptions for these terms. In the same way that the \( t^2 \) term gives interactions of the form \( S_i \cdot S_i \cdot S_i \cdot S_i \) and \( S_i \cdot S_i \cdot S_i \cdot S_i \), the \( t't' \) term induces the form \( S_i \cdot S_i + S_i \cdot S_i \) because \( \delta + \delta_2 = \delta_4 \), and the \( t'^2 \) term gives rise to \( S_i \cdot S_i + S_i \cdot S_i \) and \( S_i \cdot S_i + S_i \cdot S_i \) because \( \delta_2 + \delta'_2 = \delta_4 \) or \( \delta_5 \), where \( \delta_4 = \pm \hat{x} \pm 2\hat{y}, \pm 2\hat{x} \pm \hat{y}, \) and \( \delta_5 = \pm \hat{x} \pm 2\hat{y} \).

VI. DISCUSSIONS AND CONCLUSIONS

An effective Hamiltonian for phase fluctuations has been derived on a square lattice using the attractive Hubbard model to describe electron dynamics. We find that the effective Hamiltonian is not of the usual XY type, which maps onto a spin Hamiltonian with nearest neighbors only, but is extended XY containing spin interaction between second up to fifth neighbors. This is in contrast to the common assumption that discretization of the continuum limit Hamiltonian leads to its lattice version. In the continuum limit the BCS phase stiffness and hence the effective Hamiltonian vanish at \( T_{MF} \) because they are proportional to the number of Cooper pairs. In other words \( T_{MF} \) can be determined not only from the mean field equation for the gap but also from the phase stiffness in the continuum limit. However, this is not the case on the lattice. Since we showed that the effective Hamiltonian we obtained reduces properly to the well-known continuum limit result, this is clearly a special property of the continuum limit and does not hold on a lattice. It is interesting to note that the periodic boundary conditions in our formalism are essential to get simple results and they are those that are usually assumed for summation over the Brillouin zone. Without them the effective Hamiltonian would not necessarily end at a finite number of neighbors.

The extended feature of the effective phase Hamiltonian is reinforced when the next nearest neighbor hopping is considered in the electronic dispersion. The critical behavior is however still BKT-like but with an effective coupling which depends significantly on temperature. This arises because near the BKT transition the effective Hamiltonian reduces to the XY case but this simplification only holds in this restricted region of temperature. In particular the generalized phase Hamilto-
nian does not vanish at the mean field temperature $T_{MF}$ which is identified with the pseudogap temperature $T^*$. The crossover from BCS to Bose-Einstein corresponding to increasing $U$ and/or decreasing $n$ reduces the ratio of the BKT transition temperature to the mean field pseudogap temperature.

In the continuum limit, $1 - T_{BKT}/T_{MF} = 4T_{MF}/E_F$, where $E_F$ is the Fermi energy, for the BCS limit (large $n$ and small $U$). Since $T_{MF}/E_F$ is negligibly small for typical values of $T_{MF} \approx 20-30$ meV and $E_F \approx 800-1000$ meV, the temperature region between $T_{BKT}(= T_c)$ and $T_{MF}(= T^*)$ is negligibly small as well. However, on the lattice we find instead $1 - T_{BKT}/T_{MF} = 0.375$ for $n = 0.9$ and $U = 1.4$, which are typical values of these parameters in the BCS regime. Beyond the BCS regime (small $n$ and large $U$), $T_{BKT}/T_{MF}$ is mostly 0.5 in the continuum limit while the ratio reduces to 0.22 for $n = 0.4$ and $U = 2.8$ on the lattice. Therefore, the range for phase fluctuations between $T_c$ and $T^*$ can be much larger on the lattice as compared with the continuum limit.

In our consideration $J_1$ (or $\mathcal{J}_1$ for $t' \neq 0$) is not the BCS phase stiffness. Thus it does not have to vanish at $T_{MF}$. However, $J_{eff}$ (or $\mathcal{J}_{eff}$) is the phase stiffness near the critical region and it determines $T_{BKT}$. Nevertheless we want to mention that we cannot interpret $J_{eff}$ as the BCS stiffness in the whole temperature range. It is only near $T_{BKT}$ that $-J_{eff} \sum_{i,j>1} S_i \cdot S_j$ can represent the full Hamiltonian $\mathcal{H}_0$ that we obtained on the lattice.

We have considered only $s$-wave pairing in this paper. For cuprates $d$-wave pairing is appropriate and this case received considerable attention in the literature but only in the continuum limit. In the continuum limit the order parameter $\phi(R, r)$, where $R(r)$ is the center of mass (relative) coordinate, is represented by $\phi(R, r) = \Delta(R, r)e^{i\theta(R)}$ because the bond phase is usually replaced by the site phase. However, on the lattice it is the bonding order between the nearest sites that we must use as the building block to construct the $d$-wave order parameter. This means that we can consider phase fluctuations between the nearest neighbor building blocks in addition to the phase difference by $\pi$ between the two; therefore, we may expect that a subdominant component to the order parameter may be induced by phase fluctuations.

We neglected the so-called Landau terms associated with damping effects in this work. These terms do not enter in the static case which we have considered here. For dynamics, the Landau damping effects may play a role. Nevertheless these effects have been shown not to be important for $T \lesssim 0.6 T_{MF}$ in the case of $s$-wave superconductor in the continuum limit. However, it has also been pointed out that because of the nodal structure of the order parameter of a $d$-wave superconductor the Landau terms can have important effects even at low temperature. Therefore, to describe the dynamics of the phase fluctuations in a $d$-wave superconductor one has to consider Landau damping effects. Such effects will also be important on a lattice. An extension of the present work to include Landau terms is necessary if dynamics is considered. Further complications associated with the existence of nodal quasiparticles have been noted in Ref. 31.

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APPENDIX A: MANIPULATIONS FOR THE SECOND TRACE

In this Appendix we manipulate the second trace. Let us consider

![Graph](image_url)
\[
\sum_{K,K'} \text{tr} [G(K)G(K')] \tilde{\Sigma}^{(0)}(K - K', k') \tilde{\Sigma}^{(0)}(K' - K, k),
\]
where
\[
\tilde{\Sigma}^{(0)}(K - K', k') = i \int dX_i e^{-i(K - K') X_i} \sum_{\delta} e^{i k_i \cdot \delta} A_\delta(X_i)
\]
and
\[
A_\delta(X_i) = \sin \left( \frac{\theta_{i, i+\delta}}{2} \right) = \sum_{Q} \tilde{A}_\delta(Q) e^{i Q X_i}.
\]

Now Eq. (A1) become
\[
\sum_{K,K'} \text{tr} [G(K)G(K')] \int dX_i dX_j e^{-i(K - K')(X_i - X_j)} \times (it)^2 \sum_{\delta, \delta'} e^{i k_i \cdot \delta + i k_j \cdot \delta'} \sum_{Q,Q'} \tilde{A}_\delta(Q) e^{i Q X_i} \tilde{A}_{\delta'}(Q') e^{i Q' X_j}
\]
\[
= (it)^2 \sum_{\delta, \delta'} \sum_{Q} \tilde{A}_\delta(Q) \tilde{A}_{\delta'}(-Q) e^{-i q \cdot \delta} \sum_{K} \text{tr} [G(K)G(K - Q)] e^{i k_i \cdot (\delta - \delta')}.
\]

For the local effective action, we put \( Q = 0 \) in \( \text{tr} [G(K)G(K - Q)] \), which means that we keep only the leading term in the expansion of Eq. (A1).\(^{15,23,24}\) Note that \( \sin(\theta_{i, i+\delta}) \simeq \theta_{i, i+\delta} \sim \nabla \theta \sim q \tilde{\theta}(q) \) so that \( \sin(\theta_{i, i+\delta}) \sin(\theta_{i, i+\delta'}) \sim q^2 \tilde{\theta}(q) \tilde{\theta}(-q) \). Consequently, \( \text{tr} [G(K)G(K - Q)] \) with a finite \( Q \) gives higher order terms in the expansion. Since
\[
\sum_{Q} \tilde{A}_\delta(Q) \tilde{A}_{\delta'}(-Q) e^{-i q \cdot \delta} = \int dX_i \tilde{A}_\delta(i - \delta, \tau) \tilde{A}_{\delta'}(i, \tau),
\]
we have for Eq. (A1)
\[
t^2 \sum_{\delta, \delta'} \sum_{K} \text{tr} [G(K)G(K)] e^{i k_i \cdot (\delta - \delta')} \int dX_i \sin \left( \frac{\theta_{i, i+\delta}}{2} \right) \sin \left( \frac{\theta_{i, i+\delta'}}{2} \right).
\]

The manipulation for the second term exactly parallels the above derivation. However, as we can see, the second term is negligible because of the assumption of slow variation of the phase; therefore, we neglect it.

Now we have an effective Hamiltonian:
\[
\mathcal{H}_{eff} = t \sum_{K} \text{tr} [G(K)\tilde{\tau}_3 e^{i \mu x} \tilde{\tau}_3] \cos(k_z) \sum_{<ij>} \left[ 1 - \cos \left( \frac{\theta_{i,j}}{2} \right) \right] + \frac{1}{2} t^2 \sum_{\delta, \delta'} \sum_{K} \text{tr} [G(K)G(K)] e^{i k_i \cdot (\delta - \delta')} \sum_{i} \sin \left( \frac{\theta_{i, i+\delta}}{2} \right) \sin \left( \frac{\theta_{i, i+\delta'}}{2} \right)
\]
\[(A7)\]

For a small variation of \( \theta_{i,j} \), one can derive an effective local Hamiltonian \( \mathcal{H}_\theta \). Its derivation is straightforward so that we only briefly mention some details about it. For the second term of \( \mathcal{H}_{eff} \), if \( \delta = \delta' \), then one has \( \frac{1}{4} \text{tr} [G(K)^2] \sum_{i, \delta} (\theta_i - \theta_{i+\delta})^2 \). When \( \delta \neq \delta' \), for example \( \delta = \delta' \), one has \( \frac{1}{4} \text{tr} [G(K)^2] \cos(2k_x) \sum_{i} (\theta_i - \theta_{i+\delta})(\theta_i - \theta_{i-\delta}) \). For other cases, one can apply similar manipulation. Note that \( \delta \) and \( \delta' \) are exchangeable.

**APPENDIX B: BOUNDARY CONDITION**

Let us explain how we end up with the boundary condition. Consider
\[
\sum_{\delta, \delta'} \sum_{Q} \tilde{A}_\delta(Q) \tilde{A}_{\delta'}(-Q) e^{-i q \cdot \delta} \sum_{K} e^{i k_i \cdot (\delta - \delta')} A^{(00)}_{K,K-Q}
\]
In general if \( \theta \) The first term contributes and gives 
where \( \Lambda^{(00)} \) because 
\( \xi \) to recover the lattice constant 
we may simply put 
\( Q \) condition is satisfied by the periodic boundary condition.

Now consider 
In this appendix we show how 
\( S^{(2)} \). Now, we need to see under what condition the remaining terms are negligible. Let us transform back to the lattice space using 
\( \tilde{A}_\delta(Q) = \int dX_i A_\delta(X_i) e^{-iQX_i} \) (B2)

Then we have, for the second term,
\[
\sum_{\delta,\delta'} \sum_Q \tilde{A}_\delta(Q) \tilde{A}_{\delta'}(-Q)e^{-iQ\delta} \sum_K e^{i\mathbf{k} \cdot (\delta + \delta')} \frac{1}{2} Q^2 \left[ \frac{\partial^2}{\partial Q^2} \Lambda^{(00)} \right]_{Q=0} 
\]
(B3)

If the lattice size is large enough that we can change \( \sum_i \rightarrow \int d\mathbf{r}_i \), then assuming a periodic boundary condition \( \theta(\mathbf{r}_i + L) = \theta(\mathbf{r}_i) \), we have
\[
\int dX_i dX_i' A_\delta(\mathbf{r}_i') A_{\delta'}(\mathbf{r}_i + \delta) \frac{\partial^2}{\partial QX_i \partial X_i'} e^{iQ(X_i - X_i')} \left[ \frac{\partial^2}{\partial Q^2} \Lambda^{(00)} \right]_{Q=0} 
\]
In general if
\[
\left( \frac{\partial}{\partial X_i} \right)^n A_\delta(\mathbf{r}_i) A_{\delta'}(\mathbf{r}_i + \delta) \bigg|_{\text{boundary}} = 0 \] (B5)

we may simply put \( Q = 0 \) in \( \Lambda^{(00)} \) for \( S^{(2)} \). Since \( \theta(\mathbf{r}_i) \) is periodic, so are its derivatives. Consequently, the above condition is satisfied by the periodic boundary condition.

**APPENDIX C: REDUCTION TO THE CONTINUUM LIMIT**

In this appendix we show how \( \mathcal{H}_\theta \) reduces to the usual form in the continuum limit. In order to do so, we need to recover the lattice constant \( a \) and take the limit \( a \rightarrow 0 \) while keeping \( ta^2 \rightarrow \frac{1}{2m} \), where \( m \) is the electron mass, because \( \xi \rightarrow k^2/2m - \mu \). Let us consider first
\[
\mathcal{H}_\theta^{(1)} = t \sum_K \text{tr} \left[ G(K) \hat{\tau}_3 \epsilon^{i\mathbf{p} \cdot \mathbf{a}_3} \right] \cos(k_x a) \sum_{\langle i,j \rangle} \left[ 1 - \cos \left( \frac{\theta_{i,j}}{2} \right) \right] 
\]
\[
= t \sum_K \text{tr} \left[ G(K) \hat{\tau}_3 \epsilon^{i\mathbf{p} \cdot \mathbf{a}_3} \right] \left( 1 - \frac{1}{2} k_x a \right) \frac{1}{8} \sum_{i,\delta} \left( \theta_i - \theta_{i+\delta} \right)^2 
\]
\[
\rightarrow \sum_K \text{tr} \left[ G(K) \hat{\tau}_3 \epsilon^{i\mathbf{p} \cdot \mathbf{a}_3} \right] \int d\mathbf{r} \frac{(\nabla \theta)^2}{8m} . \] (C1)

Now consider \( \mathcal{H}_\theta^{(2)} \):
\[
\mathcal{H}_\theta^{(2)} = \frac{1}{2} t^2 \sum_{\delta,\delta'} \sum_K \text{tr} \left[ G(K)^2 \right] e^{i\mathbf{k} \cdot (\delta - \delta')} \sum_i \sin \left( \frac{\theta_{i,i+\delta}}{2} \right) \sin \left( \frac{\theta_{i,i+\delta'}}{2} \right)
\]
\[
\rightarrow \sum_K \text{tr} \left[ G(K)^2 \right] \int d\mathbf{r} \frac{(\nabla \theta)^2}{4m} . \] (C1)
\[
\approx \frac{1}{8} t^2 \sum_K \text{tr} [G(K)^2] \sum_{\delta, \delta'} \left\{ 1 - \frac{a^2}{2} [k \cdot (\delta - \delta')]^2 \right\} \sum_i \left( \theta_i - \theta_{i+\delta} \right) \left( \theta_i - \theta_{i+\delta'} \right)
\]
\[
\to \frac{1}{8m^2} \sum_K \text{tr} [G(K)^2] \int dr \left[ k_x^2 (\partial_x \theta)^2 + k_y^2 (\partial_y \theta)^2 \right]
\]
\[
= \sum_K \text{tr} [G(K)^2] k^2 \int dr \frac{(\nabla \theta)^2}{16m^2}.
\] (C2)

**APPENDIX D: OFF-DIAGONAL TERMS**

The effective Hamiltonian is
\[
\mathcal{H}_\theta = \alpha \sum_{<ij>} \theta_{ij}^2 + 2\beta \sum_i \left( \theta_{i,i+\hat{x}} \theta_{i,i+\hat{x}} + \theta_{i,i+\hat{y}} \theta_{i,i+\hat{y}} \right)
\]
\[+ \quad 2\gamma \sum_i \left( \theta_{i,i+\hat{x}} + \theta_{i,i+\hat{y}} \right) \left( \theta_{i,i+\hat{y}} + \theta_{i,i+\hat{y}} \right).\] (D1)

First let us consider the second term.
\[
2\beta \sum_i \left( \theta_{i,i+\hat{x}} \theta_{i,i+\hat{x}} + \theta_{i,i+\hat{y}} \theta_{i,i+\hat{y}} \right)
\]
\[
\approx 2\beta \sum_i \left[ \sin(\theta_{i,i+\hat{x}}) \sin(\theta_{i,i+\hat{y}}) + \sin(\theta_{i,i+\hat{y}}) \sin(\theta_{i,i+\hat{y}}) \right]
\]
\[
\approx 2\beta \sum_i \left[ (\mathbf{S}_i \times \mathbf{S}_{i+\hat{x}}) \cdot (\mathbf{S}_i \times \mathbf{S}_{i+\hat{y}}) + (\mathbf{S}_i \times \mathbf{S}_{i+\hat{y}}) \cdot (\mathbf{S}_i \times \mathbf{S}_{i+\hat{y}}) \right].\] (D2)

Applying a vector identity to this expression, we then obtain
\[
(\mathbf{S}_i \times \mathbf{S}_{i+\hat{x}}) \cdot (\mathbf{S}_i \times \mathbf{S}_{i+\hat{y}}) = \mathbf{S}_{i+\hat{x}} \cdot \mathbf{S}_{i+\hat{y}} - (\mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}})(\mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}}),\] (D3)

where we used the fact that \( \mathbf{S}_i \cdot \mathbf{S}_i = 1 \), we know that the second term becomes
\[
\beta \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j - 2\beta \sum_i \left[ \cos(\theta_{i,i+\hat{x}}) \cos(\theta_{i,i+\hat{y}}) \cos(\theta_{i,i+\hat{y}}) \right].\] (D4)

Since \( \cos(\theta_{i,i+\hat{x}}) \approx 1 - (\theta_{i,i+\hat{x}})^2/2 \), we obtain, for the second term,
\[
2\beta \sum_i \left( \theta_{i,i+\hat{x}} \theta_{i,i+\hat{x}} + \theta_{i,i+\hat{y}} \theta_{i,i+\hat{y}} \right) \approx 2\beta \sum_{<ij>} \theta_{ij}^2 + \beta \sum_{<ij>} \theta_{ij}^2 + \beta \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j.\] (D5)

It is also straightforward to show that
\[
2\gamma \sum_i \left( \theta_{i,i+\hat{x}} + \theta_{i,i+\hat{y}} \right) \left( \theta_{i,i+\hat{y}} + \theta_{i,i+\hat{y}} \right) \approx 2\gamma \sum_{<ij>} \theta_{ij}^2 + 2\gamma \sum_{<ij>\neq} \mathbf{S}_i \cdot \mathbf{S}_j.\] (D6)

**APPENDIX E: COUPLING CONSTANTS**

\[
\mathcal{J}_1 = \frac{1}{4} \left\{ t \sum_K \text{tr} [G(K)] e^{i\omega_n \tau_3} \cos(k_x) + t^2 \sum_K \text{tr} [G(K)^2] \left[ 1 + \cos(2k_x) \right]
\]
\[+ \quad 2 \cos(k_x) \cos(k_y) + 2 \left( \frac{t'}{t} \right) \cos(k_x) \cos(k_y) \right\},\] (E1)
where \( \eta \to 0^+ \) is a convergent factor.

\[
J_2 = \frac{1}{4} \left\{ -t' \sum_K \text{tr}[G(K) \hat{\tau}_3] \cos(k_x) \cos(k_y) \right. \\
+ t^2 \sum_K \text{tr}[G(K)G(K)] \left[ \cos(k_x) \cos(k_y) - 2 \left( \frac{t'}{t} \right) (\cos(k_x) + \cos(2k_x) \cos(k_y)) \right] \\
+ \left( \frac{t'}{t} \right)^2 (1 + \cos(2k_x) \cos(2k_y) + 2 \cos(2k_x)) \right\} \tag{E2}
\]

\[
J_3 = \frac{1}{8} t^2 \sum_K \text{tr}[G(K)G(K)] \left[ 1 + 2 \left( \frac{t'}{t} \right)^2 \right] \cos(2k_x) \tag{E3}
\]

\[
J_4 = \frac{1}{4} t t' \sum_K \text{tr}[G(K)G(K)] \cos(2k_x) \cos(k_y) \tag{E4}
\]

and

\[
J_5 = \frac{1}{8} t^2 \sum_K \text{tr}[G(K)G(K)] \cos(2k_x) \cos(2k_y) \tag{E5}
\]

In actual calculations, we use

\[
T \sum_{\omega_n} \text{tr}[G(k, \omega_n) \hat{\tau}_3 e^{i\eta \omega_n \hat{\tau}_3}] = 1 - \xi_k \frac{\xi_k}{E_k} \tanh \left( \frac{\xi_k}{2T} \right) \tag{E6}
\]

and

\[
T \sum_{\omega_n} \text{tr}[G(k, \omega_n)^2] = -\frac{1}{2T} \left[ 1 - \tanh^2 \left( \frac{\xi_k}{2T} \right) \right] \tag{E7}
\]
This gauge transformation results in the separation of the effective action into the mean field part and the phase fluctuation part. Thus one can do a proper theory in 2D. However, its drawback is that one needs to introduce a branch cut to have a single-valued function for the phase field, which may cause some technical complications. However, these are beyond a scope of this paper.

There might be a possibility to deal with the full expansion without requiring a boundary condition. However, we believe it is highly unlikely.

See, for example, A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Dover, New York, 1975).