Critical charge instability on verge of the Mott transition and the origin of quantum protection in high-$T_c$ cuprates

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The concept of topological excitations and the related ground state degeneracy are employed to establish an effective theory of the superconducting state evolving from the Mott insulator for high-$T_c$ cuprates. The theory includes the effects of the relevant energy scales with the emphasis on the Coulomb interaction $U$ governed by the electromagnetic U(1) compact group. The results are obtained for the layered $t - t' - t_{\perp} - U - J$ system of strongly correlated electrons relevant for cuprates. Casting the Coulomb interaction in terms of composite-fermions via the gauge flux attachment facility, we show that instanton events in the Matsubara “imaginary time”, labeled by a topological winding numbers, are essential configurations of the phase field dual to the charge. This provides a non-perturbative concept of the topological quantization and displays the significance of discrete topological sectors in the theory governed by the global characteristics of the phase field. We show that for topologically ordered states these quantum numbers play the role of an order parameter in a way similar to the Landau order parameter for conventionally ordered states. In analogy to the usual phase transitions that are characterized by a sudden change of the symmetry, the topological phase transitions are governed by a discontinuous change of the topological numbers signalled by the divergence of the zero-temperature topological susceptibility. This defines a novel type quantum criticality ruled by topologically conserved numbers rather than the Landau principle of the symmetry breaking. We show that in the limit of strong correlations topological charge is linked to the average electronic filling number and the topological susceptibility to the electronic compressibility of the system. We exploit the impact of these nontrivial U(1) instanton phase field configurations for the cuprate phase diagram which displays the “hidden” quantum critical point covered by the superconducting lobe in addition to a sharp crossover between a compressible normal “strange metal” state and a region characterized by a vanishing compressibility, which marks the Mott insulator. Finally, we argue that the existence of robust quantum numbers explains the stability against small perturbation of the system and attributes to the topological “quantum protectorate” as observed in strongly correlated systems.

I. INTRODUCTION

Superconductivity represents a remarkable phenomenon where quantum coherence effects appear at macroscopic scale. The superconducting (SC) properties, especially the perfect diamagnetism, are microscopic manifestations of the spontaneous breakdown of one of the fundamental symmetries of matter, namely the U(1) gauge symmetry. For a superconductor this introduces a state with no definite particle number, but with a definite conjugate variable identifiable with the phase. The discovery of the cuprate superconductors which is believed to emerge due to the strong electron-electron interactions, has sparked a widespread interest in physics which goes beyond the traditional Fermi-liquid framework usually employed for understanding the effect of interactions in metals. It has been recognized that the superconductivity occurs in the region of the doped Mott insulator near the Mott transition, so that the whole microscopic foundations on which BCS theory was built on cannot be accommodated to explain cuprate superconductivity. The conventional BCS theory identifies SC order as an instability of the Fermi sea. That assumes the existence of a normal Landau-Fermi-liquid which forms well above the critical temperature $T_c$, which eventually turns into a superconductor below $T_c$ due to residual attraction among low-lying quasiparticles. In cuprates, in turn, there is overwhelming evidence that superconductivity does not appear as an instability of a Landau-Fermi liquid. The reason is that the fermion quasiparticle does not seem to reflect the character of the measured low energy eigenstates. In this sense, the electron (or electron-like quasiparticle) may no longer be the appropriate way to think of elementary excitations. It is intriguing to conjecture that in the strongly correlated systems the ubiquitous competitions between the variety of possible ground states govern the essential physics - the formation of a highly degenerate state seems to open the way to transformation into alternative stable electronic configurations. Strong correlations that suppress electron motion, may transform the system into a kind of an unstable state which will be very sensible to charge and/or spin ordering. In this critical–like state the superconductivity might emerge as a competition between different ground states. Indeed, in cuprates there is clear evidence for the existence of a special doping point “hidden” near optimal doping below the SC dome where superconductivity is most robust. Such a behavior suggests that this point could be a quantum critical point (QCP) while the associated critical fluctuations might be responsible
for the unconventional normal state properties. However, it is unclear whether this QCP is “truly critical” in the sense that it is characterized by universality and scaling. For example, if excitations at QCP also carry the electrical current, then a resistivity linear in temperature, as is observed in cuprates, obtains only if the dynamical exponent is unphysically negative. The resemblance to a conventional QCP is also hampered by the lack of any clear signature of thermodynamic critical behavior. Usually, a QCP would be the end-point of a critical line below which an ordered phase takes place and it could be made manifest below the superconducting dome. Experiments appear to exclude any broken symmetry around this point although a sharp change in transport properties is observed. Unfortunately, our understanding of the underlying orders in cuprates is far from being satisfactory and identifying the nature of the putative QCP is an open question. A possible way out from this difficulty would be if the degrees of freedom that rule QCP’s are different from the energy degrees of freedom that govern the stable phases the critical point separates. Thus these “non-conventional” degrees of freedom could provide critical fluctuations beyond those of the order parameter fluctuations usually included in the standard Ginsburg-Landau-Wilson (LGW) description.

Within the LGW approach the order parameter fluctuations are implemented by constructing models which mimic the low energy properties of solids - a procedure which relies on the separability of the high and low energy scales. Under this proviso the high energy variables can be removed out yielding an effective Hamiltonian (as exemplified e.g. by the $t – J$ model) which describes the relevant low energy and long-wavelength physics. This procedure is often implemented via the projective transformation, which results in removing of high-energy degrees of freedom and replacing them with kinematical constraints. In such approaches, the high energy scale associated with the charge gap is argued to be irrelevant, hence the focus exclusively on the spin sector to characterise the Mott insulator. However, the charge transfer nature of the cuprates plays an essential role in the doped systems so that with discarding charge degrees of freedom an important part of the physics may be lost. However, there is also mounting experimental evidence which put in question the validity of the various projection schemes. For example, it has been found that above any temperature associated with ordering in both electron and hole-doped cuprates a charge gap of order 2 eV is present in the optical conductivity and a rapid reshuffling of spectral weight with hole doping. Angle-resolved photoemission spectroscopy (ARPES) also reveals a similar charge gap. Surprisingly, when superconductivity emerges, the low and high energy degrees of freedom are still coupled. It has been shown that changes in the optical conductivity occur at energies 3 eV which exceeds by two orders of magnitude the maximum of the superconducting gap. But the high energy scale involved is hard to understand unless it is assumed that the spectral weight is transferred from both the lower and the upper Hubbard bands, thus beyond the range of applicability of the pure $t – J$ model. The intimate connection between the low and high energy degrees of freedom in doped Mott insulators was firmly appreciated and termed mottness. Due to the intrinsic mixing of high and low energy degrees of freedom no low energy reduction is possible in a conventional sense, so that the doped Mott insulators are inherently asymptotically slaved. In a similar spirit a detour from the strict projection program was recently proposed in a form of the “gossamer” superconductors recognizing the role of the expensive, double-occupancy charge configurations.

While spontaneous symmetry breaking has become one of the main guiding principles in physics there are other signatures in a physical system that are associated with the topological effects. These are instrumental for a full understanding of the physics and lead to a host of rather unexpected and exotic phenomena, which are in general of a nonperturbative nature. For example, the fundamental character of a vector potential is evident in the Aharonov-Bohm (AB) effect where the topology of the U(1) group is essential: when an electron is transported in a magnetic field around a closed loop, it acquires a phase that is equal to the magnetic flux through the surface spanned by the electron path. Strongly correlated electronic system are no exception in this regard. In particular, the fractional quantum Hall (FQH) effect is the prominent representative. Here, the striking fact is that FQH systems may contain many different phases at zero temperature which have the same symmetry. Thus different states cannot be distinguished by symmetries and the Landau symmetry-breaking principle fails because also topological characteristics of the configurational space come into play. In the most interesting cases configurational spaces are not simply connected. There are space-time configurations of quantum fields which cannot be continuously deformed one into another. Further, an adiabatic motion along a noncontractible closed path in a configurational space leads to a geometric (Berry) phase acquired by the wave function. In condensed matter systems with large numbers of mutually interacting particles, the subject of Berry’s phases becomes a key issue. For example, a Berry phase distinguishes between integer and half-integer spin chains and results in different ground states and excitations. The other examples are the possible geometric phases effects on statistical transmutation that can be achieved by a “flux attachment” which now becomes a very powerful theoretical method. In many cases the topological character of the quantum field is captured by single integer, called the topological charge, or winding number of the field which classify topological excitations. These are found by integrating the so-called Chern-Simons terms which enter the Lagrangians of the theory. What is common to all the above issues is the appearance of gauge fields to characterize various interactions: field configurations which differ by a gauge transformation are to be
In the present work we argue that the important properties of cuprates are controlled by the large Mott gap and consider the representation of strongly correlated electrons as fermions with attached “flux tubes”. This introduces a conjugate U(1) phase variable, which acquires dynamic significance from the electron–electron interaction. This means that an electron is not a quasiparticle (in the Landau sense), but has a composite nature governed by the electromagnetic gauge group. Furthermore, we recognize the non-trivial topology of the electromagnetic U(1) group by observing that the fundamental group \( \pi_1(U(1)) = \mathbb{Z} \) is given by a set of integers. Therefore the elementary excitations in a strongly correlated system always carry \( 2\pi \)-kinks of the phase field characterized by the topological winding number - a quantized U(1) topological charge. Due to the nontrivial first homotopy group \( \pi_1 \) the configuration space of the quantum phase fields is multiply connected, so that inequivalent paths in the “imaginary–time” (paths that are not deformable to one another) naturally emerge. Hence, the U(1) gauge field gives rise to a “topological interaction”, which is felt by the electrons and can be separated from ordinary dynamical ones lumping them into particle “statistics”. To facilitate this task we employ the functional integral formulation of the theory that encompasses all of these topological possibilities: one has to perform the functional integral over fields defined on different topologically equivalent classes i.e. with different winding numbers. From a canonical (operator) point of view, however, the different topological sectors seem to give rise to completely different Hilbert spaces and the resultant field operators would satisfy quite complicated nonlocal commutation relations. The fact that a prospective theory of electronic states in strongly correlated electron systems must give up on either standard fermion commutation relations or standard particle conservation laws has already been pointed out. Furthermore, we exploit the impact of these topological excitations for the phase diagram of cuprates (with its various crossovers and transition lines) and show that they can induce its unusual feature: a “hidden” quantum critical point of the type that results from the topological ground-state degeneracy. It can be probed by the topological susceptibility as a robust, nonperturbative property that is related to the physical quantity of interest, namely, the diverging charge compressibility. It also provides natural description of the Mott state where the system is said to be incompressible when there is a gap in the chemical potential as a function of the electron density. This topological underpinning establishes the source of quantum protection as a collective state of the quantum field, whose excitations pertain to the whole system. Therefore, macroscopic behaviour is mostly determined by topological conservation laws which does not arise just out of a symmetry of the theory (as “conventional” conservation laws based on Noether’s theorem) but it is a consequence of the connectedness, i.e. topology of the phase space, related to the topological properties of the associated gauge group manifold.

The organization of this paper is as follows. In Section II we introduce the electronic model for cuprates which captures the layered structure and epitomizes the hierarchy of relevant energy scales, with the largest set up by the Coulomb interaction. In Section III we describe the details of the flux attachment transformation which results in the representation of strongly correlated electrons as fermions plus attached U(1) gauge “flux tubes” that leads to composite particle picture. Section IV is devoted to the basic concepts of the algebraic topology (homotopy groups) that becomes instrumental for the Feynman’s path integral formulation of quantum statistics. This is followed by Sections V and VI where the fermionic part of the theory is elaborated in terms of the momentum dependent “d-wave” spin–gap and microscopic phase stiffnesses. Here, the most important results are summarized in the effective bosonic model written with the help of the collective phase variables. This enables us to study the superconductivity as the condensation of the “flux-tubes” from the electron composite which is presented in Section VII. We elucidate there the role of doping for the superconducting order to occur and the key role played by the topological degeneracy. In the subsequent Section VIII the topological susceptibility is used to probe the change of the topological order. Here, we show that the topological susceptibility is related to the charge compressibility that diverges at the degeneracy point at zero-temperature and defines a novel type of topological quantum criticality, beyond the paradigm of the symmetry breaking. In Section IX we present calculated phase diagrams for cuprates displaying, beyond the conventional ordered states, regions that are related to the change of the topological order. Section X is dedicated to the discussion of the robustness of the ground states in cuprates and its source in the topological conservation laws. Finally, in Section XI we conclude with a summary of the results, while the Appendixxces collect material that is related to the technical part of the work.

II. ELECTRONIC MODEL FOR CUPRATES

The Hubbard model is viewed as the generic model for interacting electrons in the narrow-band and strongly correlated systems that captures the physics of Mott transition. The existence of the Mott insulator in the cuprates’ parent compounds implies that a viable theory of high–temperature superconductivity must explicitly incorporate the Mott-Hubbard gap for charge transfer. While it is believed that the basic pairing mechanism in cuprates arises from the antiferromagnetic (AF) exchange correlations it is apparent the charge fluctuations also play an essential role in doped systems. Hence the Coulomb charge fluctuations associated with double occupancy of a site are controlled by the parameter \( U \) in the Hubbard model, which also determines the strength
of the AF exchange coupling \( J \). Therefore energy scale of the charge fluctuation is characterized by the Mott gap, which is by far larger than the energy scale of magnetic fluctuations. Although the \( t-J \) model is usually viewed as the \( U \to \infty \) limit of the single band Hubbard model, the one–particle spectra of the two models differ considerably.\(^{36}\) As already mentioned, this limitation of the \( t-J \) model comes from having projected out the doubly occupied states originally contained in the Hubbard model. To explore the more flexible arrangements between \( J \) and \( U \) than encoded either in the Hubbard or \( t-J \) models we employ in the present paper a generalised \( t-t'-U-J \) model for the CuO\(_2\) plane in high-\( T_c \) superconducting.

In this way we retain basic features of both models: the charge fluctuations present in the Hubbard model (but removed from the constrained \( t-J \) model) and the robust superconducting correlations described by the exchange interaction \( J \). Furthermore, we incorporate besides the direct nearest neighbor hopping \( t \) also the next nearest neighbor \( t' \) hopping parameter, which importance in cuprates has been emphasized.\(^{37}\) A good deal of the existing literature on the cuprates invoke model Hamiltonians based only on the properties of a single CuO layer. Obviously, the interlayer structure cannot be ignored, as the measured critical temperature \( T_c \) is strongly dependent on the interlayer structure.\(^{38}\) Therefore, three dimensional (3D) coupling of planes must play an important role in the onset of superconductivity,\(^{39,40}\) which have to be incorporated by means of the interlayer couplings and the associated \( c \)-axis dispersion effects in modeling of the cuprates.\(^{41}\)

Summing up, we consider an effective one–band electronic Hamiltonian on a tetragonal lattice that emphasizes strong anisotropy and the presence of a layered CuO\(_2\) stacking sequence in cuprates: \( \mathcal{H} = \mathcal{H}_I + \mathcal{H}_J + \mathcal{H}_U \), where

\[
\begin{align*}
\mathcal{H}_I &= \sum_{\alpha \ell} \left[ -\sum_{\langle \ell r \rangle} \langle t + \delta_{r, r' \mu} \mu \rangle c_{\alpha \ell}^\dagger (r) c_{\alpha \ell} (r') \right. \\
&\quad + \sum_{\langle \ell r \rangle} t' c_{\alpha \ell}^\dagger (r) c_{\alpha \ell} (r') - \sum_{rr'} t_{\perp} (r r') c_{\alpha \ell}^\dagger (r) c_{\alpha \ell+1} (r') \right] , \\
\mathcal{H}_J &= \sum_{\ell} \sum_{\langle rr' \rangle} J \left[ \mathbf{S}_\ell (r) \cdot \mathbf{S}_\ell (r') - \frac{1}{4} n_\ell (r) n_\ell (r') \right] , \\
\mathcal{H}_U &= \sum_{r \ell} U n_\ell (r) n_{\ell \perp} (r).
\end{align*}
\]

Here \( \langle r, r' \rangle \) and \( \langle \langle r, r' \rangle \rangle \) identify summations over the nearest-neighbor and next–nearest–neighbor sites labelled by \( 1 \leq r \leq N \) within the CuO plane, respectively, while \( 1 \leq \ell \leq N_{\perp} \) labels copper-oxide layers. Subsequently, \( t \) and \( t' \) are the bare hopping integrals, while \( t_{\perp} \) stands for the interlayer coupling. The operator \( c_{\alpha \ell}^\dagger (r) c_{\alpha \ell} (r) \) creates (annihilates) an electron with spin \( \alpha \) at the lattice site \( (r, \ell) \) and \( n_\ell (r) = n_{\ell \perp} (r) + n_{\ell \parallel} (r) \) stand for number operators, where \( n_{\alpha \ell} (r) = c_{\alpha \ell}^\dagger (r) c_{\alpha \ell} (r) \) and \( \mu \) is the chemical potential. Furthermore,

\[
S_\ell^\alpha (r) = \sum_{\alpha \beta} c_{\alpha \ell}^\dagger (r) \sigma_{\alpha \beta}^\dagger c_{\beta \ell} (r)
\]

denotes the vector spin operator \( (\alpha = x, y, z) \) with \( \sigma_{\alpha \beta}^\dagger \) being the Pauli matrices. Finally, \( U \) is the on–site repulsion Coulomb energy and \( J \) the AF exchange. Owing the lattice arrangement the full electronic dispersion is given by

\[
\epsilon (k, k_z) = \epsilon_{\parallel} (k) + \epsilon_{\perp} (k, k_z),
\]

where the in-plane contribution reads

\[
\begin{align*}
\epsilon_{\parallel} (k) &= -2t \left[ \cos(ak_x) + \cos(ak_y) \right] \\
&\quad + 4t' \cos(ak_x) \cos(ak_y)
\end{align*}
\]

with \( t' > 0 \). Furthermore, the \( c \)-axis dispersion is given by

\[
\begin{align*}
\epsilon_{\perp} (k, k_z) &= 2t_{\perp} (k) \cos(ck_z), \\
t_{\perp} (k) &= t_{\perp} \left[ \cos(ak_x) - \cos(ak_y) \right]^2
\end{align*}
\]

as predicted on the basis of band calculations.\(^{43}\)

### III. ELECTRON AS A COMPOSITE OBJECT

We now provide the representation of interacting electrons as fermions plus attached “flux tubes”.\(^{44}\) This leads to a picture of composite particles which are void of the mutual interactions among fermions: the electron-electron Coulomb interaction will be transformed into the action of U(1) gauge (phase) fields governed by the effective kinetic term of “free” quantum rotors.

#### A. Fermionic action

The partition function for the system governed by the Hamiltonian in Eq.\(^{11}\) can be represented as a path integral using fermionic coherent-states. Introducing Grassmann fields \( c_{\alpha \ell} (r r'), \bar{c}_{\alpha \ell} (r r') \) that depend on the “imaginary time” \( 0 \leq \tau \leq \beta \equiv 1/k_B T \), with \( T \) being the temperature, we write the path integral for the statistical sum \( Z \) as

\[
Z = \int [Dc \bar{c}] e^{-S[\bar{c}, c]}
\]

with the fermionic action

\[
S[\bar{c}, c] = \int_0^\beta d\tau \left\{ \sum_{r \alpha \ell} \bar{c}_{\alpha \ell} (r \tau) \partial_\tau c_{\alpha \ell} (r \tau) + \mathcal{H} (\tau) \right\}.
\]

The Hubbard term in Eq.\(^{11}\) we write in a SU(2) invariant way as

\[
\mathcal{H}_U (\tau) = U \sum_{r \ell} \left\{ (1/4) n_{\ell \parallel}^2 (r \tau) - \frac{1}{2} \mathbf{S}_\ell (r \tau) \cdot \mathbf{S}_\ell (r \tau) \right\}
\]
singeing out the charge-U(1) and spin-SU(2)/U(1) sectors, where the unit vector $\Omega_{\ell}(\tau \tau')$ labels varying in space-time spin quantization axis. The spin-rotation invariance one can make explicit by performing angular integration over $\Omega_{\ell}(\tau \tau')$ at each site and time. In the following we fix our attention on the U(1) invariant charge sector leaving aside possible magnetic orderings such as antiferromagnetism. Although sometimes concurrent magnetic transitions occur with the Mott transition, the mechanism of the Mott transition is primarily independent of the symmetry breaking of spins. Thus we stress our primary interest in cuprates due to their superconducting properties and the fact that the superconductivity (resulting from condensation of charge) should not be viewed as inextricably connected with the quantum antiferromagnetism. A clear support for this point comes from the observation of the spectral weight transfer through the superconducting transition in cuprates, which cannot be explained by invoking the antiferromagnetic order: the spectral weight transfer persists well above the Neel temperature and at the doping level where antiferromagnetism is absent.

B. Gauge flux attachment transformation

To proceed, we employ the Hubbard-Stratonovich transformation to decouple the Coulomb term in Eq. (8) with the help of the fluctuating imaginary electrochemical potential $i V(t)$ conjugate to the charge number $n(t)$. Furthermore, we write the field $V(t)$ as a sum of a static $V_0(t)$ and periodic function $V'(t)$

$$\hat{V}_t(\tau \tau') = \hat{V}_t(\tau \tau + \beta) = \hat{V}_0(\tau \tau) + \hat{V}_t(\tau \tau),$$

where using Fourier series

$$\hat{V}(\tau \tau) = (1/\beta) \sum_{n=1}^{\infty} [\hat{V}(\tau \omega_n)e^{i\omega_n \tau} + \text{c.c.}],$$

with $\omega_n = 2\pi n / \beta$ ($n = 0, \pm 1, \pm 2$) being the (Bose) Matsubara frequencies. Now, we introduce the phase (or “flux”) field $\phi(t)$ via the Faraday–type relation

$$\hat{\phi}_t(\tau \tau) = \frac{\partial \hat{\phi}_t(\tau \tau)}{\partial \tau} = \hat{V}_t(\tau \tau),$$

to remove the imaginary term

$$i \int_0^\beta d\tau' \hat{\phi}_t(\tau \tau)n(t)(\tau \tau') \equiv i \int_0^\beta d\tau' \hat{V}_t(\tau \tau)n(t)(\tau \tau'),$$

for all the Fourier modes of the $V(t)$ field, except for the zero frequency by performing the local gauge transformation to the new fermionic variables $f_{\alpha \ell}(t)$:

$$c_{\alpha \ell}(\tau \tau) = \exp \left[ i \int_0^\tau d\tau' \hat{V}_t(\tau \tau') \right] f_{\alpha \ell}(\tau \tau).$$

Thus as a result of Coulomb correlations the electron acquires a phase shift similar to that in the electric (i.e. scalar) AB effect. The expression in Eq. (13) means that an electron has a composite nature made of the fermionic part $f_{\alpha \ell}(\tau \tau')$ with the attached “flux” (or AB phase) $\exp[i\phi_t(\tau \tau')]$. Here, the quantity $C_{\alpha \ell}(\tau \tau)$ defined by

$$C_{\alpha \ell}(\tau \tau) \equiv \hat{\phi}_t(\tau \tau) = \hat{V}_t(\tau \tau),$$

is the one dimensional (temporal) component Chern-Simons term that makes the minimal coupling with the fermion density field. Since the abelian Chern-Simons term is just as a total (time) derivative, the integral of it becomes simply converted by into a “surface” integral, sensitive only to the global properties of the U(1) gauge field along a “imaginary time” path that starts at imaginary time $\tau = 0$ and ends at $\tau = \beta$. Thus the paths can be divided into topologically distinct classes, characterized by a winding number defined as the net number of times the world line wraps around the system in the “imaginary time” direction. As we shall see in the next section, our considerations related to the “imaginary time” boundary conditions can be formalized using homotopically non-trivial gauge transformations for which the strength of the phase shift must be quantized, so that the gauge change of the Chern-Simons term will be an integral multiple of $2\pi$.

IV. QUANTUM STATES ON MULTIPLY CONNECTED SPACES

A. Homotopy theory

The algebraic topology and precisely the concept of homotopy groups provides the necessary background by making reference to the topological structure of the group manifold, let us say $M$. The $n$–th homotopy group $\pi_n(M)$ is a group of equivalent classes of loops that can be smoothly deformed into each other without leaving $M$, where $n$ refers to the dimensionality of the loops in question. The already mentioned AB effect is of topological nature, since mappings from the electron’s configuration space to the gauge group constitute the non-trivial homotopy group $\pi_1(U(1)) = Z$, where the elements of $Z$ are integers and represent winding numbers, i.e., U(1) topological charges. We are precisely facing a similar situation in a strongly correlated system since the electromagnetic U(1) gauge group governs the charge sector. This becomes apparent in an electrodynamic dual description of the charge in terms of the phase field, see Eq. (11), having its roots in the quantum mechanical complementarity of phase and number. In the “imaginary time” evolution of the phase, two field configurations lie in the same connected component of configurational space if they can be continuously deformed into each other. There is a natural equivalence relation between these paths called homotopy: two paths are equivalent (i.e. belong to the same class) if they can be “smoothly deformed” into each
FIG. 1: Schematic representation of the mapping from the real line $R$ (the covering group of $U(1)$) to the circle $S_1 \sim U(1)$ which is locally invertible provided the topological sector with the winding integer number $m$ which is locally invertible provided the topological sector with

other. The classes are labeled by the winding numbers and are endowed with a group structure by appropriately defining the composition of two mappings. The rule of thumb is that if the homotopy group is trivial, then there cannot be any topological field configurations in the underlying theory.

B. Homotopy classes and the path integral

If we work in the Feynman’s path integral formulation of the quantum statistics, then the statistical sum $Z$ takes a form, in which homotopically distinct paths have to be summed according to various possibilities for inequivalent quantizations (superselection sectors). Specializing to the case of the $U(1)$ group one obtains

$$Z = \sum_{m \in \pi_1(U(1))} \rho(m) Z(m)$$

(15)

Here, $m \in Z$ labels equivalence classes of homotopically connected paths and $\rho(m)$ marks the “statistical” weight which is related to a homotopy class. Furthermore, the partial sum $Z(m)$ within the $m$-th topological sector is given by the usual path integral

$$Z(m) = \sum_{m} \int [D\phi]_m \int [DF] e^{-S[\phi,f,f]}$$

(16)

with the integration restricted to the $m$-th homotopy class. Furthermore, the weights factors $\rho(m)$ form unitary irreducible representations of the homotopy group $\pi_1(U(1))$, so that the conditions for the weights are

$$|\rho(m)| = 1, \quad \rho(m_1)\rho(m_2) = \rho(m_1 \star m_2).$$

(17)

In Eq. (17) $m_1$ and $m_2$ label the homotopy classes of two the paths with common end points, while $m_1 \star m_2$ label the homotopy class of the path obtained by joining the two. In particular, the weight factor, which furnishes the representations of $Z$ takes the form $\rho(m) = e^{i\beta m}$, where $\theta \in [0,2\pi)$ is the “statistical angle” parameter. From the canonical point of view, if the configuration space of the system is not simply connected, as for the $U(1)$ group, then the quantization prescription becomes ambiguous since paths belonging to different homotopy classes can get the extra relative Berry phase factor acquired by the wave function and the $\theta$ factor represents exactly this quantization ambiguity. Moreover, the $\theta$ term cannot be traced in a perturbation theory because it has no affect upon the equations of motion. Therefore, in performing the integration in Eq. (16) one should take phase configurations that satisfy the boundary condition $\phi_0(0) = \phi_0(1) + 2\pi m_\ell(r)$ and $m_\ell(r) = 0, \pm 1, \pm 2, \ldots$. For the sake of convenience it is desirable to “untwist” the boundary condition by setting (see, Fig. 1)

$$\phi_\ell(r\tau) \rightarrow \phi_\ell(r\tau) + 2\pi \frac{\tau}{\beta} m_\ell(r).$$

(18)

Summing over all the phases $\phi_\ell(r\tau)$ amounts to integrating over the $\beta$-periodic field $\varphi_\ell(r\tau)$ and to sum over the set of integer winding numbers $\{m_\ell(r)\}$.

Explicitly, following the prescription given in Eqs. (15) and (16) we obtain for the statistical sum

$$Z = \sum_{\{m_\ell(r)\}} \int_0^{2\pi} \prod_r d\varphi_\ell(r) \int_{\varphi_\ell(r_0) = \varphi_0(r)}^{\varphi_\ell(r) = \varphi_0(r) + 2\pi m_\ell(r)} \prod_r d\varphi_\ell(r\tau) \int [DF] e^{-S[\varphi,m,f,f]},$$

(20)
with the action involving the topological Chern-Simons term and the statistical angle parameter

$$S[\varphi, m, \bar{f}, f] = \sum_{\ell} \int_0^\beta d\tau \left\{ \frac{1}{U} \sum_r \left[ \frac{\partial \varphi_r(r\tau)}{\partial \tau} + \frac{2\pi}{\beta} m_\ell(r) \right]^2 + \frac{2\mu}{U} \sum_r \left[ \frac{\partial \varphi_r(r\tau)}{\partial \tau} + \frac{2\pi}{\beta} m_\ell(r) \right] \right\} + \mathcal{H}[\phi, f, f].$$

(21)

Here, $\mathcal{H}[\phi, f, f]$ is the effective Hamiltonian that is void of the Coulomb interaction

$$\mathcal{H}[\phi, f, f] = \sum_{\ell} \int_0^\beta d\tau \left\{ \sum_{\alpha} \bar{f}_{\alpha\ell}(r\tau) \partial_\tau f_{\alpha\ell}(r\tau) - \bar{\mu} \sum_{\alpha} f_{\alpha\ell}(r\tau) f_{\alpha\ell}(r\tau) \right. \\
- \sum_{\langle r, r' \rangle} t e^{-i[\phi_{\ell}(r\tau) - \phi_{\ell}(r'\tau)]} \sum_{\alpha} \bar{f}_{\alpha\ell}(r\tau) f_{\alpha\ell}(r'\tau) + \sum_{\langle r, r' \rangle} t' e^{-i[\phi_{\ell}(r\tau) - \phi_{\ell+1}(r'\tau)]} \sum_{\alpha} \bar{f}_{\alpha\ell}(r\tau) f_{\alpha\ell+1}(r'\tau) \\
+ \sum_{\langle r, r' \rangle} t_{\perp}(r\tau') e^{-i[\phi_{\ell}(r\tau) - \phi_{\ell+1}(r'\tau)]} \sum_{\alpha} \bar{f}_{\alpha\ell}(r\tau) f_{\alpha\ell+1}(r'\tau) - J \sum_{\langle r, r' \rangle} \bar{B}_\ell(r\tau, r'\tau) B_\ell(r\tau, r'\tau) \right\},$$

(22)

where $\bar{\mu} = \mu - n_f U/2$ is the shifted chemical potential, while

$$n_f = \sum_{\alpha} \langle \bar{f}_{\alpha\ell}(r\tau) f_{\alpha\ell}(r\tau) \rangle$$

(23)

is the occupation number for the fermionic part of the electron composite. In Eq. (22), while writing the term that governs AF interaction we made use of the following representation

$$\bar{B}_\ell(r\tau, r'\tau) = \frac{1}{\sqrt{2}} [\bar{f}_{\ell\tau}(r\tau) \bar{f}_{\ell\tau}(r'\tau) - \bar{f}_{\ell\tau}(r\tau) \bar{f}_{\ell\tau}(r'\tau)],$$

(24)

which is just the singlet–pair (valence bond) operator emerging from the decomposition

$$J \sum_{\ell} \sum_{\langle r, r' \rangle} \left[ S_{\ell\tau}(r\tau) \cdot S_{\ell\tau}(r'\tau) - \frac{1}{4} n_{\ell\tau}(r\tau) n_{\ell\tau}(r'\tau) \right]$$

$$= -J \sum_{\ell} \sum_{\langle r, r' \rangle} \bar{B}_{\ell\tau}(r\tau, r'\tau) B_{\ell\tau}(r\tau, r'\tau).$$

(25)

It is obvious that a quasiparticle description (of any kind) makes sense only when the constituent objects are weakly interacting. The chief merit of the transformation in Eq. (13) is that we have managed to cast the strongly correlated problem into a system of weakly interacting f-fermions with residual interaction given by $J$, submerged in the bath of strongly fluctuating U(1) gauge potentials (on the high energy scale set by $U$) minimally coupled to f-fermions via “dynamical Peierls” phase factors. It is clear that the action of these phase factors “frustrates” the motion of the fermionic subsystem. However, as we demonstrate in the following, it is only when charge fluctuations become phase coherent the frustration of the kinetic energy is released. From Eq. (21) we can read off the explicit expression for the statistical weight

$$\rho(m) = \exp \left[ i \cdot \frac{2\mu}{U} \cdot 2\pi m_\ell(r) \right]$$

(26)

so that the statistical angle reads

$$\frac{\theta}{2\pi} = \frac{2\mu}{U}.$$  

(27)

The phase factor in Eq. (26), being a topological quantity is closely related to the concept of the geometric Berry phases. To explicate this we write explicitly the composite structure of the physical electron field using Eq. (13):

$$c_{\alpha\ell}(r\tau) = \exp \left[ i \int_0^\tau d\tau' \bar{V}_D(r\tau') \right] e^{i\gamma_B(r\tau) f_{\alpha\ell}(r\tau)}. $$

(28)

The first term in the exponential in Eq. (28) is the usual dynamical phase factor where $\bar{\phi}_\ell(r\tau) = \bar{V}_D(r\tau)$ and $\phi_\ell(r0) = \phi_\ell(r0).$ The second one, in turn, is the non-integrable Berry phase factor $2\pi \gamma_B(r\tau) = 2\pi m_\ell(r)/\beta,$ where $m_\ell(r)$ marks the integer U(1) topological number.

C. Topological ground state degeneracy

It is known that the ground state degeneracy may arise from broken symmetries. Here, we argue that the ground state degeneracy of the charge states in strongly correlated system states is a reflection of the topological properties of the system. The existence of topological features implies that the quantum eigenstates are not single-values under the continuation of the parameters in the Hamiltonian. Consider the “free” part of the action in Eq. (21) describing the dynamics of the U(1) gauge field

$$S_0[\phi] = \sum_{\ell} \int_0^\beta d\tau \left\{ \frac{1}{U} \sum_r \left[ \frac{\partial \phi_r(r\tau)}{\partial \tau} \right]^2 + \frac{2\mu}{U} \sum_r \left[ \frac{\partial \phi_r(r\tau)}{\partial \tau} \right] \right\}.$$

(29)
This is the action of a particle moving in a plane around “magnetic flux” $\Phi/\Phi_0 = 2\mu/U$. The Hamiltonian corresponding to this action is simply

$$\mathcal{H}_0[\phi] = \frac{U}{4} \sum_{\ell r} \left[ \frac{\partial}{\partial \phi_\ell(r)} - \frac{2\mu}{U} \right]^2, \quad (30)$$

with the eigenenergies given by

$$\varepsilon_0(m) = \frac{U}{4} \sum_{\ell r} \left[ m_\ell(r) - \frac{2\mu}{U} \right]^2. \quad (31)$$

The energy in Eq. (31) can be interpreted as the square of the kinetic angular momentum of a set of quantum rotors divided by the “moment of inertia” $I = 2/U$ and the allowed angular momenta are uniformly displaced from integers by $2\mu/U$, which may be any real number. The energy spectrum is labeled by integers $m_\ell(r)$ and for integer $2\mu/U$ the ground state is non-degenerate. However, for the half-odd integer $2\mu/U$ the ground state is doubly degenerate, see Fig. 2. In this case the destructive interference between even and odd topological sectors is responsible for the ground state degeneracy. As we shall see in the following, this degeneracy will be crucial in explaining the occurrence of superconductivity and anomalous properties on the verge of Mott transition, where the correspondence between the filling factor and the ground state degeneracy will also be established.

V. BARE AND DRESSED BAND PARAMETERS

With the help of the angle-resolved photoemission spectroscopy one gets a direct access to the density of low-energy electronic excited states in the momentum-energy space of Cu-O planes in cuprates. Obviously, all the interactions of the electrons are encapsulated in ARPES data, but these are still difficult to evaluate. Since the underlying band structure of the bare electrons is a priori unknown, one way to think about these interactions is to consider simply the electronic excitations as quasiparticles which are characterized by effective electronic parameters. Consequently, the tight-binding interpolation of the electronic structure is often used for fitting the experimental ARPES data for cuprates. In this type of analysis a conceptually simpler band theory is used to reveal how the strongly correlated electronic effects can be taken into account via the influence of the electronic band parameters. In the context of the present work in order to establish a link between the “bare” band parameters of the high–energy model in Eq. (1) and the “dressed” one of the low energy models we have to perform the averaging over the fluctuation of the U(1) gauge phase fields according to

$$\int [\mathcal{D}\phi] [\mathcal{D}f\mathcal{D} \bar{f}] e^{-\mathcal{S}[\phi,f,\bar{f}]} = \int [\mathcal{D}\phi] [\mathcal{D}f\mathcal{D} \bar{f}] e^{-\mathcal{S}_{LE}[f,\bar{f}]}, \quad (32)$$

where the low energy action $S_{LE}$ is given by

$$S_{LE}[f,\bar{f}] = -\ln \int [\mathcal{D}\phi] e^{-\mathcal{S}[\phi,f,\bar{f}]}. \quad (33)$$

Performing the cumulant expansion in Eq. (33) we can deduce in the lowest order the corresponding low energy fermionic Hamiltonian that has to be compared with the original one in Eq. (1):

$$\mathcal{H}_{LE} = \sum_{\ell} \left\{- \sum_{\langle\ell\ell',\alpha\rangle} (t^* + \delta_{\ell\ell'} \bar{\mu}) J_{\ell\alpha}(r) J_{\ell\alpha}(r') + \sum_{\langle\ell\ell',\alpha\rangle} t^* J^\dagger_{\ell\alpha}(r) J_{\ell\alpha}(r') - J \sum_{\langle\ell\ell',\alpha\rangle} B^\dagger_{\ell\alpha}(r) B_{\ell\alpha}(r) \right\} + \sum_{\langle\ell\ell',\alpha\rangle} t_{\perp}^* J^\dagger_{\ell\alpha}(r) J_{\ell\alpha+1}(r'), \quad (34)$$

where the dressed parameters encapsulating the effect of Coulomb interaction are given by

$$t^* = t \langle e^{-i \phi_\ell(r) - \phi_\ell(r')} \rangle \delta_{\ell\ell',1st}$$
$$t'^* = t' \langle e^{-i \phi_\ell(r) - \phi_\ell(r')} \rangle \delta_{\ell\ell',2nd}$$
$$t_{\perp}^* = t_{\perp} \langle e^{-i \phi_\ell(r) - \phi_{\ell+1}(r')} \rangle \quad (35)$$

and $\langle \ldots \rangle$ refers to the averaging over the U(1) phase field.

$$\langle \ldots \rangle \equiv \frac{\int [\mathcal{D}\phi] \ldots e^{-S_{LE}[\phi]} [\mathcal{D}\phi]}{\int [\mathcal{D}\phi] e^{-S_{LE}[\phi]}} \quad (36)$$

with, the strongly fluctuating kinetic part (on the energy scale $U$) $S_{LE}[\phi]$ given by Eq. (29). On average, the effect of this renormalization due to the presence of the phase–phase correlation functions is the effective mass enhancement of the carriers as a result of the band narrowing, so that the “dressed” bar parameters $t^*_{\perp}$ (where $t^*_X = t, t_\perp X$) are used to match electronic spectra using the low-energy scale $t - J$ model. Typically, in cuprates $t^* \sim 0.5eV, t'^* \sim 0.15 - 0.33$ and $t_{\perp}^*$ is of order of magnitude smaller than the in–plane hopping parameters.
VI. PSEUDOGAP AND PHASE STIFFNESSES

A. RVB pairs: single-particle “d-wave” gap

A routine Hubbard-Stratonovich decoupling is applied to the resonating valence bond (RVB) term in Eq. (25) to give
\[
\exp \left[ -J \int_0^\beta d\tau \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \bar{B}_\ell(\mathbf{r}, \mathbf{r}' \tau) B_\ell(\mathbf{r}, \mathbf{r}' \tau) \right] = \int [\mathcal{D}\Delta^* \mathcal{D}\Delta] e^{-S[\bar{f}, f, \Delta^*, \Delta]},
\]
(37)

where \( \Delta(\mathbf{r} \tau; \mathbf{r}' \tau') \) is the complex pair field that is non-local in space. Furthermore, the corresponding effective action is of the form
\[
S[\bar{f}, f, \Delta^*, \Delta] = \frac{1}{J} \sum_{\ell} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \int_0^\beta d\tau |\Delta_\ell(\mathbf{r}, \mathbf{r}' \tau)|^2 - \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \int_0^\beta d\tau \left\{ \frac{\Delta_\ell(\mathbf{r}, \mathbf{r}' \tau)}{\sqrt{2}} \left[ \bar{f}_\ell(\mathbf{r} \tau) f_\ell(\mathbf{r}' \tau) - f_\ell(\mathbf{r} \tau) \bar{f}_\ell(\mathbf{r}' \tau) \right] + \frac{\Delta_\ell^*(\mathbf{r}, \mathbf{r}' \tau)}{\sqrt{2}} \left[ \bar{f}_\ell(\mathbf{r} \tau) f_\ell(\mathbf{r}' \tau) - \bar{f}_\ell(\mathbf{r} \tau) \bar{f}_\ell(\mathbf{r}' \tau) \right] \right\},
\]
(38)

A saddle-point method can be applied to the action in Eq. (38) to give the self-consistency equation for the momentum-dependent gap parameter \( |\Delta(\mathbf{k})| \) belonging to the Cu-O plane. Assuming that \( \Delta(\mathbf{k}) \) is not changing along the \( c \)-direction, we can drop the layer index for this quantity. Out of the many possible mean-field translationally invariant solutions in the RVB theory the “\( \pi \)-flux” phase is selected here because of its relation to the “d-wave” symmetry of the pseudogap in cuprates. It is governed by the equation
\[
1 = \frac{J}{N} \sum_k \frac{\eta^2(k)}{2E(k)} \tanh \left( \frac{\beta E(k)}{2} \right),
\]
(39)

where, \( \eta(k) = \cos(k_x a) - \cos(k_y a) \) with the quasiparticle spectrum of the fermionic part of the electron composite,
\[
E^2(k) = \left[ \epsilon_\uparrow^*(k) - \mu \right]^2 + |\Delta(k)|^2
\]
(40)

and
\[
\Delta(k) = \Delta[\cos(ak_x) - \cos(ak_y)].
\]
(41)

The gap parameter is a quantity with the short-range property, \( \lim_{|\mathbf{r} - \mathbf{r}'| \to 0} \Delta(\mathbf{r} - \mathbf{r}') = 0 \), essentially tied to local correlations on neighboring sites. As we see in the following, the presence of the “d-wave” pair function \( \Delta(k) \) is not a signature of the superconducting state - it merely marks the region of non-vanishing phase stiffness. However, the presence of \( \Delta(k) \) should be visible e.g., in ARPES spectra that picture the momentum-space occupation and therefore can detect the dispersion \( E(k) \) with a gap for single particle excitations.15

B. Microscopic phases stiffnesses

We can take advantage of the effective fermionic action in Eq. (38) which is now quadratic in the Grassmann field variables that can be integrated out without any difficulty yielding a fermionic determinant:
\[
Z = \int [\mathcal{D}\phi] e^{-S_0[\phi] + \text{Tr} \ln \hat{G}^{-1}},
\]
(42)

where
\[
\hat{G}^{-1} = \hat{G}^{-1}_o - \mathbf{T} = \left( \mathbf{1} - \mathbf{T}\hat{G}_o \right) \hat{G}_o^{-1}
\]
(43)

is the effective propagator of the theory, while
\[
\mathbf{T} \equiv [\mathbf{T}]_{\ell \ell'}(\mathbf{r}, \mathbf{r}' \tau') =
\begin{cases} 
  te^{-i[\phi(\mathbf{r} \tau) - \phi(\mathbf{r}' \tau)]]} & \delta_{\ell \ell'} \delta_{|\mathbf{r} - \mathbf{r}'|,1st} \delta_3 \delta(\tau - \tau') \\
  t' e^{-i[\phi(\mathbf{r} \tau) - \phi(\mathbf{r}' \tau)]} & \delta_{\ell \ell'} \delta_{|\mathbf{r} - \mathbf{r}'|,2nd} \\
  + t_\perp(\mathbf{r} - \mathbf{r}') e^{-i[\phi(\mathbf{r} \tau) - \phi(\mathbf{r}' \tau)]]} & \delta_{\ell \ell'} \delta_{|\mathbf{r} - \mathbf{r}'|,1st} \\
  \equiv \hat{T} + \hat{T}' + \hat{T}_\perp 
\end{cases}
\]
(44)

is the matrix composed of the hopping integrals and phase factors. Furthermore,
\[
\left[\hat{G}_o^{-1}\right]_{\ell}(\mathbf{r}, \mathbf{r}' \tau') = \left[ \left( \frac{\partial}{\partial \tau} - \delta_{3 \mu} \right) \delta_{\ell, \ell'} + \frac{\Delta_\ell(\mathbf{r}, \mathbf{r}' \tau)}{\sqrt{2}} \right] \delta_3 \delta(\tau - \tau')
\]
(45)
stands for the inverse of the “free” fermion propagator containing the gap $\Delta$ field. Here,
\[
\hat{\sigma}_+ = \frac{1}{2}(\hat{\sigma}_1 + i\hat{\sigma}_2),
\]
\[
\hat{\sigma}_- = \frac{1}{2}(\hat{\sigma}_1 - i\hat{\sigma}_2),
\]
where $\hat{\sigma}_a$ ($a = 1, 2, 3$) are the Pauli matrices acting in the Nambu spinor space, so that
\[
\hat{G}_o(r\tau' r\tau) = \left[ G(r\tau' r\tau') F(r\tau' r\tau') - G(r\tau' r\tau) F(r\tau' r\tau') \right],
\]
Using the self-consistency solution, Eq. (39), and Fourier transforming to the frequency and momentum domain one obtains
\[
\hat{G}_o(k\nu_n) = \left( \frac{-\nu_n + \mu}{\nu_n + \mu + |\Delta(k)|^2} \right),
\]
where $\nu_n = (2n + 1)\pi/\beta$ are the (Fermi) Matsubara frequencies, $n = 0, \pm 1, \pm 2, \ldots$. Now, expanding the trace of the logarithm in Eq. (49) we obtain up to the second order in the hopping matrix elements
\[
\text{Tr} \ln \hat{G}^{-1} = \frac{1}{2} \text{Tr} \left( \hat{G}_o \hat{\nabla}^2 \right) - \frac{1}{2} \text{Tr} \left( \hat{G}_o \hat{\nabla}_\perp^2 \right) + \ldots.
\]
Finally, by performing summations over frequencies and momenta that are implicitly assumed in the trace operation in Eq. (49) we obtain an effective action expressed in the U(1) phase fields
\[
S_{ph}[\phi] = \sum_\ell \int_0^\beta d\tau \left\{ \sum_r \left[ \frac{1}{U} \delta^2_\phi(r\tau) + \frac{2\mu}{U} \phi_\ell(r\tau) \right] - \sum_{(rr')} J_{\parallel}(\Delta) \cos[2\phi_\ell(r\tau') - 2\phi_\ell(r'\tau')] - \sum_{(rr')} J_{\parallel}'(\Delta) \cos[\phi_\ell(r\tau') - \phi_\ell(r'\tau')] - \sum_r J_{\perp}(\Delta) \cos[2\phi_\ell(r\tau) - 2\phi_{\ell+1}(r\tau)] \right\},
\]
In our case $U \gg J, J', J_{\perp}$ so that the microscopic phase stiffnesses can be regarded as residual interactions to the dominant kinetic term of the phase model in Eq. (50).

This justifies the retention of only the lowest order non-vanishing terms in the electron hopping $t$ and $t'$ in Eq. (10) since for the ensuing microscopic phase stiffnesses one has, e.g., $J_{\parallel}(\Delta) \sim t/U$ and $J_{\parallel}'(\Delta) \sim t'/U$, respectively. All the stiffnesses in Eq. (50) (see also Eq. (A4) in Appendix A) rest on the single-particle gap due to the in-plane momentum space pairing among fermionic parts of the electron composites governed by the AF exchange $J$: when $\Delta(k) = 0$ all the phase stiffnesses collapse. While $J_{\parallel}$ and $J_{\perp}$ depend on the square of the corresponding hopping elements, the stiffness $J_{\parallel}'$ is different: it depends linearly on $t'$ and governs the process of correlated particle-hole motion. Collective pair transfer events are costly for large $U$, so that excitonic coherent charge transfer dominates the in-plane charge motion. The inter-plane stiffness $J_{\perp}$ is essential, however, in establishing bulk superconductivity via the Josephson-like interplanar coupling.

VII. FROM THE MOTT INSULATOR TO SUPERCONDUCTOR

A. ODLRO vs. charge frustration

Because of the composite nature of the electron field in strongly correlated system the occurrence of superconductivity requires both the condensation of the of fermion pairs described by $\bar{\psi}_f(r\tau'), \psi_f(r\tau)$ as well as the phase coherence which follows form the condensation of “flux tubes” $e^{i\phi(r\tau)}$ attached to the $f$-fermions. Thus, non-vanishing of the pair–wave function $\Delta$ is not a sufficient signature of the off–diagonal long–range order (ODLRO). We can deduce this relationship from the definition of the superconducting order parameter which implies,
\[
\Psi_{\ell\ell'}(r\tau, r'\tau') = \langle \bar{c}_{\ell\ell}(r\tau) c_{\ell'\ell'}(r'\tau') \rangle
\]
\[
= \delta_{\ell\ell'} \langle \bar{f}_{\ell\ell}(r\tau) f_{\ell'\ell'}(r'\tau') e^{-i[\phi(r\tau) - \phi(r'\tau')]} \rangle
\]
\[
\rightarrow \delta_{\ell\ell'} \Delta(r\tau, r'\tau) \psi_0^\ell
\]
where $\psi_0 = e^{i\phi_{\ell}(r\tau)}$. The condensation of the “flux-tubes” from the electron composite has a transparent physical explanation. The phase factors which are introduced into the hopping elements by the gauge transformation in Eq. (13) frustrate the motion in the fermionic subsystem. However, when charge fluctuations become phase coherent, as signalled by $\langle e^{i\phi(r\tau)} \rangle \neq 0$, the frustration of the kinetic energy is released. The role of the gap parameter $\Delta$ also becomes apparent: pairing among fermionic parts of the electron composites is a necessary precondition for the existence of the microscopic phase stiffnesses (c.f. Eq. (A2)), and, thereby, for the whole superconducting order. The opposite is obviously not true: the pseudogap state with $\Delta = 0$ may be phase incoherent. However, the appearance of bulk phase coherence in the presence of large Coulomb interaction $U$, whose energy scale by far exceeds that of microscopic phase stiffnesses, is not so obvious. Therefore in the following we elucidate the instrumental role of doping, since for the superconducting order to occur the system should be brought in the vicinity of the degeneracy point, that is on the brink of change of the topological order.

B. Effective NLσM

To proceed, we replace the phase degrees of freedom in Eq. (40) by the unimodular complex scalar $z_\ell(r\tau) =
where the unimodularity constraint can be imposed using
Dirac δ-functional, thus bringing the partition function
where the unimodularity constraint can be imposed using
Dirac δ-functional, thus bringing the partition function
into the following form:

\[
Z = \int [D^2 z] \prod_{\ell} \delta \left( |z_\ell(rr)|^2 - 1 \right) e^{-S[z,z^*]}.
\] (53)

The (non-linear) unimodularity constraint can be conveniently resolved with the help of a real Lagrange multiplier λ, so that the phase action in Eq. (50) can be suitably expressed by the effective non-linear σ-model (NLσM) represented by the action

\[
S[z, z^*] = \sum_\ell \int_0^\beta d\tau \left\{ -\sum_\ell \int_0^\beta d\tau' z^*_\ell(rr)\gamma^{-1}(\tau - \tau')z_\ell(rr) - 2J_\parallel(\Delta) \sum_{\langle rr' \rangle} \left[ 1/2 z^*_\ell(rr)z_{\ell+1}(rr') + c.c. \right]^2 \right. \\
\left. - J_\perp^2(\Delta) \sum_\langle rr' \rangle \left[ 1/2 z^*_\ell(rr)z_{\ell+1}(rr') + c.c. \right] \right\},
\] (54)

where

\[
\begin{align*}
\gamma(\tau - \tau') &= \frac{1}{Z_0} \int [D\phi] e^{i\phi_\ell(rr) - \phi_\ell(rr')} e^{-S^{(0)}_{\text{eff}}[\phi]}, \\
Z_0 &= \int [D\phi] e^{-S^{(0)}[\phi]},
\end{align*}
\] (55)

is the phase–phase correlation function calculated with the action in Eq. (29) (see Appendix B). Since a part of the action in Eq. (40) is quartic in the unimodular z-fields we employ the mean-field like decoupling

\[
\begin{align*}
\left[ 1/2 z^*_\ell(rr)z_{\ell+1}(rr') + c.c. \right]^2 \rightarrow \\
\langle z^*_\ell(rr)z_{\ell+1}(rr') \rangle \left[ z^*_\ell(rr)c_{\ell+1} + c.c. \right] + \text{c.c.}
\end{align*}
\] (56)

to perform the closed-form integration over z-variables in Eq. (55). Here, the average \( \langle \ldots \rangle \) should be determined with the resulting effective action. To justify Eq. (56), we observe that, formally, Eq. (55) follows from the decoupling of quartic terms in Eq. (54) with the help of suitable Hubbard-Stratonovich transformation and subsequent use of the saddle-point method with respect to the emerging auxiliary variables. Next, we introduce the Fourier transformed variables becomes

\[
S[z, z^*] = \frac{1}{\beta NN_N} \sum_{q=0}^{\beta} z^* (q, \omega_n) \Gamma^{-1}(q, \omega_n) z(q, \omega_n),
\] (58)

where

\[
\Gamma^{-1}(q, \omega_n) = \lambda - J(q) + \gamma^{-1}(\omega_n)
\] (59)

is the inverse propagator for the z-fields and

\[
\begin{align*}
J(q) &= J^{\parallel}(\Delta) \left[ \cos(k_x a) + \cos(k_y a) \right] \\
&+ J^{\perp}(\Delta) \cos(k_x a) \cos(k_y a) \\
&+ J^{\perp}\left( \Delta \right) \cos(k_z c)
\end{align*}
\] (60)

is the dispersion associated with the microscopic phase stiffnesses, where

\[
\begin{align*}
\tilde{J}^{\parallel}(\Delta) &= \tilde{J}^{\parallel}(\Delta) |z^*_\ell(rr)z\ell(r + 1_{st}, \tau) | \\
\tilde{J}^{\perp}(\Delta) &= \tilde{J}^{\perp}(\Delta) |z^*_\ell(rr)z\ell+1(r) |
\end{align*}
\] (61)

Furthermore, \( \gamma_0(\omega_n) \) is the Fourier transform of the bare phase propagator in Eq. (55), see Appendix B.

C. SC critical boundary

At the critical boundary demarcating the long-range ordered phase-coherent true superconducting state the static and uniform “order parameter” susceptibility diverges, so that the suitable condition that can be read off from the action in Eq. (55) is

\[
\Gamma^{-1}(0, 0)|_{\lambda=\lambda_c} = 0
\] (62)
which fixes the Lagrange parameter $\lambda$ at the transition boundary and within the ordered state. The parameter $\lambda_c$ is given by the solution of the unimodularity constraint equation:

$$1 = \frac{1}{\beta NN_\perp} \sum_{q,\omega_n} \Gamma(q,\omega_n).$$

(63)

The emerging ground-state phase diagram is depicted in Fig. 4. It exhibits a periodic arrangement of phase incoherent Mott-insulating lobes with the superconducting state above and between them. Apparently, at the degeneracy point $\mu_c$ defined by

$$2\mu_c = \frac{1}{2}$$

(64)

the superconducting state is most robust. Clearly, the above picture resembles that of a system described by the well known Bose-Hubbard Hamiltonian as a generic Hamiltonian for strongly correlated bosons. It covers the physics originating from the competition between the repulsive and kinetic term of the Hamiltonian, whose magnitude are proportional, in the present setting, to the parameters $U$ and phase stiffnesses, respectively. Moreover, this similarity is not accidental, since this is just an example of statistical transmutation where bosons emerge as fermions with attached “flux tubes” as a result of the gauge transformation $\phi$. Within the phase coherent superconducting state order parameter is given by

$$1 - \psi^2 = \frac{1}{\beta NN_\perp} \sum_{q,\omega_n} \Gamma(q,\omega_n) \Big|_{\lambda=\lambda_c}.$$  

(65)

With the aid of Eq. (65) and (66), by performing the summation over Bose Matsubara frequencies, we obtain

$$1 - \psi^2 = \frac{1}{4 NN_\perp} \sum_q \frac{1}{\sqrt{2J(0) - J(q)} + h^2 \left(\frac{2\mu}{U}\right)} \left\{ \coth \left[ \frac{\beta U}{4} \left( \sqrt{2J(0) - J(q)} - h^2 \left(\frac{2\mu}{U}\right) \right) - h^2 \left(\frac{2\mu}{U}\right) \right] \right\}$$

where $h(x - 1/2) = x - [x]$, while $[x]$ is the greatest integer less than or equal to $x$. The remaining summation over the momenta can be efficiently performed by resorting to the lattice density of states as explained in Appendix C. The parameter $\psi$ as a function of temperature and the chemical potential is depicted in Fig. 4 which shows substantial enhancement of this quantity near the degeneracy point. Note that the three-dimensional anisotropic lattice structure is essential, since even a very small interplanar coupling renders the phase transition in the 3D universality class as observed in cuprates. Thus, the absence of $t_\perp$ will suppress the bulk critical temperature to zero, because for isolated stack of two-dimensional layers the NL$\sigma$M strictly predicts $T_c = 0$, in agreement with the Mermin-Wagner theorem.

VIII. TOPOLOGICAL CRITICALITY AT THE DEGENERACY POINT

In the preceding paragraphs we have shown that a theory of strongly interacting electrons can be transformed to an equivalent description of weakly interacting fermions which are coupled to the “fluxes” of the strongly fluctuating U(1) gauge field. In regard to the nonperturbative effects, we realized the presence of an additional parameter, the topological angle $\theta/2\pi \equiv 2\mu/U$, which related to the chemical potential. We argued that the configuration space for the phase field $\phi$ consists of distinct topological sectors, each characterized by an integer, entering the weight factors in the functional integral and counts the topological excitations of the system. On the other hand, the ground state degeneracy depends also on the topology of the configurational space and the transition we encountered at $\theta/2\pi = 1/2$ corresponds to an abrupt change of the ground state that is not related to any visible symmetry breaking. However, the existence of different ground states that are related to the topological properties of the interacting electronic system is a hallmark of the topological order. The latter is not associated with the symmetry breaking pattern, so it cannot be characterized by conventional order parameters in the Landau sense. We argue that the ground state degeneracy can be parametrized by a topological order parameter being the average of the topological charge, i.e., the elements of the homotopy group of the U(1) gauge group and this parameter has a direct physical significance: in the large-$U$ limit the electron density (i.e. the filing factor) is just given the mean topological charge rather than the number of fermionic oscillators. Furthermore, in analogy to the Landau theory where the divergence of the order parameter susceptibility signals the
FIG. 3: The ground state phase diagram resulting from the effective action in Eq. (50). Here, in the filling-control transition, the control parameter is the chemical potential, which is conjugate to the carrier density. The picture shows the arrangement of Mott-insulating (incompressible) lobes MI, with topological order characterized by the winding number $m = 0$ and $m = 1$, respectively, with the phase coherent superconducting ground state between and above them. For large Coulomb energy $U$, the phase coherent state is only possible in the vicinity of the degeneracy point $2\mu/U = 1/2$. The curves are plotted for different ratios of the inter- to intra-layer couplings as input parameters: $J_\perp/J_\parallel = 0.001, 0.01$ and 0.1 (from the top to the bottom) and show the proliferation of the superconducting state as the stack of coupled two-dimensional planes system crosses from 2D to 3D behavior.

phase transition between states with different symmetry, to indicate the change between different topologically ordered states, we introduce the topological susceptibility being a derivative of the mean topological charge with respect to the statistical angle $\theta$. Its divergence is related to the existence of distinct “vacua”, which cross in energy at the degeneracy point. Subsequently, we show that the topological susceptibility has a direct physical relevance, since it is related to the charge compressibility. It diverges at the degeneracy point at $T = 0$ and thus defines a novel type of topological quantum criticality, beyond the Landau paradigm of the symmetry breaking.

A. Topological charge and the electron density

In addition to the Coulomb energy $U$ and temperature, the chemical potential $\mu$ plays a crucial role in Mott transition, since it controls the electron filling $n_e$. An immediate implication of the composite nature of the electrons is that the electron occupation number (i.e., the average number of of electrons per site in the Cu-O plane)

$$n_e = \frac{1}{N} \sum_{\alpha \ell} \langle \bar{c}_{\alpha \ell}(r \tau)c_{\alpha \ell}(r \tau) \rangle$$

(67)

consists of the fermion occupation coming from the fermionic part of the composite and a topological contribution resulting from the “flux-tube” attachment:

$$\langle \sum_{\alpha} \bar{c}_{\alpha \ell}(r \tau)c_{\alpha \ell}(r \tau) \rangle = \langle \sum_{\alpha} \bar{f}_{\alpha \ell}(r \tau)f_{\alpha \ell}(r \tau) \rangle + \frac{2}{iU} \langle \partial_{\tau} \phi_{\ell}(r \tau) \rangle.$$ (68)

The appearance of the topological contribution in Eq. (68) is not surprising given the fact that “statistical angle”, see Eq. (26), depends on the chemical potential and the occupation number is just its conjugate quantity. Owing that the U(1) topological charge (the winding number) is given by

$$m_{\ell}(r) = \frac{1}{2\pi} \int_{\phi_{\ell}(r)}^{\beta} d\tau \dot{\phi}_{\ell}(r \tau) = \frac{1}{2\pi} \int_{\phi_{\ell}(r) + 2\pi m_{\ell}(r)}^{\phi_{\ell}(r)} d\phi_{\ell}(r \tau)$$

(69)

the mean value of the density of the topological charge can be written after performing Legendre transformation as

$$n_b = \frac{2\mu}{U} + \frac{2}{U} \left\langle \frac{1}{i} \frac{\partial \phi_{\ell}(r \tau)}{\partial \tau} \right\rangle.$$ (70)
Therefore the average electron occupation number \( n_e \) is given by
\[
n_e = n_f + n_b - \frac{2\mu}{U}.
\] (71)

In the limit of strong (weak) correlations \( n_e \) interpolates between topological \( n_b \) (fermionic \( n_f \)) occupation numbers. Clearly, in the large–\( U \) limit \( \mu \to n_f U / 2 \), so that \( n_e \to n_b \) and the system behaves as governed entirely by density of topological charge. The latter behaves in the large \( U \) limit as the typical density of hard-core bosons showing characteristic “staircase” behavior, see Figs. 4 7. Indeed, in this limit the system is described by the quantum rotor action in Eq. (29), in which the probability distribution function of the density of topological charge is gaussian and the problem has single-site character that can be analytically solved in a closed form:
\[
n_{ob}(\mu) = \frac{2\mu}{U} \frac{1}{\beta} \frac{\partial h}{\partial \theta} \left[ \frac{n_b}{2\pi i} e^{-\beta U/4} \right] \] (72)

\[
n_b(\lambda) = n_{ob}(\mu) - \frac{1}{2NN_\perp} \sum_q \left\{ \coth \left[ \frac{\beta U}{2} \left( \sqrt{\frac{2[\mathcal{J}(0) - \mathcal{J}(q)]}{U}} + \delta \lambda + h^2 \left( \frac{2\mu}{U} \right) + h \left( \frac{2\mu}{U} \right) \right) \right] - \coth \left[ \frac{\beta U}{4} \left( \sqrt{\frac{2[\mathcal{J}(0) - \mathcal{J}(q)]}{U}} + \delta \lambda + h^2 \left( \frac{2\mu}{U} \right) - h \left( \frac{2\mu}{U} \right) \right) \right] \right\}.
\] (75)

with \( \delta \lambda = \lambda - \lambda_0 \). Here, the parameter \( \lambda \) is self-consistently determined via Eq. (30) whereas \( \lambda_0 \) is given by the solution of Eq. (42). The summation over the wave vectors can be conveniently performed with the help of the lattice density of states.

B. Topological susceptibility and charge compressibility

Mott insulators have a clear distinction from metals by vanishing of the charge compressibility at zero temperature, while this quantity have a finite value in metals. In physical terms, the charge compressibility measures the stiffness to the twist of the phase of the wave function in the “imaginary time” direction. As we have shown, in the limit of strong correlations the physical properties of the system are governed by the fluctuations of the topological charge. Thus, the effects connected with the nontrivial topological configurations of the gauge fields can be tested by performing the second derivative of the free energy with respect to the statistical parameter \( \theta \), see Eq. (27), which gives the topological susceptibility, i.e., the connected part of the two-point correlator of the by making use of the Jacobi theta-function identity
\[
\frac{\partial }{\partial \theta} \left( \frac{n_b}{2\pi i} e^{-\beta U/4} \right) = \sum_{m=1}^{\infty} \frac{(-1)^m 4\pi i q^m}{1 - q^{2m}} \sinh(2\pi mv). (73)
\]

The calculation of the mean topological density for the interacting problem, i.e. with the full phase action given by Eq. (30) involving phase stiffnesses is a bit demanding since spatial correlations have to be included, as well. However, we can resort to the unimodular-filed NLsM description given in Eq. (52). The result for \( n_b \) both within the Mott lobe and in the superconducting region is given by
\[
n_b = \begin{cases} n_b(\lambda), & \text{within MI} \\ n_b(\lambda_0) - 2\psi^2 h \left( \frac{2\mu}{U} \right), & \text{within SC} \end{cases}
\] (74)

where \( \psi \) is the order parameter given by Eq. (60), while topological charge densities at zero momentum:
\[
\chi_t = \frac{1}{Z} \sum_{m \pi_1(U(1))} \frac{\partial^2 \rho(m)}{\partial \theta^2} Z(m) - \left[ \frac{1}{Z} \sum_{m \pi_1(U(1))} \frac{\partial^2 \rho(m)}{\partial \theta^2} Z(m) \right]^2.
\] (76)

In Eq. (70), as a result of the non-trivial topology in the group manifold group caused by the non-simply connected structure, the partition functions \( Z(m) \) are given by the functional integrals taken over the field configurations in the topological class \( m \) only. The full partition function \( Z \), as defined by Eq. (15) involves all topological sectors. Since the statistical angle parameter \( \theta \) (and thereby the chemical potential \( \mu \)) acts as a ground state selector, the topological susceptibility can be conveniently employed to detect transition between different topologically ordered states. Since these are labeled by the average topological charge, the abrupt change of this quantity will be signalled by the divergence of \( \chi_t \) at the degeneracy point
\[
\lim_{\mu \to \mu_c} \chi_t(T = 0, \mu) = \infty,
\] (77)
FIG. 5: Evolution of the fermionic occupation number \( n_f \) with increasing correlations at \( T = 0 \) and for \( t^* = 1 \text{eV}, t^* = 0.5 \text{eV}, t^* = 0.25 \text{eV}, \) and \( t^*/t^* = 0.5 \). For large values of the Coulomb to band energy ratio the fermionic filling factor behaves as \( n_f \sim (\mu/U)^2 \).

where \( \mu_c \) is the value of the chemical potential at the degeneracy point. The topological susceptibility in Eq. (76) can be directly linked with the physical quantities, namely the charge compressibility

\[
\kappa = \frac{\partial n_e}{\partial \mu},
\]

which expresses the total density response of the system to a local change of the chemical potential. It is related to the shift of the electron chemical potential as a function of electron density which can be measured e.g. through the shifts of spectral features in photoemission spectra. Taking the derivative of Eq. (71) with respect to the chemical potential we obtain

\[
\frac{U}{2} \kappa = \frac{U}{2} \frac{\partial n_b}{\partial \mu} + \frac{U}{2} \frac{\partial n_f}{\partial \mu} - 1.
\]

While the fermionic contribution \( \frac{\partial n_f}{\partial \mu} \) is regular, for the bosonic part \( \frac{\partial n_b}{\partial \mu} \) one gets

\[
2\pi \chi_t = \frac{U}{2} \frac{\partial n_b}{\partial \mu}.
\]

Therefore in the large \( U \)-limit the charge compressibility is entirely governed by the topological susceptibility and serves to distinguish that \( \chi_t \) is zero in a Mott insulating region while it remains finite superfluid region and diverges at the degeneracy point.

C. Electron mass enhancement at the degeneracy point

Another remarkable aspect of the transition from one topologically ordered state to another is the great enhancement of the effective mass \( m_e^* \) of the electrons due to the collapse of electron kinetic energies due to the formation of the degenerate state at \( 2\mu/U = 0.5 \). To estimate the change of \( m_e^* \) we calculate

\[
\frac{m_e^*}{m_e} = \frac{\partial^2 \epsilon(\mathbf{k})/\partial k^2 |_{k=0}}{\partial^2 \epsilon(\mathbf{k})/\partial k^2 |_{k=0}} = \frac{1}{R},
\]

where

\[
R = \langle e^{-i[\phi(\mathbf{r}) - \phi(\mathbf{r'})]} \rangle |_{r - r'| = d}
\]

is the band renormalization factor, see Eq. (85), where \( d \) stands for the lattice vector connecting nearest-neighbors sites on a two-dimensional lattice. Figure 8 illustrates the evolution of the effective mass as a function of temperature in the vicinity of the degeneracy point. Interestingly, at \( 2\mu/U = 0.5 \) which marks the “topological quantum critical point” the electronic matter in its charge aspect
FIG. 7: (Color online) Average topological number $n_b$ as a function of temperature and chemical potential for $U = 4\text{eV}$, $J = 0.15\text{eV}$, $t^* = 0.5\text{eV}$, $t'^*/t^* = 0.25$, $t_1^* = 0.01\text{eV}$, and different temperatures $T = 1\text{K}$, $50\text{K}$, $115\text{K}$ and $300\text{K}$ from the top to the bottom.

is very “soft” (see, Fig.9) making it very susceptible to transformation into alternative stable electronic configurations, namely to superconductivity, which we are going to analyze.

IX. PHASE DIAGRAM FOR CUPRATES

There has been a considerable amount of controversy regarding the observed pseudogap phenomena in cuprates. One general class of theories views the pseudogap phase as resulting from performed pairs. The cuprates, however, are not in the strict Bose condensation (“local pair”) limit, since the photoemission still reveals the presence of a large Fermi surface. Furthermore, in the Bose limit, the chemical potential would actually be located beneath the bottom of the energy band, which is also not the case. The other class of scenarios (coined as “competing order”) consider the pseudogap as not intrinsically related to superconductivity, but rather proclaim it as competitive with superconductivity. Most of these proposals involve either a charge density wave or spin density wave, usually without long range order. However, if there is a phase transition underlying pseudogap formation, a direct thermodynamic evidence (i.e. non-analytic behavior of the specific heat, the susceptibility, or some other correlation function of the system) must show up in existing experiments. Unfortunately, none of the spectroscopic data support a picture where the pseudogap phase represents a phase with true long range order. For the temperature-doping phase diagrams the two delineated above scenarios generally predict that the pseudogap characteristic temperature $T^*(x)$ merges with $T_c(x)$ on the overdoped side (“precursor” scenario) or $T^*(x)$ falls from a high value at low doping, comparable to the exchange energy to zero at a critical doping point inside the superconducting dome (“competing order” picture). Below we show that both scenarios are consistently accommodated within the presence of topological order, degeneracy point and accompanying phase coherence around it, as shown in Fig.10. We see the evolution of the charge compressibility $\kappa$ as a function of the chemical potential from the Mott insulator with $\kappa = 0$ (at $2\mu/U = 1$) to a point of degeneracy on the brink of the particle occupation change at $2\mu/U = 1/2$ where $\kappa = \infty$ at $T = 0$. This is also the point on the phase diagram from which the superconducting lobe emanates. It is clear that, the nature of the divergence of $\kappa$ here has nothing to do with singular fluctuations due to spontaneous symmetry breaking as in the “conventional” phase transition. Rather, this divergent response appears as a kind of topological protection built in the system against the small changes of $\mu$. Further, $\kappa \to \infty$ implies that $\partial\mu/\partial n_e$ becomes vanishingly small at $T = 0$ which results in the chemical potential pinning, as observed in high-$T_c$ cuprates.

A. Low energy scale pseudogap temperature $T^*$

In the pseudogap state at high temperatures one thus finds the coexistence of two distinct components; a
state with gaped fermionic excitations (described by the fermionic part of the composite electron) and incoherent charge excitations (given by the attached “flux-tube”), which, as the temperature is lowered, enter the superconducting state. The pseudogapped state is largely unaffected by the superconducting transition and does not participate directly in the superconducting behavior. As explained above the underlying mechanism for the appearance of a gapped state with non-vanishing $\Delta$ is intimately connected with the antiferromagnetic correlations represented by the AF exchange $J$. We identify the temperature for which $\Delta$ sets in with the pseudogap temperature $T^\ast$. This is also the temperature at which the microscopic phase stiffnesses in Eq. (A2) vanish, so that

$$\left\langle e^{-\beta(\phi(r)-\phi'(r'))}\right\rangle \to 0.$$  

(83)

Using results of Sec.VIA, the fermionic filling factor $n_f$ defined by Eq. (23) can be computed explicitly as

$$n_f - 1 = -\frac{1}{N} \sum_k \left[ \frac{\epsilon^\ast(k) - \mu}{E(k)} \right] \tanh \left[ \frac{\beta E(k)}{2} \right].$$  

(84)

With the help of Eq. (83) and using Eq. (39) and we obtain that at $T^\ast$

$$\frac{1}{J} = \frac{1}{2|\mu|} \tanh \left( \frac{\beta|\mu|}{2} \right),$$  

$$n_f - 1 = \frac{\bar{\mu}}{|\mu|} \tanh \left( \frac{\beta|\mu|}{2} \right).$$  

(85)

By eliminating the chemical potential from Eq. (84) we get

$$\frac{k_B T^\ast}{J} = \frac{|n_f - 1|}{\ln \left[ -\frac{2|n_f - 1| + (n_f - 1)^2 + 1}{2|n_f - 1| - (n_f - 1)^2 - 1} \right]}$$  

(86)

revealing that $T^\ast$ is a universal function of the fermionic filling number $n_f$. Approaching half-filing ($n_f = 1$) we can infer from Eq. (56) that

$$\lim_{n_f \to 1} k_B T^\ast(n_f) = \frac{J}{4 \ln(3)} \approx 0.228J \equiv k_B T^\ast_{max},$$  

(87)

where $T^\ast_{max}$ is the maximum value of the pseudogap temperature $T^\ast$. For $J = 0.15eV$ we obtain $T^\ast_{max} = 396K$, see Fig. 12.

B. Effect of doping on AF exchange and $x-T$ phase diagram for cuprates

It is well known that the antiferromagnetic exchange $J$ originates from the interplay between on-site repulsion ($U$) and the delocalization energy ($t$). The effect can be derived straightforwardly by expanding the energy to the second order in the hopping matrix element. This involves virtual double occupation and can be represented by an exchange process taking place on neighboring lattice sites:

$$\begin{align*}
| \uparrow, \downarrow \rangle & \xrightarrow{\frac{1}{U}} | \uparrow, \downarrow, 0 \rangle \xrightarrow{\frac{1}{U}} | \downarrow, \uparrow \rangle \\
| \uparrow, \downarrow \rangle & \xrightarrow{\frac{1}{U}} | 0, \uparrow, \downarrow \rangle \xrightarrow{\frac{1}{U}} | \uparrow, \downarrow \rangle
\end{align*}$$  

(88)

which yields a contribution $\sim t^2/U$. There are also processes that are prohibited by the Pauli exclusion principle...
such as |↑,↑⟩ → 0. However, with increasing hole doping (i.e., departing from the half-filling) a given electron has fewer neighboring electrons to pair with, which results in degradation of the exchange process described in Eq.\ref{eq:J_eff}. Therefore, the AF exchange is leading to an effective interaction which is a steadily decreasing function of \(x\), vanishing at the critical doping \(x_c\):

\[
J_{\text{eff}}(x) = J(1 - Kx),
\]

where \(K\) is treated as the lattice connectivity and the factor of \(K = 4\) is the coordination number on the 2D square lattice. Therefore, the vanishing of \(J_{\text{eff}}\) determines the critical doping value \(x_c = 0.25\). It is clear by inspecting Eq.\ref{eq:J_eff} that diminishing of the AF exchange with doping will spoil the RVB pairing of the fermionic part of the electron composite by suppressing the \(d\)-wave gap function \(\Delta(k)\). Since phase stiffnesses in Eq.\ref{eq:phase_stiffness} rest on \(\Delta(k)\) the doping dependence of \(J_{\text{eff}}(x)\) can be directly translated into the calculation of the \(x-T\) phase diagram that involves the doping effect on \(J_{\text{eff}}\), see Fig.\ref{fig:phase_diagram}. By comparing Fig.\ref{fig:phase_diagram} and Fig.\ref{fig:phase_diagram} we can clearly see that the diminishing of the superconductivity in the overdoped region is just the result of the pair-breaking effect triggered by the doping dependent AF exchange.

To summarize: \(T^*(x)\) demarcates the region of non-zero microscopic phase stiffnesses which persist in the region characterized by the non-vanishing of the spin gap, as observed in high-frequency conductivity measurements. The origin of the spin gap is purely electronic and results from the restricted space of available states that strongly correlated excitations on neighboring sites encounter. It is described by the resonating valence bond singlet \(d\)-wave spin pairing of the fermionic part of the electron composite and is controlled by the AF super-exchange parameter \(J\). The coincidence of the Fermi surface with the minimum gap locus as obtained from ARPES measurements also supports of a pairing gap interpretation of the pseudogap.

C. Crossover to the “strange metal” state at \(T_s\):
high energy scale feature

The doping-dependent characteristic temperature \(T^*\) in Eq.\ref{eq:J_eff}, at which this pseudogap opens is in the underdoped region significantly larger than \(T_c\). The physical reason for this is transparent: \(T^*\) marks the region of non-vanishing phase stiffness, albeit without global phase coherence (that appears at much lower temperature \(T_c\)). However, when the copper oxide superconductor is driven in the normal state by applying a high magnetic field, a clear pseudogap feature at a similar energy scale to the superconducting gap is observed in the quasiparticle tunnelling spectra and the pseudogap feature persists up to the highest applied fields and does not depend on the magnetic field. Surprisingly, the Hall coefficient does not vary monotonically with doping but rather exhibits a sharp change at the optimal doping level for superconductivity. This observation would support the idea that two competing ground states underlie the high-temperature superconducting phase. From this perspective one has to conclude that any prospective order consistent with these observations implies that the pseudogap coexists with superconductivity and is essentially unchanged by a large applied external field. It is clear that sudden onset of the pseudogap at critical doping right at the point where the rigidity of the condensate wave function is at its maximum would be very difficult to reconcile with the precursor scenario, but is very consistent with the onset of correlations which compete with superconductivity. This is precisely the outcome of the topological order which differentiates the electronic ground state into two states labeled by the topological winding number and with the degeneracy point separating them. It controls a remarkable concurrence between normal state properties and the ground-state superconducting order setting up a unique critical doping point in the phase diagram where the transport properties change very suddenly and where superconductivity is most robust. Therefore we identify the crossover line \(T_g(x)\) where the charge compressibility undergoes a sudden change as an additional boundary hidden in the cuprate phase diagram, see Fig.\ref{fig:phase_diagram}. It is important to realize that in contrast to \(T^*(x)\) the crossover line \(T_g(x)\) is controlled by the highest energy scale in the problem, namely the Mott scale set up by \(U\). This explains why the anomalous behavior still persists even the superconducting order is suppressed, e.g. by the strong magnetic field.

Considering the Hall effect one has to conclude that the mobile carrier density varies considerably with both doping and temperature. On the other hand, the ARPES Fermi surface remain essentially unchanged in the whole of the metallic doping range suggesting a constant density of states. These apparently contradictory results could be reconciled by observing that ARPES is sensitive to the momentum-space occupation and therefore detect the excitation described by the fermionic part of the electron composite, whereas the charge transport properties are governed mainly by the “flux tubes” which constitute charge collective variables. Given fact that the inverse of the Hall coefficient is proportional to the number of carriers \(1/R_H \sim n_e\) and \(n_e\) is governed by the topological charge \(n_T\) it is apparent why \(1/R_H\) jumps in the vicinity of the QCP that is of topological origin.

X. QUANTUM PROTECTORATE

It is often difficult to formulate a fully consistent and adequate microscopic theory of complex cooperative phenomena and great advances in the solid-state physics are to a great extent due to the use of simplified and schematic model representations for the theoretical interpretation. In particular, the method of model Hamiltonians has proved to be very effective. However, as it was recently argued, ab-initio computations have failed com-
FIG. 10: (Color online) Finite temperature phase diagram: the superconducting lobe \( T_c(\xi) \) translated from the chemical potential \( \xi \equiv \mu \) (upper right panel) to the particle occupation number \( \xi \equiv n_b \) (lower left panel). Shaded area: the density plot of the charge compressibility \( \bar{\kappa} = \frac{U\kappa}{2} \). The degeneracy point \( (T = 0, \frac{\mu}{U} = \frac{1}{2}) \), where \( \kappa \) diverges transforms into the critical line on the \( n_b - T \) phase diagram. Upper left panel: \( \kappa \) and \( n_b \) as a function of temperature for \( T = 0.1U \) showing the transition from the incompressible Mott state at \( 2\mu/U = 1 \) to a highly compressible region around the degeneracy point. The values of the parameters for creation of the plots are the same as in Fig. 9.

FIG. 11: (Color online) Temperature–doping \( (x = 1 - n_b) \) phase diagram calculated for the doping independent AF exchange \( J \) (for the values of the parameters, see Fig. 9). Depicted is the superconducting lobe (bounded by the critical temperature \( T_c(x) \)) and the pseudogap temperature \( T^* \) which marks the region of non-vanishing microscopic phase stiffnesses (below \( T^*(x) \)). Shaded area: intensity plot of the charge compressibility \( \kappa \) diverging along the critical \( T = 0 \) line (see, previous figure).

in general, \textit{impossible} to calculate from first principles. However, as we saw, a system with many microscopic degrees of freedom can have ground states whose degeneracy is determined by the topology of the system. Prototypes of this kind of systems are provided by fractional quantum Hall effect. For example, the ground state degeneracy in FQH liquids is not a consequence of symmetry of the Hamiltonian. It is robust against arbitrary perturbations, even impurities that break the symmetries in the Hamiltonian. Thus the topological ground state degeneracy on non-trivial manifolds provides a precise theoretical distinction between a topological and conventional order. The Hilbert space of quantum states decomposes into distinct topological sectors, each sector remaining isolated under the action of local perturbations. This is a signature of its topological nature. Choosing the states from ground states in different sectors protects these states from unwanted mixing through the change of system parameters- protection within the sector is secured through a gapped excitation spectrum. In particular, we found that for strong correlations the system is governed by the topological Chern numbers. However, the Chern number is a topologically conserved quantity...
and is “protected” against the small changes of system parameters. Being an integer it can not change at all if it has to change continuously. However, changing the interaction by a large amount may cause abrupt changes in ground state properties described by a different topological quantum number, which leads to a change of topological order. This kind of stability might be generic for quantum systems governed by topologically non-trivial groups manifolds. Therefore one is left not only with the low-energy principle (the classic prototype being the Landau Fermi liquid), but the emergent physical phenomena are regulated also by topological principles that have a property of their insensitivity to microscopics and this quantum protectorate functions under certain topological environments, through conserving of topological charges.

XI. SUMMARY AND DISCUSSION

In the present work focusing on the $t-t'-t_\perp-U-J$ model it is shown that the topological excitations of charge given by the collective $U(1)$ phase field in a form of “flux tubes” attached to fermions can reproduce many robust features present in the phase diagram of high-$T_c$ cuprates, thus substantiating one of the emerging paradigms in the condensed matter physics, namely the ubiquitous competitions in strongly correlated systems. The fundamental entities that carry charge (and spin) in the copper oxides are no longer the usual Landau quasiparticles but the “flux tube” fermion composites, so that the charge is no longer tied to the Fermi statistics. When charges are “liberated” then they can condense leading to superconductivity. This picture naturally leads to the pseudogap physics that is observed in the underdoped cuprates, which originates from the momentum pairing (in a $d$-wave pattern) of the fermionic parts of the electron composite controlled by the antiferromagnetic superexchange $J$. This underlines the necessity of the fundamental concept of fermion pairing in achieving the superconductivity. In the mathematical structure of the theory the gauge field is governed by the $U(1)$ Chern-Simons term in the action of purely topological nature. From the canonical point of view the Hilbert space of a quantum theory has a non-trivial structure marked by the topological sectors which corresponds to a set of degenerate ground states. The topological ground state degeneracy provides a precise theoretical distinction between a topological and conventional order: states with the same conventional broken symmetries may still be distinguished from each other on the basis of whether they are characterized by different topological quantum numbers captured by the homotopy theory gauge group manifold. In this paper, it has been shown that physics of the Mott transition is successfully covered in a topological framework. The natural order parameter for the Mott transition is the topological charge related to electron concentration for the filling-control scenario that selects topologically ordered states. Expectation value of the density of topological charge, determines also a dominant contribution to the topological susceptibility which, in turn, is related to the charge compressibility of the system. It diverges at the degeneracy point at zero-temperature and defines a novel type of topological quantum criticality, beyond the Landau paradigm of the symmetry breaking. Although the charge compressibility is completely suppressed in the Mott insulator because of the Mott gap, the criticality on the “strange metallic” side can be described adequately by the divergence of the charge compressibility at zero temperature. This critical enhancement of the density fluctuations extends to finite-temperature and is controlled by the Mott energy scale. This gives rise to another crossover line hidden in the cuprate phase diagram, where the charge compressibility undergoes a sudden change to the “strange metal” state. The crossover is governed by the Coulomb energy $U$, so that the density fluctuations at the instability towards the superconductivity surpass the effects of the spin fluctuation mechanisms governed by the antiferromagnetic exchange extensively studied for the cuprate superconductors. This clearly demonstrates the inseparability of the high-energy Mott scale from the low-energy physics.
in the cuprate problem and redefines the role of the chemical potential from a quantity that simply demarcates the boundary between filled and empty states to a selector of topologically ordered electronic ground state.

**APPENDIX A: MICROSCOPIC PHASE STIFFNESSES**

The microscopic phase stiffnesses to the lowest order in the hopping amplitudes are given by

\[ J_{||}(\Delta) = \frac{2t^2}{N\beta} \sum_{\mathbf{k}v_n} F^*(\mathbf{k}v_n)F(\mathbf{k}v_n) \]

\[ J_{\perp}(\Delta) = \frac{t'}{\beta N} \sum_{\mathbf{k}v_n} \cos(ak_x) \cos(ak_y)G(\mathbf{k}v_n) \]

\[ J_{\perp}(\Delta) = \frac{1}{N} \sum_q \frac{t^2}{\beta N} \sum_{\mathbf{k}v_n} F^*(\mathbf{k}v_n)F(\mathbf{k}v_n). \] (A1)

Explicitly, after performing frequency and momentum sums in Eq. (A1) we obtain

\[ J_{||}(\Delta) = \frac{t^2}{4} \int_{-2}^{2} dx dy  \frac{x^2 y^2}{y^2 - x^2} \rho(x) \rho(y) \times \left\{ \frac{\tan \left( \frac{1}{2} \beta \epsilon(x) \right)}{\epsilon(x)} - \frac{\tan \left( \frac{1}{2} \beta \epsilon(y) \right)}{\epsilon(y)} \right\}, \]

\[ J_{\perp}(\Delta) = -t' \mu \int_{-2}^{2} dx \frac{\tilde{\rho}(x)}{\epsilon(x)} \tan \left( \frac{1}{2} \beta \epsilon(x) \right), \]

\[ J_{\perp}(\Delta) = \frac{9t^2 \left| \Delta \right|^2}{16} \int_{-2}^{2} dx \frac{x^2 \rho(x)}{e^{\beta \epsilon(x)}} \left\{ 2 \tanh \left[ \frac{\beta \epsilon(x)}{2} \right] - \beta \epsilon(x) \operatorname{sech}^2 \left[ \frac{\beta \epsilon(x)}{2} \right] \right\}. \] (A2)

Here, \( \epsilon(x) = \sqrt{\mu^2 + \left| \Delta \right|^2 x^2} \) and

\( \rho(x) = \left( \frac{1}{\pi^2} \right) K \sqrt{1 - (x^2/4)} \)

\( \rho'(x) = \rho(x) - \left( \frac{2}{\pi^2} \right) E \sqrt{1 - (x^2/4)} \) (A3)

where \( K(x) \) and \( E(x) \) are the complete elliptic integrals of the first and second kind, respectively.

**APPENDIX B: PHASE-PHASE CORRELATION FUNCTION**

By performing the functional integration over the phase variables in Eq. (53) we obtain

\[ \gamma^{-1}(\tau - \tau') = \frac{\vartheta_3^{2t \mu} + \pi \frac{\tau - \tau'}{\beta}, e^{\frac{4t \mu}{\beta}}}{\vartheta_3^{2t \mu}, e^{-\frac{4t \mu}{\beta}}} \times \exp \left\{ -\frac{U}{4} \left[ \tau - \tau' \right] - \left( \frac{\tau - \tau'}{\beta} \right)^2 \right\}, \] (B1)

where \( \vartheta_3(z, q) \) is the Jacobi theta function which comes from the topological part of the functional integral over the phase variables. The function \( \vartheta_3(z, q) \) is defined by

\[ \vartheta_3(z, q) = 1 + 2 \sum_{n=1}^{\infty} \cos(2nz)q^{n^2} \] (B2)

and is \( \beta \)-periodic in the imaginary-time \( \tau \) as well as in the variable \( 2\mu/\beta \) with the period of unity. Fourier transforming one obtains

\[ \gamma(\omega_n) = \frac{1}{Z_0} \sum_{m=-\infty}^{\infty} \frac{\vartheta \exp \left[ -\frac{\beta U}{2} \right]}{1 - 4 \left[ (m + 2)\beta - 2\mu \omega_n \right]^2}, \] (B3)

where

\[ Z_0 = \exp \left[ \frac{\beta \mu^2}{\beta U/4} \right] \theta_3 \left( \frac{\beta \mu}{2\pi i}, e^{-\beta U/4} \right) \] (B4)

is the partition function for the “free” rotor Hamiltonian in Eq. (59).

**APPENDIX C: LATTICE DENSITY OF STATES**

In this Appendix we give the explicit formulas for the densities of states (DOS) for the anisotropic three-dimensional lattice that is helpful for evaluation of the sums over the momenta that appear in Section VII and VIII of the present paper. Our starting point is the dispersion relevant for the two-dimensional lattice with next-nearest interactions:

\[ E(\mathbf{k}) = -2t \cos(ak_x) - 2t \cos(ak_y) + 4t' \cos(ak_x) \cos(ak_y) = 2t \left[ -\cos(ak_x) - \cos(ak_y) + r \cos(ak_x) \cos(ak_y) \right]. \] (C1)

The choice of such a dispersion is obviously motivated by its relevance as a simple means of modelling the quasiparticle band in the high-\( T_c \) cuprates. The density of states reads:

\[ \rho(E) = \int_{-\pi/\alpha}^{\pi/\alpha} \frac{dk_x}{(2\pi/\alpha)} \int_{-\pi/\alpha}^{\pi/\alpha} \frac{dk_y}{(2\pi/\alpha)} \times \delta[E - E(\mathbf{k})] \equiv \frac{1}{2t} \tilde{\rho}(\epsilon) \] (C2)

with

\[ \tilde{\rho}(\epsilon) = \frac{K}{\pi^2 \sqrt{1 + \frac{\epsilon}{\tau}}} \left[ \Theta(2 + r - \epsilon) \times \Theta(\epsilon + r) + \Theta(-r - \epsilon) \Theta(\epsilon + 2 - r) \right], \] (C3)

where \( \epsilon = E/2t \) and \( r = 2t'/t \). Here \( \Theta(x) \) is the Heavyside (unit-step) function. The expression in Eq. (C3) is valid for \( r \leq 1 \). For \( r > 1 \) one has to make the replacement \( \tilde{\rho}(\epsilon) \rightarrow |\Re\tilde{\rho}(\epsilon)| \).
The effect of inter-planar (c-axis) interaction can be incorporated as well via the following dispersion

\[ E_{3d}(k) = E(k) - 2t_z \cos(\epsilon q_z). \]  

(C4)

In the presence of \( t_z \) the system is a three-dimensional anisotropic one for which the density of states becomes

\[ \rho_{3d}(E) = \int_{-\pi/a}^{\pi/a} \frac{dx}{2\pi} \int_{-\pi/b}^{\pi/b} \frac{dy}{2\pi} \int_{-\pi/c}^{\pi/c} \frac{dz}{2\pi} \times \]

\[ \times \delta\left[E - E_{3d}(k)\right] = \frac{1}{2\pi} \tilde{\rho}_{3d}(\epsilon). \]  

(C5)

Performing the integration over \( \kappa_z \) we obtain

\[ \rho_{3d}(E) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\xi \tilde{\rho}(\xi) \theta\left[\xi^2 - (\epsilon - \xi)^2\right]. \]  

(C6)

in a form of the convolution involving previously calculated DOS in Eq. (C3).

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