Composite quasiparticles and the “hidden” quantum critical point 
in the topological transition scenario of high-$T_c$ cuprates

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The quantum interference effects due to the Aharonov-Bohm-type phase factors are studied in the layered $t - t' - t_\perp - U - J$ strongly correlated system relevant for cuprates. Casting Coulomb interaction in terms of composite-fermions via the flux attachment facility, we argue that $U(1)$ compact group instanton events labelled by a topological winding number are essential configurations of the phase field dual to the charge. The impact of these topological excitations is calculated for the phase diagram which displays the “hidden” quantum critical point of a novel type.

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The discovery of high-temperature superconductors (HTSC) and follow-up studies of strongly correlated (SC) fermionic systems reveal that an explanation of their unusual properties appears unlikely in a way of thinking rooted in an independent electron picture. It is widely accepted that the central issue in the high-temperature superconducting cuprates is physics of the doped Mott insulator [1]. There are also strong indications [2], that much of their behavior is governed by the proximity to a kind of quantum critical point (QCP). However, in approaches to the HTSC one customary concentrates on the low-energy physics usually discarding the hallmark of SC systems - the high energy scale given by the Coulomb interaction $U$ by projecting out double-occupancy charge configurations. A detour from the strict projection program was recently proposed in a form of the “gossamer” superconductor [3], recognizing the role of correlations among expensive double-occupancy charge configurations.

Moreover, a SC electronic system can have non-trivial topological properties which can be described by gauge fields [4]: a phase of the many-body wave function might be arbitrary but correlations among the local phases of its constituents can bring unusual gauge structures [5]. Quantum theories with topological properties have raised considerable interest in connection with a wide range of problems, among them, the Aharonov-Bohm (AB) effect [6], which establishes the reality of the electromagnetic gauge potential, is a typical example. In fact, the AB effect forms only the prelude to the even more general class of topological phenomena which are possible in gauge theories. In particular, the fractional quantum Hall effect [7, 8] is the prominent representative. A succinct account [9] of the latter is given in terms of new particles called composite fermions (CF) by casting electron-electron correlation in terms of vortex attachment facility to grasp the intricate many-particle behavior [7].

In the present paper recognizing the significance of the AB non-integrable phase factor we consider, inspired by the CF idea, the representation of strongly correlated electrons as a fermions plus attached “flux tubes”. This effectively removes most of the electron-electron interaction from the problem and leads to composite particles which are almost void of mutual interactions. Furthermore, taking into account the proper topology of the phase field dual to the charge, we recognize that the elementary excitations in strongly correlated system always carry $2\pi$-kinks of the phase field characterized by the topological winding number. We reveal the impact of these topological excitations for the phase diagram of cuprates and show that they can induce its unusual feature: a “hidden” quantum critical point of a novel type that is not related to the symmetry breaking.

We consider an effective one-band electronic Hamiltonian on a tetragonal lattice that emphasize strong anisotropy and the presence of a layered CuO sequence in cuprates: $\mathcal{H} = \mathcal{H}_t + \mathcal{H}_J + \mathcal{H}_U$, where

$$
\mathcal{H}_t = \sum_{\alpha\ell} \left[ -\sum_{\langle\mathbf{r}\mathbf{r}'\rangle} (t + \mu \delta_{\mathbf{r}\mathbf{r}'}) c_{\alpha\ell}^\dagger(\mathbf{r}) c_{\alpha\ell}(\mathbf{r}') + \sum_{\langle\mathbf{r}\mathbf{r}'\rangle} t' c_{\alpha\ell}^\dagger(\mathbf{r}) c_{\alpha\ell}(\mathbf{r}') - \sum_{\mathbf{r}\mathbf{r}'} t_\perp(\mathbf{r}\mathbf{r}') c_{\alpha\ell}^\dagger(\mathbf{r}) c_{\alpha\ell+1}(\mathbf{r}') \right],
$$

$$
\mathcal{H}_J = \sum_{\ell} \sum_{\langle\mathbf{r}\mathbf{r}'\rangle} J \left[ \mathbf{S}_\ell(\mathbf{r}) \cdot \mathbf{S}_\ell(\mathbf{r}') - \frac{1}{4} n_{\ell}(\mathbf{r}) n_{\ell}(\mathbf{r}') \right],
$$

$$
\mathcal{H}_U = \sum_{\ell \mathbf{r}} U n_{\ell}(\mathbf{r}) n_{\ell}(\mathbf{r}).
$$

(1)

Here, $\langle\mathbf{r}, \mathbf{r}'\rangle$ and $\langle\langle\mathbf{r}, \mathbf{r}'\rangle\rangle$ identifies summation over the nearest-neighbor and next-nearest-neighbor sites labeled by $1 \leq r \leq N$ within the CuO plane, respectively, with $t, t'$ being the bare hopping integrals, while $1 \leq \ell \leq N_\perp$ labels copper-oxide layers and $t_\perp$ stands for the inter-layer coupling. The operator $c_{\alpha\ell}^\dagger(\mathbf{r}) c_{\alpha\ell}(\mathbf{r})$ creates (annihilates) an electron of spin $\alpha$ at the lattice site $(\mathbf{r}, \ell)$. Next, $S_\alpha^a(\mathbf{r}) = \sum_{\alpha\beta} c_{\alpha\ell}^\dagger(\mathbf{r}) \sigma_{\alpha\beta}^a c_{\beta\ell}(\mathbf{r})$ ($a = x, y, z$) stands for spin and $n_{\ell}(\mathbf{r}) = n_{\ell}(\mathbf{r}) + n_{\ell}(\mathbf{r})$ number operators, respectively, where $n_{\ell}(\mathbf{r}) = c_{\alpha\ell}^\dagger(\mathbf{r}) c_{\alpha\ell}(\mathbf{r})$ and $\mu$ is the
chemical potential. Subsequently, $U$ is the on-site repulsion Coulomb energy of the order of bandwidth and $J$ the antiferromagnetic (AF) exchange. The values of $J$ in cuprates are known to be not strongly dependent on materials with the magnitude of 0.1–0.16 eV. The electronic dispersion is $\epsilon(k_x, k_z) = \epsilon(k_x) + \epsilon(k_z)$, where the in-plane contribution is $\epsilon(k_x) = -2t [\cos(k_x) + \cos(k_y)] + 4t' \cos(k_x) \cos(k_y)$ with $t' > 0$. Furthermore, the $c-$axis dispersion is $\epsilon(k_x, k_z) = 2t_\perp(k_x) \cos(k_z)$, while $t_\perp(k) = t_\perp[\cos(k_x) - \cos(k_y)]^2$ as predicted on the basis of band calculations.

We write the partition function $Z = \int [\mathcal{D}c\bar{c}] e^{-S[c, \bar{c}]}$ with the action $S[c, \bar{c}] = \int_0^\beta d\tau \sum_{\alpha r} \bar{c}_\alpha(r) \partial_\tau c_\alpha(r) + \mathcal{H}(\tau)$ using coherent-state fermionic path integral over Grassmann fields $\bar{c}_\alpha(r), c_\alpha(r)$ depending on the “imaginary time” $0 \leq \tau \leq \beta \equiv 1/k_B T$ with $T$ being the temperature. The last term in Eq.11 we write as $\mathcal{H}_U(\tau) = \sum_{\ell} (1/4) n_{\ell}^2(\tau) - \mathcal{S}_f(r) \cdot \mathcal{S}_f(r)^* \big)$ singling out the charge $U(1)$ and spin sector in $SU(2)/U(1)$ coset space, where the unit vector $\mathcal{S}_f(r)$ sets varying in space-time spin quantization axis $\mathcal{S}_f$. In the following we fix our attention on $U(1)$ invariant charge sector, and use Hubbard-Stratonovich transformation to decouple the Coulomb term giving rise to fluctuating imaginary “voltage” $iV_\tau(r)$ conjugate to the number of charged particles $n_\ell(r)$. Furthermore, we write the field $V_\ell(r)$ as a sum of a static $V_0(r)$ and periodic function $V_\tau(r) \equiv V_0(r) + \beta\cdot V(r)$ using Fourier series $V(r) = \sum_{\omega} V(\omega) e^{i\omega \tau} + c.c.$ 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 $\phi_\ell(r)$ via the Faraday–type relation

$$\phi_\ell(r) = \frac{\partial \phi_\ell(r)}{\partial \tau} = \tilde{V}_\ell(r),$$

(2)

The last term in Eq.(1) we write as $i \int_0^\beta d\tau \tilde{V}_\ell(r) n_\ell(r) \equiv i \int_0^\beta d\tau \tilde{V}_\ell(r) n_\ell(r) \equiv i \int_0^\beta d\tau \tilde{V}_\ell(r) n_\ell(r)$ for all the Fourier modes of the $V_\tau(r)$ field, except for the zero frequency by performing the local gauge transformation to the new fermionic variables $f_\alpha(r)$:

$$c_\alpha(r) = \exp \left[ i \int_0^\tau d\tau' \tilde{V}_\ell(r) \right] f_\alpha(r)$$

(3)

Thus, as a result of Coulomb correlations the electron acquire a phase shift similar to that in the electric (i.e. scalar) AB effect [6]; Eq.8 means that an electron has a composite nature made of the fermionic part $f_{\alpha r}$ with the attached “flux” (or AB phase) $\exp[i \phi_\ell(r)]$. The transformed action $S[c, \bar{c}] \to S[\phi, \tilde{f}, \tilde{f}]$ then reads

$$S[\phi, \tilde{f}, \tilde{f}] = \sum_\ell \int_0^\beta d\tau \left\{ \frac{1}{U} \sum_r \left[ \frac{\partial \phi_\ell(r)}{\partial \tau} \right]^2 + \frac{2\mu}{U} \sum_r \frac{1}{\tilde{f}_\alpha(r)} \frac{\partial \phi_\ell(r)}{\partial \tau} - \mu \sum_{\alpha r} \tilde{f}_\alpha(r) f_\alpha(r) \right\} + \sum_{\ell\ell'} t_\parallel(r) e^{-i[\phi_\ell(r)-\phi_{\ell+1}(r')] \sum_\alpha \tilde{f}_\alpha(r) f_\alpha(r')} - \sum_{\ell\ell'} t_\perp(r) e^{-i[\phi_\ell(r)-\phi_{\ell+1}(r')] \sum_\alpha \tilde{f}_\alpha(r) f_\alpha(r')} - J \sum_{\ell\ell'} \tilde{B}(r', r') \tilde{B}(r, r')$$

(4)

where $\mu = \nu J U/2$ and $n_f = \langle \tilde{f}_\alpha(r) f_\alpha(r) \rangle$ is the occupation number for $f-$fermions while $\tilde{B}(r, r') = (1/\sqrt{2})[\tilde{f}_{\tau}(r) \tilde{f}_{\tau}(r') - \tilde{f}_{\tau}(r) \tilde{f}_{\tau}(r')]$ is the singlet pair (valence bond) operator $[13]$. The chief merit of the transformation in Eq.4 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, it is only when charge fluctuations become phase coherent the frustration of the kinetic energy is released. On average, the effect of this frustrated motion

is the effective mass enhancement of carriers due to the band narrowing, so that the “dressed” band parameters $t'_{X} = t_{X} \langle e^{i[\phi_\ell(r)-\phi_{\ell+1}(r)]} \rangle$ (where $t_X = t, t', t_\perp$) are used to match electronic spectra of HTSC using low-energy scale $t - J$ model [11]. Typically, in cuprates $t'_{*} \sim 0.5$ eV, $t''/t' \sim 0.15 - 0.35$ and $t'_{*}$ is of order of magnitude smaller than the in-plane hopping parameters [10].

Because for SC system the charge quantization matters, the electromagnetic $U(1)$ group governing the phase field is compact, i.e. $\phi_\ell(r)$ has the topology of a circle ($S_1$). Genuine topological effects can arise due to non-homotopic mappings of the configuration space onto the gauge group $S_1 \to U(1)$. The total time derivative Berry phase [13] imaginary term in Eq.4 is nonzero due to phase field configurations with $\phi_\ell(r) - \phi_{\ell}(r) = 2\pi m_\ell(r)$
where \( m_\ell(r) = 0, \pm 1, \pm 2, \ldots \) marks the U(1) winding (or Chern) number. Therefore, the proper integration measure over \( \phi \) in a multiply-connected domain is then [16]:

\[
\int [D\phi] \ldots = \sum_{\{m_\ell(r)\}} \int_0^{2\pi} \prod_r d\theta_\ell(r) \times \int_{\phi_\ell(r(t)) = \phi_\ell_0(r)} d\phi_\ell(r) \prod_r d\phi_\ell(r) \ldots 
\]

where in each topological sector the integration goes over the gauge potentials with the Chern number equal to \( m_\ell(r) \). This is an important observation since these global topological effects are not encoded in the operator algebra of the original \( c_{\alpha \ell}(r), c_{\alpha \ell}^\dagger r) \) operators.

To address the issue of the phase order we trace over the fermionic degrees of freedom using Eq. [14] to obtain an effective action is the phase field:

\[
S[\phi] = \sum_\ell \int_0^\beta dr \left\{ \sum_r \left[ \frac{1}{U} \phi_\ell^2(r) + \frac{2\mu}{U} 1 \phi_\ell(r) \right] - \sum_{<rr'>} J_\parallel(\Delta) \cos[2\phi_\ell(rr') - 2\phi_\ell(r'r')] - \sum_{<rr'>} J'_\parallel(\Delta) \cos[\phi_\ell(rr') - \phi_\ell(r'r')] - \sum_r J_\perp(\Delta) \cos[2\phi_\ell(rr') - 2\phi_\ell(r+1)(rr')] \right\},
\]

(6)

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

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

(7)

\[
J'_\parallel(\Delta) = -t'\bar{\mu} \int_2^2 dx \frac{\bar{\rho}(x)}{\epsilon(x)} \tanh \left[ \frac{1}{\beta} \epsilon(x) \right],
\]

\[
J_\perp(\Delta) = \frac{4\pi^2 |\Delta|^2}{16} \int_{-2}^2 dx \frac{x^2 \rho(x)}{\epsilon(x)} \left\{ 2 \tanh \left[ \frac{\beta \epsilon(x)}{2} \right] - \beta \epsilon(x) \sech^2 \left[ \frac{\beta \epsilon(x)}{2} \right] \right\}.
\]

Here, we denote \( \epsilon(x) = \sqrt{\mu_1^2 + |\Delta|^2 x^2} \) and \( \rho(x) = (1/\pi^2)K(\sqrt{1 - (x^2/4)}) \) while \( \bar{\rho}(x) = \rho(x) - (2/\pi^2)E(\sqrt{1 - (x^2/4)}) \), where \( K(x) \) and \( E(x) \) are the complete elliptic integrals of the first and second kind, respectively [14]. While \( J_\parallel \) and \( J_\perp \) depend on the square of the corresponding hopping elements, which render them similar to the Josephson pair tunneling amplitudes, the stiffness \( J'_\parallel \) is different: it depends linearly on \( t' \) and governs the process of correlated particle-hole motion. Collective pair (and in general multiple charge) tunneling events are costly for large \( U \), so that excitonic coherent charge transfer dominates the in-plane physics [17]. The inter-plane stiffness \( J_\perp \) is essential, however, in establishing bulk superconductivity via the Josephson coupling. All the stiffnesses in Eq. [7] rest on a gap due to the in-plane momentum space pairing of the \( f \)-fermions induced by AF exchange \( J \) a Gorkov-type decoupling of the valence bond term in Eq. [14] readily gives for the gap parameter \( |\Delta(k)| \)

\[
1 = \frac{J}{N} \sum_k |\cos(k_xa) - \cos(k_ya)|^2 \tanh \left[ \frac{\beta |\Delta(k)|}{2} \right]
\]

(8)

with the quasiparticle spectrum of the \( f \)-fermions, \( E^\pm(k) = [|\epsilon_\perp^+(k)|^2 + |\Delta(k)|^2]^1/2 \) and \( \Delta(k) = \Delta(|\cos(k_xa) - \cos(k_ya)|) \). Obviously, 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. The state with truly off-diagonal long range order is signalled by \( \langle e^{i\phi_\ell(r'r')} \rangle \neq 0 \) marking the macroscopic quantum phase coherence. To proceed, we introduce the unimodular complex scalar \( z_\ell(r') = e^{i\phi_\ell(r')} \) and rewrite the partition function as \( Z = \int [D^2 z] \prod_r \delta \left( |z_\ell(r)|^2 - 1 \right) e^{-S[z,z']}, \) where the unimodularity constraint can be imposed with a real Lagrange multiplier \( \lambda \), so that the effective action reads

\[
S[z,z'] = \frac{1}{\beta NN_\perp \sum_{q\in\Lambda} \sum_{\omega\in\Delta} z(q, \omega) N^{-1}(q, \omega) z(q, \omega) z(q, \omega)}. \]

(9)

Here, \( q \equiv (k_x, k_y) \) and \( N^{-1}(q, \omega) = \lambda - \Sigma(q, \omega) + \gamma_0(q, \omega) \). Subsequently, \( \Sigma_{\tau'}(r, r'; r) \) = \( J_\perp \delta_{\tau'\tau} \delta_{r-r'} \equiv J_\perp \delta_{\tau'\tau} \delta_{r-r'} \), while the \( d_{1st} \) and \( d_{2nd} \) are the lattice vectors connecting nearest neighbors and next-nearest neighbors in the CuO plane, respectively. Furthermore, \( \gamma_0(q, \omega) \) is the Fourier transform of the bare phase correlator \( \langle e^{i[\phi_\ell(r]'(r') - \phi_\ell(r')(r')]} \rangle \) originating from the kinetic and topological part of the action in Eq. [14]. Using Poisson summation formula we obtain

\[
\left( e^{-i[\phi_\ell(r'r) - \phi_\ell(r')(r')]} \right) \left| \right>_0 = \frac{\partial}{\partial \beta} \left( \frac{2\pi \mu}{\beta} + \frac{\pi \beta |\Delta|^2}{\beta} \right) \left( \frac{2\pi \mu}{\beta} e^{-2\pi^2 \beta |\Delta|^2} \right) \times \exp \left( \frac{-U}{\beta} \left( |\tau | - |\tau' | - \frac{(\tau - \tau')^2}{\beta} \right) \delta_{\tau'\tau} \delta_{\ell'\ell} \right). \]

(10)
be obtained after a Legendre transformation. The resulting temperature-chemical potential phase diagram is depicted in Fig.1. First, it shows that $T_c$ correlates with the diagonal hopping $t'$ in accord with the observation that the next-nearest-neighbor hopping dominates the variation of the maximum $T_c$ in hole doped cuprates\cite{15}. Further, the phase diagram in Fig.1 exhibits the special point at $\mu_c$ defined by $2\mu_c/U = 1/2$ away from the incompressible Mott state at $2\mu_c/U = 1$ from which the superconducting lobe emanates. In cuprates there is clear evidence for the existence of a special doping point $x_c$ in the lightly-overdoped region where superconductivity is most robust. Such behavior indicates this point could be a QCP while the associated critical fluctuations might be responsible for the unconventional normal state behavior \cite{16}. However, the resemblance to a conventional QCP is incomplete due to the lack of any clear signature of thermodynamic critical behavior: a QCP is generally the endpoint of a line of phase transition. Experiments appear to exclude any broken symmetry around this point although a sharp change in transport properties is observed \cite{19} and $\partial \mu_c/\partial x$ becomes vanishingly small due to slow chemical potential shift implying a divergence of charge susceptibility \cite{20}. We argue that due topological excitations indeed such a singularity arises at $\mu_c$ in the local charge susceptibility $\chi_c = \partial n_c/\partial \mu$ where $n_c \equiv \langle \tilde{c}_{\alpha}(\mathbf{r})c_{\alpha}(\mathbf{r}) \rangle$ is the electron filling. From Eq.\ref{eq:1} we readily obtain that $n_c = n_f + n_b - 2\mu_c/U$ where the topological contribution is given by $n_b = 2\mu_c/U - (2/iU)\langle \phi(\mathbf{r}) \rangle$. In the large-$U$ limit $\mu \rightarrow n_fU/2$ so that $n_c \rightarrow n_b$, which means, via Eq.\ref{eq:2}, that for strong correlations $n_e$ is governed by the topological winding numbers rather then the number of fermionic oscillators. However, the winding number is a topologically conserved quantity and is “protected” against the small changes of $\mu$. Being an integer it can not change at all if it has to change continuously. For substantial perturbations the ground state crosses over abruptly to other eigenstates: $n_b$ can change only when level degeneracies occur which happens at isolated discrete values of $2\mu_c/U$.

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