Nexus between quantum criticality and the chemical potential pinning in high-$T_c$ cuprates

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For strongly correlated electrons the relation between total number of charge carriers $n_e$ and the chemical potential $\mu$ reveals for large Coulomb energy the apparently paradoxical pinning of $\mu$ within the Mott gap, as observed in high-$T_c$ cuprates. By unravelling consequences of the non-trivial topology of the charge gauge U(1) group and the associated ground state degeneracy we found a close kinship between the pinning of $\mu$ and the zero-temperature divergence of the charge compressibility $\kappa \sim \partial n_e / \partial \mu$, which marks a novel quantum criticality governed by topological charges rather than Landau principle of the symmetry breaking.

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The location of the chemical potential $\mu$ is a fundamental issue for theories of doped high-$T_c$ cuprates. However, the understanding of the observed doping dependence of $\mu$ in cuprates remains a puzzle. In the case of LSCO, the angle-resolved photoemission spectroscopy studies [1, 2] have shown that in underdoped samples, the chemical potential is pinned above the top of the lower Hubbard band. The photoemission measurements of core levels also shows that $\mu$ does not move with hole doping in the underdoped region [3]. The observed shift in the chemical potential as a function of the electron density $n_e$ is related to the charge compressibility $\kappa$ or the charge susceptibility $\chi_e$ via $\kappa^{-1} = (1/n_e)(\partial \mu / \partial n_e)$ and $\chi_e = \partial n_e / \partial \mu$, respectively. In Fermi liquid theory (FLT) the parameter $\kappa$ is proportional to the effective mass $m^*$ of the quasiparticles, thus the absence of a shift $(\kappa \rightarrow \infty)$, quite peculiar from the viewpoint of the rigid-band model, would imply the divergence of the effective mass. The pinning behavior of $\mu$ can be made plausible for a system where charge carriers are segregated, e.g., in a stripe form [4]. However, it is hard to imagine how the property $m^* \rightarrow \infty$ might arise due to inhomogeneities, since the mass enhancement appears to result from the physics of the uniform liquid [5]. Anyway, the behavior of $\mu$ is quite peculiar from the viewpoint of the FLT of the metallic states and signals a dramatic reorganization of the electronic structure of cuprates with doping.

Given the fact that the electron density appears (besides the temperature $T$) as a control parameter, it follows from scaling and thermodynamic considerations that the existence of quantum phase transitions [6] and associated zero–temperature quantum critical points might be a part of the physics of high-$T_c$ cuprates. Indeed, in cuprates there is clear evidence for the existence of a special doping point in the lightly-overdoped region where superconductivity is most robust. Such behaviour indicates this point could be a quantum critical point (QCP) while the associated critical fluctuations might be responsible for the unconventional normal state behaviour [7]. However, it is unclear whether this QCP is “truly critical” in the sense that it is characterized by universality and hyperscaling. The resemblance to a conventional QCP is hampered by the lack of any clear signature of thermodynamic critical behavior. Experiments appear to exclude any broken symmetry around this point although a sharp change in transport properties is observed [8].

Understanding these novel phenomena in cuprates are challenging tasks. In the celebrated Hubbard model, which epitomizes the character of strongly correlated electrons the degeneracy of energy states renders the usual perturbation theory inapplicable. However, there is an intimate relation between the ground state degeneracy and the topology of the system- much of the quantum information is encoded in phase relations of the many-body wave function [9]. The non-integrable Berry phase factors [10] of the topological origin that the eigenvectors of the Hubbard Hamiltonian possesses can produce the interference akin to the Aharonov-Bohm effect [11] in an electromagnetic field giving rise to more exotic elementary excitations [12].

In this work, we explore Mott transitions from the non-magnetic insulator to a superconductor induced by doping and show that the process is governed by the topological structure of the electromagnetic compact gauge U(1) group. As a result collective instanton excitations of the phase field (dual to the charge) arise with a great degree of stability, governed by gauge flux changes by an integer multiples of $2\pi$, which labels the ground state degeneracy. The associated abrupt transition between different “vacua” allows us to make link between the unusual behavior of the chemical potential and a novel type of quantum criticality that goes beyond the paradigm of the symmetry breaking.

We consider an effective one–band electronic Hamiltonian on a tetragonal lattice that emphasises strong anisotropy and the presence of a layered CuO2 stacking
sequence in cuprates: \( \mathcal{H} = \mathcal{H}_{t-J} + \mathcal{H}_U + \mathcal{H}_{\perp} \), where
\[
\mathcal{H}_{t-J} = \sum_{\alpha \ell} \left[ -t \sum_{\langle \mathbf{r}, \mathbf{r'} \rangle} c_{\alpha \ell}^{\dagger} (\mathbf{r}) c_{\alpha \ell} (\mathbf{r'}) + \sum_{\langle \mathbf{r}, \mathbf{r'} \rangle} t' c_{\alpha \ell}^{\dagger} (\mathbf{r}) c_{\alpha \ell} (\mathbf{r'}) - \mu \sum_{\mathbf{r}} c_{\alpha \ell}^{\dagger} (\mathbf{r}) c_{\alpha \ell} (\mathbf{r}) \right]
+ \sum_{\ell} \left( \sum_{\langle \mathbf{r}, \mathbf{r'} \rangle} J \left[ S_\mathbf{r} (\mathbf{r}) \cdot S_\mathbf{r} (\mathbf{r'}) - \frac{1}{4} n_{\mathbf{r}} (\mathbf{r}) n_{\mathbf{r}} (\mathbf{r'}) \right] \right). \tag{1}
\]

Here \( \langle \mathbf{r}, \mathbf{r'} \rangle \) denotes summation over the nearest-neighbour and next-nearest-neighbour sites labelled by \( 1 \leq \mathbf{r} \leq N \) within the CuO plane, respectively, with \( t, t' \) being the bare hopping integrals \( t', t > 0 \), while \( 1 \leq \ell \leq N_\perp \) labels copper-oxide layers. The operator \( c_{\alpha \ell}^{\dagger} (\mathbf{r}) c_{\alpha \ell} (\mathbf{r}) \) (annihilates) an electron of spin \( \alpha \) at the lattice site \( (\mathbf{r}, \ell) \), \( S_\mathbf{r} (\mathbf{r}) = \sum_{\alpha \beta} c_{\alpha \ell}^{\dagger} (\mathbf{r}) \sigma_{\alpha \beta}^{\ell} c_{\beta \ell} (\mathbf{r}) \) \((a = x, y, z) \) stands for spin and \( n_{\mathbf{r}} (\mathbf{r}) = n_{t \ell} (\mathbf{r}) + n_{\ell \mu} (\mathbf{r}) \) number operators, respectively, where \( n_{\alpha \ell} (\mathbf{r}) = c_{\alpha \ell}^{\dagger} (\mathbf{r}) c_{\alpha \ell} (\mathbf{r}) \), \( \mu \) is the chemical potential and \( J \) the antiferromagnetic (AF) exchange. The Hubbard term is \( \mathcal{H}_U = \sum_{\mathbf{r} \ell} U n_{t \ell} (\mathbf{r}) n_{\ell \mu} (\mathbf{r}) \) with the on-site repulsion Coulomb energy \( U \), while \( \mathcal{H}_{\perp} = - \sum_{\mathbf{r} \ell} t_\perp (\mathbf{r}) c_{\alpha \ell}^{\dagger} (\mathbf{r}) c_{\alpha \ell+1} (\mathbf{r'}) \) facilitates the interlayer coupling, where \( t_\perp (\mathbf{r}) \) is the interlayer hopping with the \( c-\)axis dispersion \( c_\perp (k_x, k_z) = 2t_\perp (k) \cos (k_z) \), while \( t_\perp (\mathbf{r}) = t_\perp \left[ \cos (ak_x) - \cos (ak_y) \right] \) as predicted on the basis of band calculations.\(^{15}\)

We write the partition function \( Z = \int [\mathcal{D} \mathcal{C} \mathcal{D} \mathcal{E}] e^{-S_\text{tot}[\mathcal{C}, \mathcal{E}]} \) with the action
\[
S_\text{tot}[\mathcal{C}, \mathcal{E}] = \int_0^\beta d\tau \sum_{\alpha \ell \mathbf{r}} \left[ \bar{c}_{\alpha \ell} (\mathbf{r}) \partial_\tau c_{\alpha \ell} (\mathbf{r}) + \mathcal{H} (\mathbf{r}) \right] \tag{2}
\]
using coherent-state fermionic path integral over Grassmann fields depending on the "imaginary time" \( 0 \leq \tau \leq \beta = 1/k_B T \). Further, we write the Hub-

The electromagnetic U(1) group governing the phase field is compact, i.e. \( \phi_\ell (\mathbf{r}) \) has the topology of a circle \( (S_1) \), but topological effects can arise due to non-homotopic mappings of the configuration space onto the gauge group \( S_1 \rightarrow U(1) \). To obtain the complete nature of the physical electron field we write explicitly:
\[
c_{\alpha \ell} (\mathbf{r}) = \exp \left[ i \int_0^\tau d\tau' \bar{V}_{\ell \ell'} (\mathbf{r}) \right] e^{i\phi_\ell (\mathbf{r})} f_{\alpha \ell} (\mathbf{r}). \tag{3}
\]

The first term in the exponential in Eq. 3 is the usual dynamical phase factor where \( \theta_\ell (\mathbf{r}) = \bar{V}_{\ell \ell'} (\mathbf{r}) \) and \( \theta_\ell (\mathbf{r}) = \theta_\ell (\mathbf{r}) \). The second one is the non-integrable Berry phase factor: \( \gamma_{\ell \ell'} (\mathbf{r}) = 2\pi m_\ell (\mathbf{r}) / \beta \), where \( m_\ell (\mathbf{r}) \) marks the integer U(1) winding number. Working backwards we can now formulate the path integral for the partition function. For this we concentrate on closed paths (or world lines) in the imaginary time \( \tau \) that start at position \( \mathbf{r} \) at imaginary time \( \tau = 0 \) and end at the same position at \( \tau = \beta \), which fall into distinct, disconnected (homotopy) classes labelled by the winding number.\(^{16}\)

Homotopically distinct paths can be summed according to various possibilities for inequivalent quantizations (superselection sectors) according to the formula:
\[
Z = \sum_{\{m_\ell (\mathbf{r})\}} \prod_{\mathbf{r} \ell} d\theta_\ell (\mathbf{r}) \int \frac{\phi_\ell (\mathbf{r} \beta) = \phi_\ell (\mathbf{r}) + 2\pi m_\ell (\mathbf{r})}{\phi_\ell (\mathbf{r}) = \phi_\ell (\mathbf{r})} \prod_{\mathbf{r} \ell} d\theta_\ell (\mathbf{r}) \int [\mathcal{D} \mathcal{F} \mathcal{D} \mathcal{F}] e^{-S[\theta, m, \bar{f}, f]},
\]
\[
S[\theta, m, \bar{f}, f] = \sum_{\ell} \int_0^\beta d\tau \left\{ \frac{1}{U} \sum_{\mathbf{r}} \left[ \frac{\partial \theta_\ell (\mathbf{r})}{\partial \tau} + \frac{2\pi}{\beta} m_\ell (\mathbf{r}) \right]^2 + \frac{2\mu}{U} \sum_{\mathbf{r}} \frac{1}{i} \left[ \frac{\partial \theta_\ell (\mathbf{r})}{\partial \tau} + \frac{2\pi}{\beta} m_\ell (\mathbf{r}) \right] + H \left[ \bar{f}_{\alpha \ell} (\mathbf{r}), f_{\alpha \ell} (\mathbf{r}), \theta_\ell (\mathbf{r}), m_\ell (\mathbf{r}) \right] \right\}. \tag{4}
\]
The first order in time derivative term in Eq. (1) is just the
topological action which does not affect the equa-
tion of motions but influences statistics [12]. The gauge
transformation in Eq. (1) introduces phase factor into
the hopping elements of the hamiltonian which frustrate
the motion of the fermionic subsystem. However, when
charge fluctuations become phase coherent is signalled by
\(\langle e^{i\phi_\tau}\rangle \neq 0\) the frustration of the kinetic energy is re-
leased. To proceed, we trace over the fermionic degrees
of freedom in Eq. (4) and introduce the unimodular com-
plex scalar \(z_\tau = e^{i\phi_\tau}\) via another Fadeev-Popov
resolution of unity

\[
1 = \int [D^2z] \prod_{\tau\ell} \delta (|z_\tau(r_\ell)|^2 - 1) \times \Re \left[ z_\tau(r_\ell) - e^{i\phi_\tau(r_\ell)} \right] \Im \left[ z_\tau(r_\ell) - e^{i\phi_\tau(r_\ell)} \right],
\]

(5)

where the unimodularity constraint can be imposed with a real Lagrange multiplier \(\lambda\).

The partition function then becomes

\[
Z = \int [D^2z] \prod_{\tau\ell} \delta (|z_\tau(r_\ell)|^2 - 1) e^{-S[z, z^*]} = \beta^{N_\ell} \sum_{\omega_n} g_{\omega_n} e^{i\omega_n|z_\tau(r_\ell)|^2}\]

The phase-coherence boundary is \(\lambda = \sum_{\omega_n} \Gamma_\lambda(\omega_n)\).

Here, \(q = (k, \ell)\) and at criticality, the condition \(\Gamma_{q_0}^{-1}(\omega_n) = 0\) fixes the Lagrange parameter while

\[
\Gamma_\perp(\omega_n) = \lambda - \Sigma(q, \omega_n) + \gamma^{-1}(\omega_n),
\]

\[
\Sigma(q, \omega_n) = J_\|^{(\perp)}(\Delta) \cos(ak_x) \cos(ak_y)
\]

\[
+ \sum_q \frac{\xi_k}{NN} \Gamma_{q=\omega}(\omega_n) \left[ J_\|^{(\perp)}(\Delta) + J_\perp(\Delta) \cos(ck_z) \right],
\]

(6)

where \(\xi_k = \cos(ak_x) + \cos(ak_y)\) Furthermore, \(\gamma_0(\omega_n)\) is the Fourier transform of the bare phase correlator \(\langle e^{-i\phi_\tau(r_\ell) - \phi_\ell(r_\tau')}\rangle\) originating from the kinematic and
topological part of the action in Eq. (1).

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

(7)

where \(Z_0 = \exp(2\theta^2/\beta)\) and \(\theta \approx 1\) is the Jacoby theta function which is \(\beta\)-periodic in \(\tau\) as well as in the variable \(2\mu/\beta\) and \(\mu\) with the period of unity. The micro-
scope phase stiffnesses to the lowest order in the hopping
amplitudes are given by

\[
J_\|^{(\perp)}(\Delta) = \frac{1}{2} \beta N \sum_{\nu} \left[ \mu_{\nu}^{\perp} + \mu_{\nu}^{\perp} + |\Delta(\nu_\perp)|^2 \right],
\]

(8)

\[
J_\perp(\Delta) = -\frac{\beta}{2} \sum_{\nu_\perp} \frac{\cos(ak_{\nu_\perp})}{\nu_\perp^{\perp} + \mu_{\nu_\perp}^{\perp} + |\Delta(\nu_\perp)|^2},
\]

(9)

where \(\mu_\perp = \mu_\perp(\nu_\perp)\).

The relaxation of the \(\Delta\) parameter \(\lambda\) is the oc-
clusion number for \(\Delta\) and \(\nu_\perp = \pi(2n + 1)/\beta\)
and \(n_\perp = 0, \pm 1, \pm 2\) stand for the Fermi Matsubara frequency.

The stiffnesses in Eq. (1) rest on the “d-wave” pair am-
plitude \(\Delta(\nu_\perp) = |\Delta(\nu_\perp)|\) where \(\eta_\perp = \cos(ak_{\nu_\perp}) - \cos(ak_{\nu_\perp})\) due to the
in-plane momentum space pairing of the \(\nu_\perp\)-fermions. A
Gorkov-type decoupling of the AF exchange term in
Eq. (1) using the valence bond operator \(\pi\) readily gives
for the gap parameter: \(1 = \frac{1}{N} \sum_k \frac{\beta}{2\beta} \tanh \left[ \frac{\beta}{2} \xi_k \right] \) with
the quasiparticle spectrum, \(\xi_k = |\epsilon_k(\nu_\perp) - \mu_\perp|^2 + |\Delta(\nu_\perp)|^2\).

Here, \(\xi_k(\nu_\perp)\) is effective in-plane bond dispersion
due to the frustrated motion of the carriers in the fluctu-
ting “bath” of U(1) gauge potentials, so that the actual
tight-binding parameters are “dressed” ones \(\xi_\perp = \xi_k(\nu_\perp) - \mu_\perp + \mu_\perp\) where \(\xi_\perp = t_X(\nu_\perp) - \phi_\perp(r_\perp)\) is the occupation number
given by the mean value of the winding numbers

\[
n_\perp(\mu) = n_0(\mu) + 1 \sum_{q\omega_n} \Gamma_{q}(\omega_n) \partial_\mu^{-1}(\omega_n)
\]

(10)

FIG. 1: (Color online) The critical temperature \(T_c\) as a func-
tion of the chemical potential \(\mu\) together with the density
plot of the charge susceptibility \(\chi_c \equiv U_c/2\) for \(t^* = 0.5\times\)
and \(t^*/t^* = 0.3\), \(t^*/t^* = 0.01\times\), \(J = 0.15\times\) and \(U = 4\times\). Inset:
\(\chi_c\) and the occupation number \(n_\perp\) for \(T = 0.1\times\).

Inset: \(\chi_c\) and the occupation number \(n_\perp\) for \(T = 0.1\times\).
where we made use of the relation

$$\frac{\partial \theta_3(iv,q)}{\theta_3(iv,q)} = \sum_{m=1}^{\infty} \frac{(-1)^m 4\pi q^m}{1 - q^{2m}} \sinh(2\pi mv). \quad (11)$$

In the limit of strong (weak) correlations \(n_e\) interpolates between topological \(n_b\) (fermionic \(n_f\)) occupation numbers. In the large–\(U\) limit \(\mu \rightarrow n_fU/2\), so that \(n_e \rightarrow n_b\) and the system behaves as governed entirely by U(1) topological charges which play the role of “quasiparticles”. It is straightforward now to calculate the charge compressibility \(\kappa\). The result is given in Fig.1 along with the outcome for the superconducting phase boundary. We see the evolution of \(\kappa\) with decreasing \(n_e\), (i.e. hole doping) 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 \(2\mu/U = .5\) 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, \(\kappa \rightarrow \infty\) implies that the and \(\partial \mu/\partial n_e\) becomes vanishingly small at \(T = 0\) which results in the chemical potential pinning, see Fig.2, where the temperature dependence of \(\mu\) is also shown in the inset. In cuprates \(\mu(T)\) can be accessed via the measurement of the work function [21], the available data for YBCO clearly indicates the temperature behav-

ior of \(\mu\) characteristic for a bosonic system.

To conclude, new type of quantum numbers must be invoked to explain topologically induced QCP in cuprates and the associated pinning of the chemical potential. Topological effects arise as stable, non-perturbative, collective excitations of the phase field (dual to the charge), which carry novel topological characteristics. These are the winding numbers of U(1) group: \(m(n) = \frac{1}{2\pi} \int_0^\beta d\tau \phi(\tau)\) that become topological conserved quantities. It is exactly the appearance of these topological charges that render the system “protected” against small changes of the hamiltonian’s parameters. This novel conservation 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 symmetry group.

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