Quantum phase transitions: from Mott insulators to the cuprate superconductors

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Parent compound of the high temperature superconductors: $\text{La}_2\text{CuO}_4$

Band theory

Half-filled band of Cu 3d orbitals – ground state is predicted by band theory to be a metal.

However, $\text{La}_2\text{CuO}_4$ is a very good insulator
Parent compound of the high temperature superconductors: \( \text{La}_2\text{CuO}_4 \)

**A Mott insulator**

\[
H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j
\]

\( \vec{S}_i \Rightarrow \text{spin operator with angular momentum } S=1/2 \)

Ground state has long-range spin density wave (Néel) order at wavevector \( \mathbf{K} = (\pi, \pi) \)

Spin density wave order parameter:

\[
\langle \vec{\phi} \rangle \neq 0
\]

\[
\vec{\phi} = \eta_i \frac{\vec{S}_i}{S} ; \quad \eta_i = \pm 1 \text{ on two sublattices}
\]
Parent compound of the high temperature superconductors: $\text{La}_2\text{CuO}_4$

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$\vec{S}_i \Rightarrow$ spin operator with angular momentum $S=1/2$

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\( \vec{S}_i \) ⇒ spin operator with angular momentum \( S = 1/2 \)

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\]
Superconductivity in a doped Mott insulator

Introduce mobile carriers of density $\delta$ by substitutional doping of out-of-plane ions e.g. $\text{La}_{2-\delta}\text{Sr}_\delta\text{CuO}_4$

Doped state is a paramagnet with $\langle \tilde{\phi} \rangle = 0$

and also a high temperature superconductor with the BCS pairing order parameter $\langle \Psi_{\text{BCS}} \rangle \neq 0$.

$\Rightarrow$ With increasing $\delta$, there must be one or more quantum phase transitions involving

(i) onset of a non-zero $\langle \Psi_{\text{BCS}} \rangle$

(ii) restoration of spin rotation invariance by a transition from $\langle \tilde{\phi} \rangle \neq 0$ to $\langle \tilde{\phi} \rangle = 0$

First study magnetic transition in Mott insulators..............
Outline

A. Magnetic quantum phase transitions in “dimerized” Mott insulators
   *Landau-Ginzburg-Wilson (LGW) theory*

B. Mott insulators with spin $S=1/2$ per unit cell
   *Berry phases, bond order, and the breakdown of the LGW paradigm*

C. Cuprate Superconductors
   *Competing orders and recent experiments*
A. Magnetic quantum phase transitions in “dimerized” Mott insulators:

Landau-Ginzburg-Wilson (LGW) theory:
Second-order phase transitions described by fluctuations of an order parameter associated with a broken symmetry
M. Matsumoto, B. Normand, T.M. Rice, and M. Sigrist, cond-mat/0309440.
Coupled Dimer Antiferromagnet


\[ S = \frac{1}{2} \text{ spins on coupled dimers} \]

\[
H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j
\]

\[ 0 \leq \lambda \leq 1 \]
$\lambda$ close to 0

Weakly coupled dimers
$\lambda$ close to 0

Weakly coupled dimers

Paramagnetic ground state

$\left\langle \tilde{S}_i \right\rangle = 0$, $\left\langle \tilde{\phi} \right\rangle = 0$

$\frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$
$\lambda$ close to 0

Weakly coupled dimers

Excitation: $S=1$ *triplon*
Weakly coupled dimers

\[ \lambda \text{ close to } 0 \]

\[
\begin{align*}
\lambda & \approx 0 \\
\text{Excitation: } S=1 \text{ triplon}
\end{align*}
\]

\[
\begin{align*}
\Phi &= \frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)
\end{align*}
\]
Weakly coupled dimers

\[ \lambda \text{ close to 0} \]

\[ \downarrow \uparrow - \uparrow \downarrow = 2 \]

Excitation: \( S=1 \) triplon

\[ = \frac{1}{\sqrt{2}} \left( \left| \uparrow \downarrow \right> - \left| \downarrow \uparrow \right> \right) \]
$\lambda$ close to 0

Weakly coupled dimers

\[ \begin{align*}
\downarrow & \uparrow - \uparrow & \downarrow = & \frac{1}{2} \left( \lvert \uparrow \downarrow \rangle - \lvert \downarrow \uparrow \rangle \right) \\
\end{align*} \]

Excitation: $S=1$ triplon
\( \lambda \) close to 0  \hspace{2cm} \text{Weakly coupled dimers}

\[ \frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) \]

Excitation: \( S=1 \) \textit{triplon}
$\lambda$ close to 0

Weakly coupled dimers

$\frac{\omega_{xx}}{2} + \frac{\omega_{yy}}{2} + \frac{c_p^2}{2\Delta} \rightarrow$

Energy dispersion away from antiferromagnetic wavevector $\varepsilon_p = \Delta + \frac{c_x^2 p_x^2 + c_y^2 p_y^2}{2\Delta}$

$\Delta \rightarrow$ spin gap

Excitation: $S=1$ triplon (exciton, spin collective mode)
For quasi-one-dimensional systems, the triplon linewidth takes the exact universal value $1.20 k_B T e^{-\Delta/k_B T}$ at low T. This result is in good agreement with observations in CsNiCl$_3$ (M. Kenzelmann, R. A. Cowley, W. J. L. Buyers, R. Coldea, M. Enderle, and D. F. McMorrow Phys. Rev. B 66, 174412 (2002)) and Y$_2$NiBaO$_5$ (G. Xu, C. Broholm, G. Aeppli, J. F. DiTusa, T.Ito, K. Oka, and H. Takagi, preprint).
Coupled Dimer Antiferromagnet
$\lambda$ close to 1

Weakly dimerized square lattice
Weakly dimerized square lattice

Excitations:
2 spin waves (magnons)

\[ \varepsilon_p = \sqrt{c_x^2 p_x^2 + c_y^2 p_y^2} \]

Ground state has long-range spin density wave (Néel) order at wavevector \( K = (\pi, \pi) \)

spin density wave order parameter: \( \bar{\phi} = \eta_i \frac{\vec{S}_i}{\vec{S}} \); \( \eta_i = \pm 1 \) on two sublattices


Neutron Diffraction Study of the Pressure-Induced Magnetic Ordering in the Spin Gap System TlCuCl$_3$

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Fig. 3. Temperature dependence of the magnetic Bragg peak intensity for $Q = (1,0,-3)$ reflection measured at $P = 1.48$ GPa in TlCuCl$_3$.
$\lambda_c = 0.52337(3)$
M. Matsumoto, C. Yasuda, S. Todo, and H. Takayama,

\[ \lambda_c = 0.52337(3) \]


LGW theory for quantum criticality

Landau-Ginzburg-Wilson theory: write down an effective action for the antiferromagnetic order parameter $\bar{\phi}$ by expanding in powers of $\bar{\phi}$ and its spatial and temporal derivatives, while preserving all symmetries of the microscopic Hamiltonian.

$$S_\phi = \int d^2 x d\tau \left[ \frac{1}{2} \left( (\nabla_x \bar{\phi})^2 + \frac{1}{c^2} (\partial_\tau \bar{\phi})^2 + (\lambda_c - \lambda) \bar{\phi}^2 \right) + \frac{u}{4!} (\bar{\phi}^2)^2 \right]$$

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For $\lambda < \lambda_c$, oscillations of $\bar{\phi}$ about $\bar{\phi} = 0$ constitute the *triplon* excitation.

B. Mott insulators with spin \( S=1/2 \) per unit cell:

*Berry phases, bond order, and the breakdown of the LGW paradigm*
Mott insulator with two $S=1/2$ spins per unit cell
Mott insulator with one $S=1/2$ spin per unit cell
Mott insulator with one $S=1/2$ spin per unit cell

Ground state has Neel order with $\tilde{\phi} \neq 0$
Mott insulator with one $S=1/2$ spin per unit cell

Destroy Neel order by perturbations which preserve full square lattice symmetry e.g. second-neighbor or ring exchange. The strength of this perturbation is measured by a coupling $g$.

Small $g \Rightarrow$ ground state has Neel order with $\langle \tilde{\phi} \rangle \neq 0$

Large $g \Rightarrow$ paramagnetic ground state with $\langle \tilde{\phi} \rangle = 0$
Mott insulator with one $S=1/2$ spin per unit cell

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Possible large $g$ paramagnetic ground state (Class A) with $\langle \tilde{\phi} \rangle = 0$
Mott insulator with one $S=1/2$ spin per unit cell

Possible large $g$ paramagnetic ground state (Class A) with $\langle \phi \rangle = 0$

Such a state breaks the symmetry of rotations by $n\pi / 2$ about lattice sites, and has $\langle \Psi_{\text{bond}} \rangle \neq 0$, where $\Psi_{\text{bond}}$ is the bond order parameter

$$\Psi_{\text{bond}}(i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i \arctan(r_j - r_i)}$$
Mott insulator with one $S=1/2$ spin per unit cell

\[
\Psi = \sum_i \Psi_{\text{bond}}(i)
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$$\Psi_{\text{bond}} (i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i \arctan(r_j - r_i)}$$
Mott insulator with one $S=1/2$ spin per unit cell

Another state breaking the symmetry of rotations by $n\pi/2$ about lattice sites, which also has $\langle \Psi_{\text{bond}} \rangle \neq 0$, where $\Psi_{\text{bond}}$ is the bond order parameter.

$$\Psi_{\text{bond}}(i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i \arctan(r_j - r_i)}$$
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$$\Psi_{\text{bond}}(i) = \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j e^{i\arctan(r_j-r_i)}$$
Resonating valence bonds

Different valence bond pairings resonate with each other, leading to a resonating valence bond liquid, (Class B paramagnet) with $\langle \Psi_{\text{bond}} \rangle = 0$


Such states are associated with non-collinear spin correlations, $Z_2$ gauge theory, and topological order.


Resonance in benzene leads to a symmetric configuration of valence bonds

*(F. Kekulé, L. Pauling)*
Excitations of the paramagnet with non-zero spin

\( \langle \Psi_{\text{bond}} \rangle \neq 0; \text{Class A} \)
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\( S = \frac{1}{2} \) spinons, \( Z_\alpha \), are confined into a \( S = 1 \) triplon, \( \tilde{\phi} \)

\( \tilde{\phi} \sim Z_\alpha \tilde{\sigma}_{\alpha\beta} Z_\beta \)
Excitations of the paramagnet with non-zero spin

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*\( S=1/2 \) spinons, \( z_\alpha \), are confined into a \( S=1 \) triplon, \( \tilde{\phi} \)

\[ \tilde{\phi} \sim z_*^* \tilde{\sigma}_{\alpha \beta} z_\beta \]

*\( S=1/2 \) spinons can propagate independently across the lattice
Quantum theory for destruction of Neel order

Ingredient missing from LGW theory:
Spin Berry Phases

\[ e^{iSA} \]
Quantum theory for destruction of Neel order

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Quantum theory for destruction of Neel order

Discretize imaginary time: path integral is over fields on the sites of a cubic lattice of points $a$. 
Quantum theory for destruction of Neel order

Discretize imaginary time: path integral is over fields on the sites of a cubic lattice of points \( a \)

Recall \( \vec{\phi}_a = 2\eta_a \vec{S}_a \rightarrow \vec{\phi}_a = (0,0,1) \) in classical Neel state;

\( \eta_a \rightarrow \pm 1 \) on two square sublattices ;
Quantum theory for destruction of Neel order

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\[ S. \text{ Sachdev and K. Park, } Annals \text{ of Physics, } 298, \text{ 58 (2002)} \]
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$$2A_{a\mu} \rightarrow 2A_{a\mu} - \gamma_{a+\mu} + \gamma_a$$

Change in choice of $\vec{\phi}_0$ is like a “gauge transformation”

Quantum theory for destruction of Neel order

Discretize imaginary time: path integral is over fields on the sites of a cubic lattice of points $a$

Recall $\phi_a = 2\eta_a S_a \rightarrow \phi_a = (0,0,1)$ in classical Neel state;

$\eta_a \rightarrow \pm 1$ on two square sublattices;

$A_{a\mu} \rightarrow \text{half} \ oriented \ area \ of \ spherical \ triangle$

formed by $\phi_a$, $\phi_{a+\mu}$, and an arbitrary reference point $\phi_0$

$2A_{a\mu} \rightarrow 2A_{a\mu} - \gamma_{a+\mu} + \gamma_a$

Change in choice of $\phi_0$ is like a “gauge transformation”

The area of the triangle is uncertain modulo $4\pi$, and the action has to be invariant under $A_{a\mu} \rightarrow A_{a\mu} + 2\pi$

Quantum theory for destruction of Neel order

**Ingredient missing from LGW theory:**

**Spin Berry Phases**

\[
\exp\left(i \sum_a \eta_a A_{a\tau}\right)
\]

Sum of Berry phases of all spins on the square lattice.

\[
= \exp\left(i \sum_{a,\mu} J_{a\mu} A_{a\mu}\right)
\]

with "current" \(J_{a\mu}\) of static charges \(\pm 1\) on sublattices.
Quantum theory for destruction of Neel order

Partition function on cubic lattice

\[ Z = \prod_a \int d\vec{\phi}_a \delta\left(\vec{\phi}_a^2 - 1\right) \exp\left(\frac{1}{g} \sum_{a,\mu} \vec{\phi}_a \cdot \vec{\phi}_{a+\mu}\right) \]

LGW theory: weights in partition function are those of a classical ferromagnet at a “temperature” \( g \)

Small \( g \) ⇒ ground state has Neel order with \( \langle \vec{\phi} \rangle \neq 0 \)

Large \( g \) ⇒ paramagnetic ground state with \( \langle \vec{\phi} \rangle = 0 \)
Quantum theory for destruction of Neel order

Partition function on cubic lattice

$$Z = \prod_a \int d\vec{\varphi}_a \delta\left(\vec{\varphi}_a^2 - 1\right) \exp\left(\frac{1}{g} \sum_{a,\mu} \vec{\varphi}_a \cdot \vec{\varphi}_{a+\mu} + i \sum_a \eta_a A_{a\tau}\right)$$

Modulus of weights in partition function: those of a classical ferromagnet at a “temperature” $g$

Small $g \Rightarrow$ ground state has Neel order with $\langle \vec{\varphi} \rangle \neq 0$

Large $g \Rightarrow$ paramagnetic ground state with $\langle \vec{\varphi} \rangle = 0$

Berry phases lead to large cancellations between different time histories $\Rightarrow$ need an effective action for $A_{a\mu}$ at large $g$

Simplest large $g$ effective action for the $A_{a\mu}$

\[ Z = \prod_{a,\mu} \int dA_{a\mu} \exp \left( \frac{1}{2e^2} \sum \cos \left( \Delta_\mu A_{a\nu} - \Delta_\nu A_{a\mu} \right) + i \sum \eta_a A_{a\tau} \right) \]

with $e^2 \sim g^2$

This is compact QED in 3 spacetime dimensions with static charges $\pm 1$ on two sublattices.

Analysis by a duality mapping shows that this theory is *always* in a phase with $\langle \Psi_{\text{bond}} \rangle \neq 0$ (Class A paramagnet).

The gauge theory is in a *confining* phase (spinons are confined and only $S=1$ triplons propagate).

Proliferation of monopoles in the presence of Berry phases.


Ordering by quantum fluctuations
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Phase diagram of $S=1/2$ square lattice antiferromagnet

Neel order
\[
\langle \tilde{\phi} \rangle \sim \langle z^*_\alpha \tilde{\sigma}_{\alpha\beta} z_\beta \rangle \neq 0
\]

Bond order $\langle \Psi_{\text{bond}} \rangle \neq 0$
(associated with condensation of monopoles in $A_\mu$),
\[
S = 1/2 \text{ spinons } z_\alpha \text{ confined},
\]
\[
S = 1 \text{ triplon excitations}
\]

Second-order critical point described by
\[
S_{\text{critical}} = \int d^2x d\tau \left[ |(\partial_\mu - iA_\mu)z_\alpha|^2 + r |z_\alpha|^2 + \frac{u}{2} (|z_\alpha|^2)^2 + \frac{1}{4e^2} (\partial_\mu A_\nu - \partial_\nu A_\mu)^2 \right]
\]
at its critical point $r = r_c$, where $A_\mu$ is non-compact

Bond order in a frustrated $S=1/2$ XY magnet


First large scale (> 8000 spins) numerical study of the destruction of Neel order in a $S=1/2$ antiferromagnet with full square lattice symmetry

\[
H = 2J \sum_{\langle ij \rangle} \left( S_i^x S_j^x + S_i^y S_j^y \right) - K \sum_{\langle ijkl \rangle} \left( S_i^+ S_j^- S_k^+ S_l^- + S_i^- S_j^+ S_k^- S_l^+ \right)
\]
Mott insulators with spin $S=1/2$ per unit cell:

*Berry phases, bond order, and the breakdown of the LGW paradigm*

*Order parameters/broken symmetry*  
+  
*Emergent gauge excitations, fractionalization.*
C. Cuprate superconductors:
*Competing orders and recent experiments*
Minimal LGW phase diagram with $\bar{\phi}$ and $\Psi_{BCS}$

Quantum phase transitions

- **Paramagnetic Mott Insulator**
  - $\langle \bar{\phi} \rangle = 0$, $\langle \Psi_{BCS} \rangle = 0$

- **Magnetic Mott Insulator**
  - $\langle \bar{\phi} \rangle \neq 0$, $\langle \Psi_{BCS} \rangle = 0$

- **Superconductor**
  - $\langle \bar{\phi} \rangle = 0$, $\langle \Psi_{BCS} \rangle \neq 0$

- **Magnetic Superconductor**
  - $\langle \bar{\phi} \rangle \neq 0$, $\langle \Psi_{BCS} \rangle \neq 0$

La$_2$CuO$_4$
Quantum phase transitions

Minimal LGW phase diagram with $\bar{\phi}$ and $\Psi_{BCS}$

- $\langle \bar{\phi} \rangle = 0$, $\langle \Psi_{BCS} \rangle = 0$
  - Paramagnetic Mott Insulator

- $\langle \bar{\phi} \rangle = 0$, $\langle \Psi_{BCS} \rangle \neq 0$
  - Superconductor

- $\langle \bar{\phi} \rangle \neq 0$, $\langle \Psi_{BCS} \rangle = 0$
  - Magnetic Mott Insulator

- $\langle \bar{\phi} \rangle \neq 0$, $\langle \Psi_{BCS} \rangle \neq 0$
  - Magnetic Superconductor

La$_2$CuO$_4$

High temperature superconductor

Spin density wave order $K \neq (\pi, \pi)$

Spirals... Shraiman, Siggia
Stripes... Zaanen, Kivelson...
Quantum phase transitions

Paramagnetic Mott Insulator

\[ \langle \phi \rangle = 0, \langle \Psi_{BCS} \rangle = 0 \]

Magnetic Mott Insulator

\[ \langle \phi \rangle \neq 0, \langle \Psi_{BCS} \rangle = 0 \]

La\textsubscript{2}CuO\textsubscript{4}
Quantum phase transitions

\[
\langle \phi \rangle = 0, \quad \langle \Psi_{BCS} \rangle = 0
\]

\[
\langle \phi \rangle \neq 0, \quad \langle \Psi_{BCS} \rangle = 0
\]

Paramagnetic Mott Insulator

Magnetic Mott Insulator

Bond order

Neel order

La\_2CuO\_4
Large N limit of a theory with Sp(2N) symmetry: yields existence of bond order and \( \delta \)-wave superconductivity

Magnetic, bond and superconducting order

Bond order

Neel order

La$_2$CuO$_4$

Localized holes

Large $N$ limit of a theory with Sp$(2N)$ symmetry: yields existence of bond order and d-wave superconductivity

Scattering off spin density wave order with

$$\langle \vec{S}_i \rangle = \vec{N} \cos(\vec{Q} \cdot \vec{r}_i + \alpha)$$

$$\vec{Q} = 2\pi \left( \frac{1}{2}, \frac{1}{2} \pm \frac{1}{8} \right) \text{ and } 2\pi \left( \frac{1}{2} \pm \frac{1}{8}, \frac{1}{2} \right)$$

At higher energies, semiclassical theory predicts that peaks lead to spin-wave ("light") cones.
Neutron scattering measurements of La_{15/8}Ba_{1/8}CuO_4 (Zurich oxide)

At higher energies, semiclassical theory predicts that peaks lead to spin-wave ("light") cones.

La_{5/3}Sr_{1/3}NiO_4

Ni has $S = 1$; $\mathbf{Q} = 2\pi \left( \frac{1}{2} \pm \frac{1}{6}, \frac{1}{2} \pm \frac{1}{6} \right)$

La$_{5/3}$Sr$_{1/3}$NiO$_4$

Spin waves: $J=15$ meV, $J'=7.5$meV

Scattering off spin density wave order with

$$\langle \vec{S}_i \rangle = \bar{N} \cos(\vec{Q} \cdot \vec{r}_i + \alpha)$$

$$\vec{Q} = 2\pi \left( \frac{1}{2}, \frac{1}{2} \pm \frac{1}{8} \right) \text{ and } 2\pi \left( \frac{1}{2} \pm \frac{1}{8}, \frac{1}{2} \right)$$

At higher energies, semiclassical theory predicts that peaks lead to spin-wave ("light") cones.
Observations in La$_{15/8}$Ba$_{1/8}$CuO$_4$ are very different and do not obey spin-wave model.

Similar spectra are seen in most hole-doped cuprates.

Red lines: triplon excitation of a 2 leg ladder with exchange $J=100$ meV

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Spectrum of a two-leg ladder

J. M. Tranquada et al., cond-mat/0401621
Possible simple microscopic model of bond order

- M. Vojta and T. Ulbricht, cond-mat/0402377
- G.S. Uhrig, K.P. Schmidt, and M. Grüninger, cond-mat/0402659
- M. Vojta and S. Sachdev, unpublished.

J. M. Tranquada et al., cond-mat/0401621
Numerical study of coupled ladder model,
G.S. Uhrig, K.P. Schmidt, and M. Grüninger,
cond-mat/0402659
J. M. Tranquada et al., cond-mat/0401621

G.S. Uhrig, K.P. Schmidt, and M. Grüninger, cond-mat/0402659
I. Theory of quantum phase transitions between magnetically ordered and paramagnetic states of Mott insulators:


B. *S=1/2 square lattice*: Berry phases induce bond order, and LGW theory breaks down. Critical theory is expressed in terms of emergent fractionalized modes, and the order parameters are secondary.
Conclusions

II. Competing spin-density-wave/bond/superconducting orders in the hole-doped cuprates.

• Main features of spectrum of excitations in LBCO modeled by LGW theory of quantum critical fluctuations in the presence of static bond order across a wide energy range.


Conclusions

III. Breakdown of LGW theory of quantum phase transitions with magnetic/bond/superconducting orders in doped Mott insulators?