HTS 2020 Modelling

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Mean-field approximation for a model HTSC cuprate

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Outline

- Introduction
- Electron-lattice effects for cuprates
- Hole superconductivity in parent T′-cuprates
- Model of charge triplets and on-site composite boson
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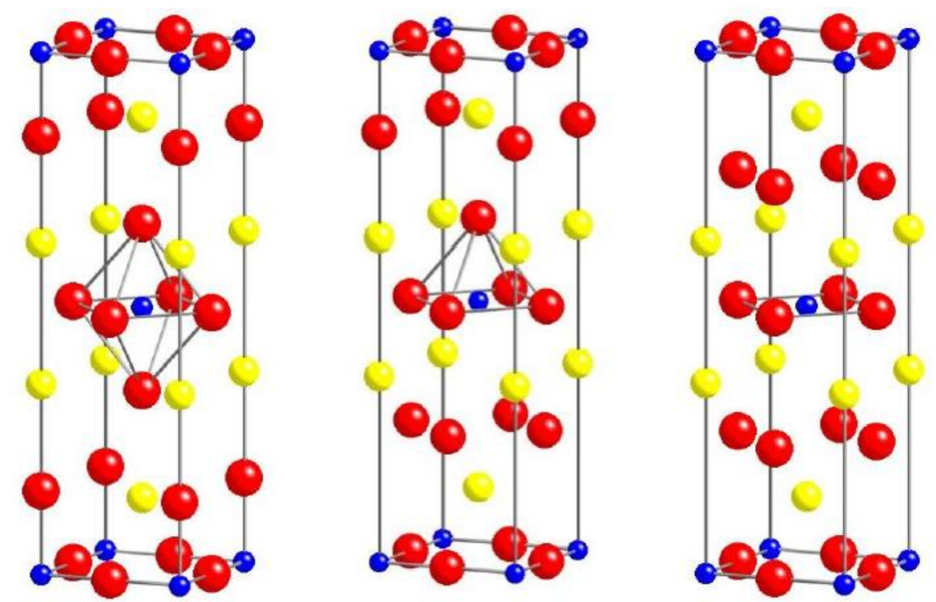
- Fermi-liquid phase
- Large negative-*U* model
- Effective field theory
- Phase diagram for the model cuprate
- Summary

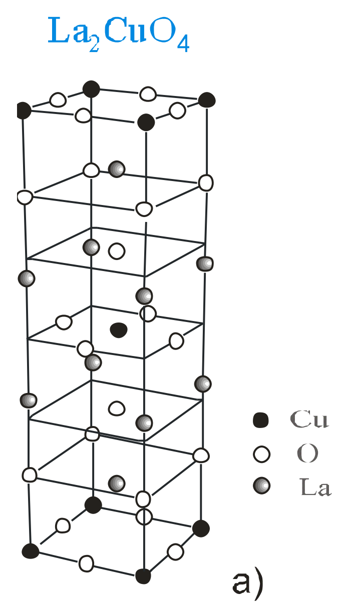
Crystal structure of HTSC cuprates: CuO_4 plaquette as a basic element of crystal and electronic structure

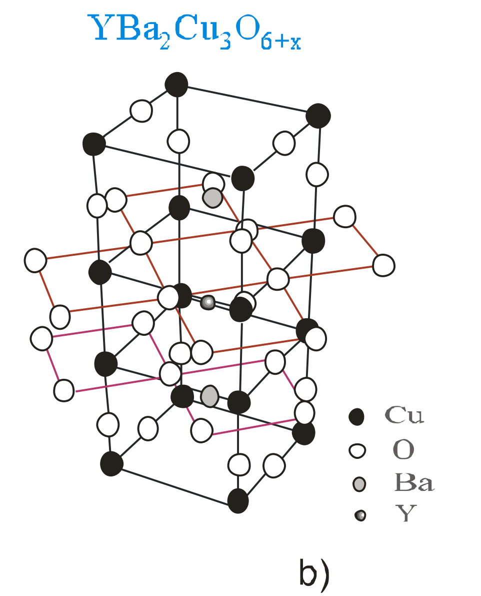


K_2NiF_4 (T) | T^* | Nd_2CuO_4 (T')

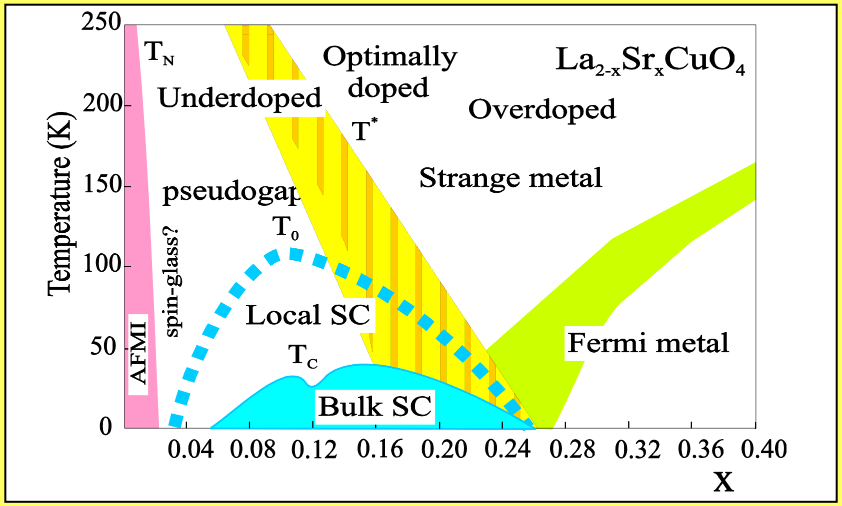
(a) | (b) | (c)

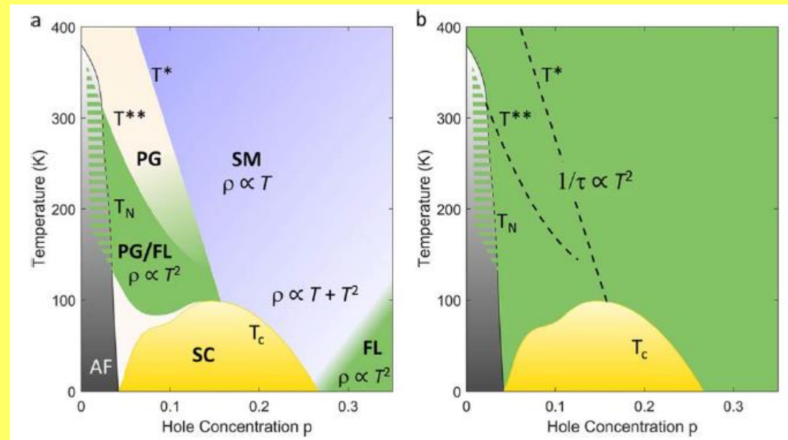
Two-apex | One-apex | No-apex





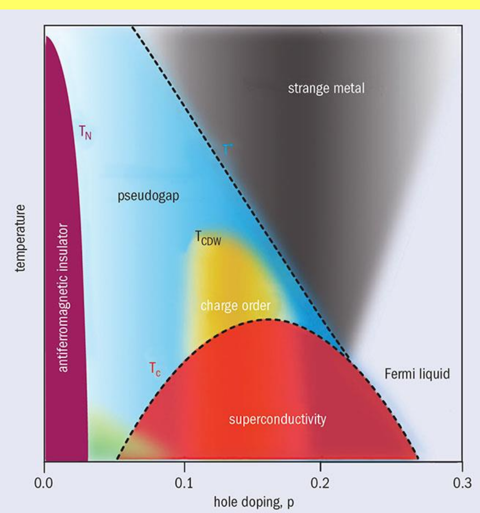
Typical T-x phase diagrams for the hole doped cuprates

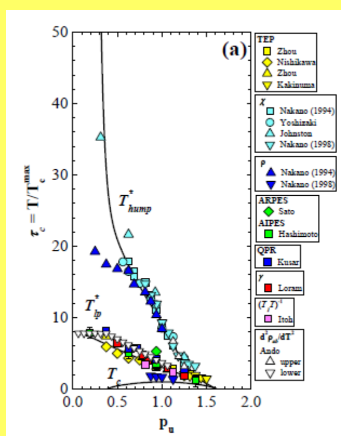




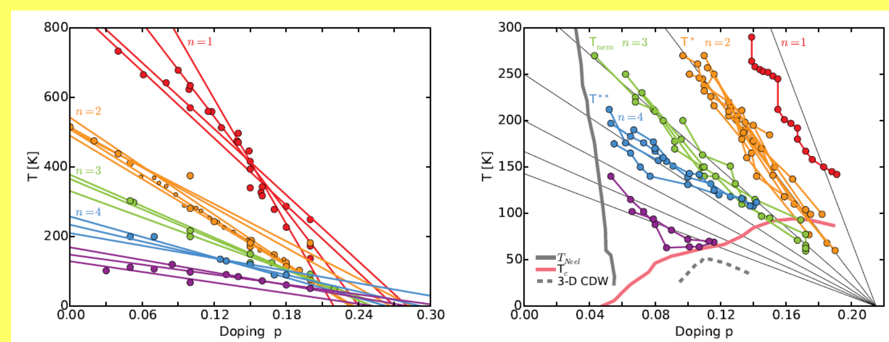
N. Barišić et al., New J. Phys. 21 (2019) 113007

$HgBa_2CuO_{4+\delta}$





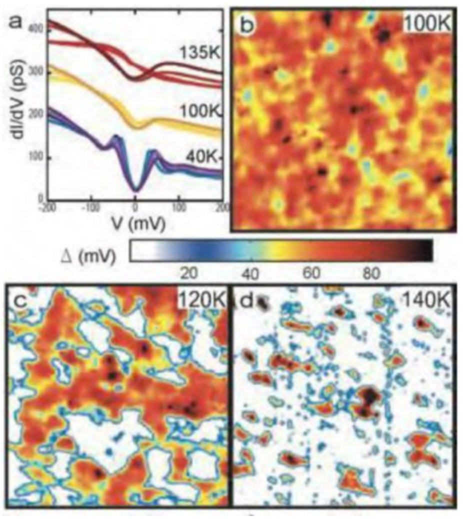
T. Honma and P.H. Hor, PRB 77, 184520 (2008)



$La_{2-x}Sr_xCuO_4$ $YBa_2Cu_3O_{6+\delta}$

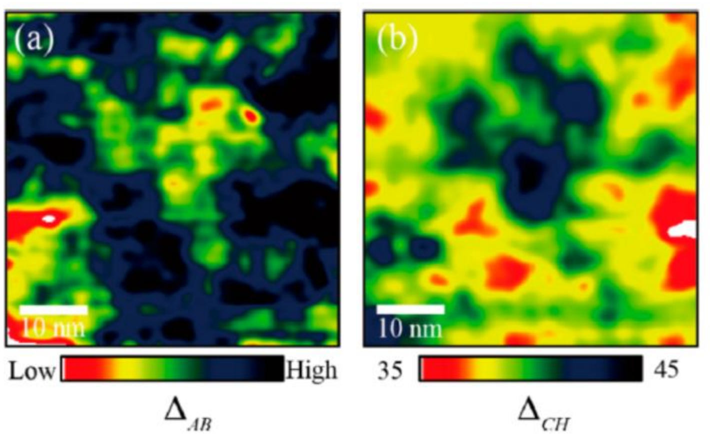
Sacksteder, V. *JSNM* **33,** 43 (2020).

Inhomogeneous nanoscale electronic gaps (INSEG) states



Gap evolution for Bi2212 (Tc=93 K) at different temperatures (Gomes, K. et al. Nature **447**, 569 (2007):)

…we find that pairing gaps nucleate in nanoscale regions above Tc. These regions proliferate as the temperature is lowered, …"



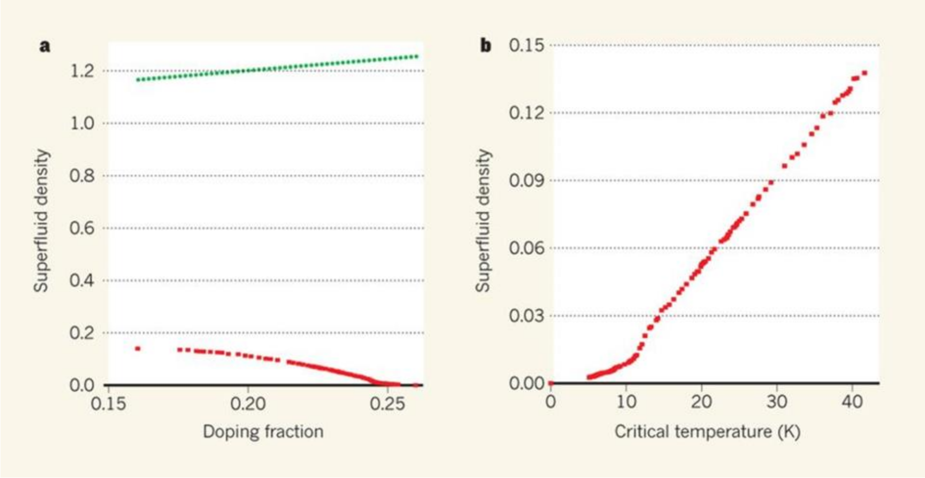
Energy gaps in Bi2212: Scanning tunneling microscopy (STM) against scanning Josephson tunneling microscopy (SJTM)

The gap map revealed by SJTM is anticorrelated to the gap map revealed by the conventional STM method using coherence peaks. This may suggest that the "superconducting gap" defined by coherence peaks cannot simply be assumed to be related to the superconductivity alone (S.H. Joo et al. Nano Lett. 2019, 19, 1112)

T. Honma, P. H. Hor, Physica C 509, 11 (2015):
"… we find that the two pseudogaps are connected to two specific coverages of the CuO2 plane by inhomogeneous nanoscale electronic gaps (INSEG) state: the 50% and 100% coverages of the CuO2 planes by INSEG correspond to the upper and lower pseudogaps, respectively."

Despite many years of tremendous efforts, the problem of unconventional normal and superconducting properties of 2D cuprates remains unsolved … Why?

The fact is that, despite many experimental and theoretical findings, our "superconducting community" cannot refuse the familiar BCS paradigm based on a metallic scenario with a quasiparticle k-momentum description of single-particle states and the search for a "superconducting glue" for the Cooper pairing in k-space



Superfluid density/unit cell for La2-xSrxCuO4 as a function of the doping level (a) and critical temperature (b). Experimental data by red, BCS theory predictions by green.
(I.Bozovic et al., Nature 536, 309 (2016))

Electron-lattice effects do work in cuprate beyond the BCS theory

The exclusion of the BCS mechanism as the main candidate for explaining the HTSC in cuprates does not mean excluding the important, if not decisive, role of the electron-lattice effects for explaining the unusual behavior of cuprates.

The main effect of the electron-lattice interaction in cuprates is not the effect of Cooper pairing, but the effect of suppression of local and nonlocal electron correlations.

Main effect of electron-lattice relaxation which makes parent cuprates as a basis for HTSC

- Anomalously small magnitude of the «thermal» charge transfer (CT) gap, or the electron-hole (EH)-dimer formation energy:

$U_{th} \approx 0.5$ **eV** (T-cuprates), $U_{th} \approx -0.0$ **eV** (T′-cuprates),

as compared with large magnitude of the optical CT gap:

$U_{opt} \approx 2.0$ **eV** (T-cuprates), $U_{opt} \approx 1.5$ **eV** (T′-cuprates)

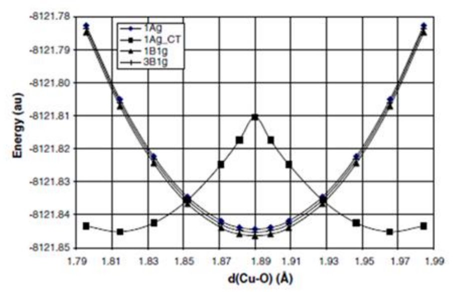
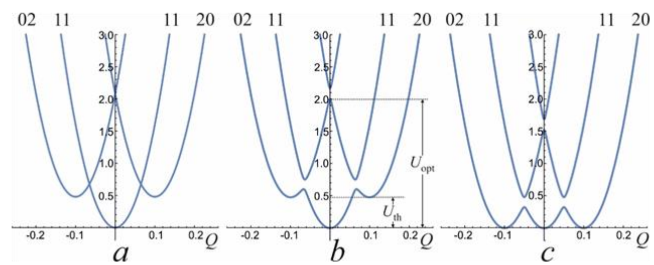


Fig. 1. Calculated PES for the cluster $Cu_4O_{20}^{32-}$ representing a CuO_2 plane.

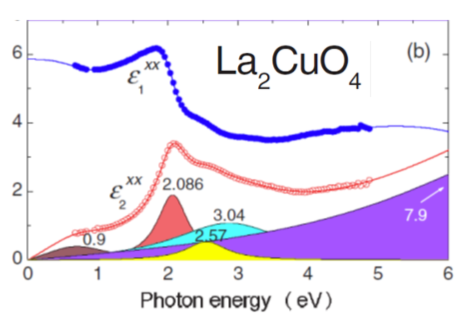
S. Larsson, Physica C 460 1063 (2007)

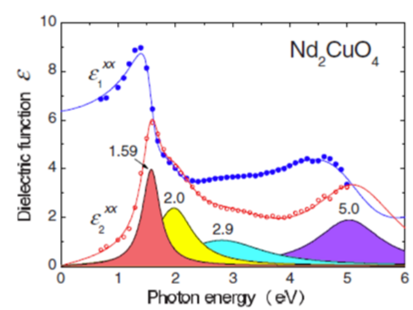


T-cuprates (*a*,*b*): $U_{th} \approx 0.5$ eV

T′-cuprates(*c*): $U_{th} \approx 0$ eV

Optical spectra of parent cuprates: T-La_2CuO_4 and T′-Nd_2CuO_4



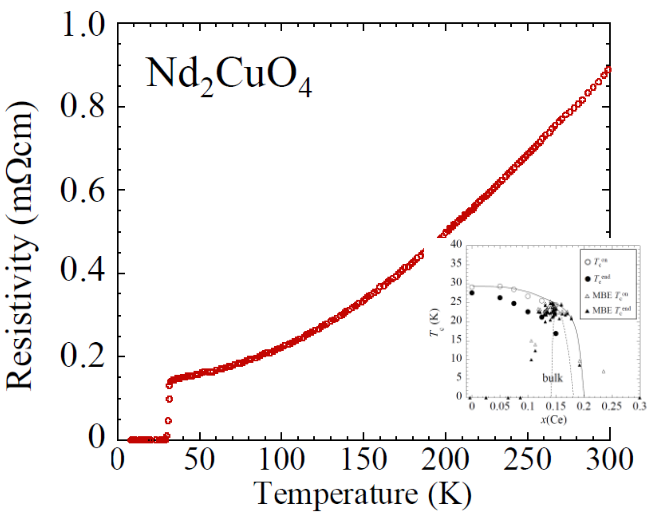


R. V. Pisarev, V. V. Pavlov, A. M. Kalashnikova, A. S. Moskvin, Phys. Rev. B **82**, 224502 2010

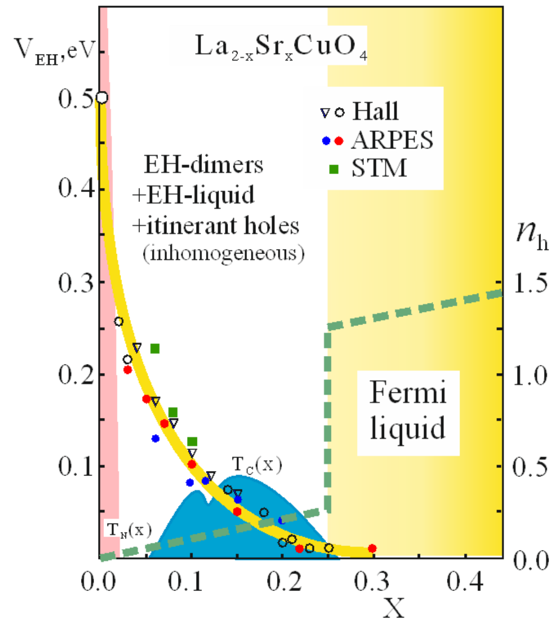
HTSC in parent “true” T′-cuprates vs doping induced HTSC in T-cuprates

T′-puzzle:

unconventional superconductivity in parent “true” T′-cuprate Nd_2CuO_4



M. Naito, Y. Krockenberger, A. Ikeda, H. Yamamoto Physica C: Superconductivity and its Applications **523**, 28 (2016).



Y. Ando, Y. Kurita, S. Komiya, S. Ono, and K. Segawa, Phys. Rev. Lett. **92**, 197001 (2004); S. Ono, Seiki Komiya, and Yoichi Ando, Phys. Rev. B **75**, 024515 (2007).

L.P. Gorkov and G B Teitelbaum, Phys. Rev. Lett. **97** 247003 (2006); J. Phys.: Conf. Ser. **108**, 12009 (2008).

A.S. Moskvin, Phys. Rev. B **84**, 075116 (2011).

Doping dependence of the EH-dimers “dissociation” energy $U^*_{th} = U_{th} + V_{EH}$ in hole-doped cuprates points to its dramatic fall with deviation from half-filling due to a strong screening of the local and nonlocal correlation parameters U_{th} and V_{EH}

Main effect of electron-lattice relaxation which makes parent cuprates as a basis for HTSC

Instability regarding the charge transfer

$$Cu^{2+} + Cu^{2+} \rightarrow Cu^{1+} + Cu^{3+}\ (Cu^{3+} + Cu^{1+}),$$

or rather

$$[CuO_4]^{6-} + [CuO_4]^{6-} \rightarrow [CuO_4]^{7-} + [CuO_4]^{5-}$$

with the disproportionation and formation of the system both of individual and coupled electron $[CuO_4]^{7-}$ and hole $[CuO_4]^{5-}$ centers (EH-dimers)

In other words, all three charge centers $[CuO_4]^{7-,6-,5-}$ (charge triplet) must be considered on equal footing

Charge triplet model for cuprates

Our scenario for 2D cuprates is based on obvious assumption that the low-energy physics is determined by coexistence in the CuO_2 planes of charge triplets formed by the $[CuO_4]^{7-,6-,5-}$ centers (only nominally $Cu^{1+,2+,3+}$). The $[CuO_4]^{7-,6-,5-}$ centers to be many-electron atomic species with strong p-d covalence and strong intra-center correlations cannot be described within any conventional (quasi)particle approach. We combine the three centers into a pseudospin S = 1 triplet following the spin-magnetic analogy proposed by Rice and Sneddon (PRL,1981) to describe the three charge states (Bi^{3+},Bi^{4+},Bi^{5+}) of the bismuth ion in $BaBi_{1-x}Pb_xO_3$ and use the traditional spin algebra.

CuO_4-centers
Charge triplets, spin-charge quartets

Center	cluster	nominal	Pseudospin S=1 projection	Conventional spin	Orbital state
electron	$[CuO_4]^{7-}$	Cu^{1+}	$M_S = -1$	0	A_{1g}
parent	$[CuO_4]^{6-}$	Cu^{2+}	$M_S = 0$	1/2	B_{1g}
hole	$[CuO_4]^{5-}$	Cu^{3+}	$M_S = +1$	0	A_{1g}

On-site “Zhang-Rice” hole boson

- $[CuO_4]^{7-}$ – on-site vacuum state $|0\rangle$
- $[CuO_4]^{6-}$ – b_{1g}-hole; $|b_{1g}\rangle=0.83|d\rangle+0.55|p\rangle$
- $[CuO_4]^{5-}$ – Zhang-Rice singlet
- $|ZR\rangle=(-0.38\,|d^2\rangle+0.82\,|dp\rangle-0.44\,|p^2\rangle)=\hat{B}^{\dagger}\,|0\rangle$
- Two-hole ZR-state forms an on-site composite hole boson with $d^2_{x^2-y^2}$ -symmetry
- $[CuO_4]^{5-}=\hat{B}^{\dagger}[CuO_4]^{7-}; |+1\rangle=\hat{B}^{\dagger}|-1\rangle$

The S=1 spin algebra implies eight independent nontrivial pseudospin operators (and corresponding on-site order parameters)

$$S_0 = S_z; S_\pm = \mp \frac{1}{\sqrt{2}}\left(S_x \pm i S_y\right); S_z^2; T_\pm = \{S_z, S_\pm\}; S_\pm^2$$

For pseudospin systems (semi-hard-core bosons, HTSC cuprates)

$S_\pm, T_\pm$ – "single particle" creation/annihilation operators;

$S_\pm^2$ – "two-particle" creation/annihilation operators;

$\frac{1}{2N}\sum_i \langle S_{iz} \rangle = \Delta n$ – deviation from half-filling

- Novel Fermi-type operators

$$\hat{P}_{\pm} = \frac{1}{2}\left(\hat{S}_{\pm} + \hat{T}_{\pm}\right);\ \hat{N}_{\pm} = \frac{1}{2}\left(\hat{S}_{\pm} - \hat{T}_{\pm}\right)$$

realize transitions

$$Cu^{2+} \leftrightarrow Cu^{3+} \text{ or } Cu^{1+} \leftrightarrow Cu^{2+}$$

These are the creation/annihilation operators for holes ($\hat{P}_{\pm}$) and electrons ($\hat{N}_{\pm}$), respectively, on the vacuum half-filled band.

Then the “single particle” transport can be written as follows

$$H_{kin}^{(1)} = -\frac{1}{2}\sum_{\langle ij\rangle}\left[t^{p}P_{i+}P_{j-} + t^{n}N_{i+}N_{j-} + \frac{1}{2}t^{pn}\left(P_{i+}N_{j-} + N_{i+}P_{j-}\right) + h.c.\right]$$

“Cartesian” hermitian form for pseudospin operators

$$\hat{S}_{\pm}^{2} = \frac{1}{2}\left[\left(\hat{S}_{x}^{2} - \hat{S}_{y}^{2}\right) \pm i\left\{\hat{S}_{x}, \hat{S}_{y}\right\}\right]$$
$$= \hat{B}_{1} \pm i\hat{B}_{2}$$

$$\hat{P}_{\pm} = \frac{1}{2}\left(\hat{P}_{1} \pm i\hat{P}_{2}\right); \;\; \hat{N}_{\pm} = \frac{1}{2}\left(\hat{N}_{1} \pm i\hat{N}_{2}\right)$$

“Vector” form: $\hat{\boldsymbol{B}}\left(\hat{B}_{1}, \hat{B}_{2}\right); \; \hat{\boldsymbol{P}}\left(\hat{P}_{1}, \hat{P}_{2}\right); \; \hat{\boldsymbol{N}}\left(\hat{N}_{1}, \hat{N}_{2}\right)$

Effective spin-pseudospin Hamiltonian

$$\hat{H} = \hat{H}_{pot} + \hat{H}_{kin}^{(1)} + \hat{H}_{kin}^{(2)} + \hat{H}_{ex} \,,$$

$$\hat{H}_{pot} = \sum_{i} (\Delta S_{iz}^2 - \mu S_{iz}) + \frac{1}{2} \sum_{ij} V_{ij} S_{iz} S_{jz} \,,$$

$$\hat{H}_{kin}^{(1)} = - \sum_{i<j} \sum_{\nu} [t_{ij}^{p} \hat{P}_{i+}^{\nu} \hat{P}_{j-}^{\nu} + t_{ij}^{n} \hat{N}_{i+}^{\nu} \hat{N}_{j-}^{\nu} + \frac{1}{2} t_{ij}^{pn} (\hat{P}_{i+}^{\nu} \hat{N}_{j-}^{\nu} + \hat{P}_{i-}^{\nu} \hat{N}_{j+}^{\nu}) + h.c.] \,,$$

$$\hat{H}_{kin}^{(2)} = - \sum_{i<j} t_{ij}^{b} (\hat{S}_{i+}^2 \hat{S}_{j-}^2 + \hat{S}_{i-}^2 \hat{S}_{j+}^2) \,,$$

$$\hat{H}_{ex} = \frac{1}{4} \sum_{i<j} J_{ij} \boldsymbol{\sigma}_i \boldsymbol{\sigma}_j \,,$$

где $\boldsymbol{\sigma} = 2\hat{P}_0 \mathrm{s}$, $\hat{P}_0 = 1 - \hat{S}_z^2$ — оператор локальной спиновой плотности.

"Cartesian" form for spin-pseudospin Hamiltonian

$$\mathcal{H} = \Delta \sum_{i} \hat{S}_{zi}^2 + V \sum_{\langle ij \rangle} \hat{S}_{zi}\hat{S}_{zj} + Js^2 \sum_{\langle ij \rangle} \hat{\boldsymbol{\sigma}}_i \hat{\boldsymbol{\sigma}}_j$$

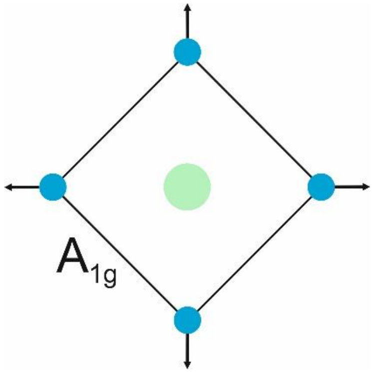
$$- \mathbf{h}s \sum_{i} \hat{\boldsymbol{\sigma}}_i - \mu \sum_{i} \hat{S}_{zi} - \frac{t_b}{2} \sum_{\langle ij \rangle} \hat{\mathbf{B}}_i \hat{\mathbf{B}}_j - \frac{t_p}{2} \sum_{\langle ij \rangle \nu} \hat{\mathrm{P}}_i^{\nu} \hat{\mathrm{P}}_j^{\nu}$$

$$- \frac{t_n}{2} \sum_{\langle ij \rangle \nu} \hat{\mathrm{N}}_i^{\nu} \hat{\mathrm{N}}_j^{\nu} - \frac{t_{pn}}{4} \sum_{\langle ij \rangle \nu} \left(\hat{\mathrm{P}}_i^{\nu} \hat{\mathrm{N}}_j^{\nu} + \hat{\mathrm{N}}_i^{\nu} \hat{\mathrm{P}}_j^{\nu} \right)$$

On-site pseudospin-lattice coupling

- Breathing mode

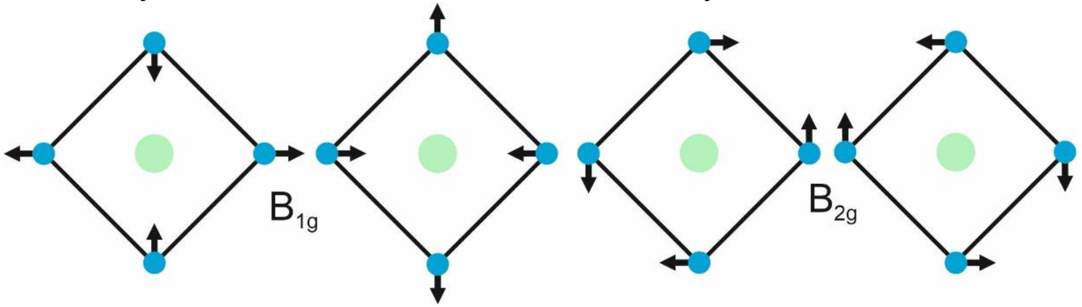
$$\widehat{H}_{e-l}^{(A)} = \sum_i \left(a_1 \hat{S}_{iz} + a_2 \hat{S}_{iz}^2\right) Q_i\left(A_{1g}\right)$$



- Rhombic modes

$$\widehat{H}_{e-l}^{(B)} = b_1 \sum_i \left(\hat{S}_{i+}^2 + \hat{S}_{i-}^2\right) \boldsymbol{Q}_i\left(B_{1g}\right) - i b_2 \sum_i \left(\hat{S}_{i+}^2 - \hat{S}_{i-}^2\right) \boldsymbol{Q}_i\left(B_{2g}\right)$$

$$= b_1 \sum_i \left(\hat{S}_{ix}^2 - \hat{S}_{iy}^2\right) \boldsymbol{Q}_i\left(B_{1g}\right) + b_2 \sum_i \left\{\hat{S}_{ix}, \hat{S}_{iy}\right\} \boldsymbol{Q}_i\left(B_{2g}\right)$$



On-site "lattice" energy

$$H_{lat}^{(A)} = \frac{1}{2}\sum_{i>j} K_{ij}(A_{1g})Q_i(A_{1g})Q_j(A_{1g})$$

$$H_{lat}^{(B)} = \frac{1}{2}\sum_{i>j}\left(K_{ij}(B_{1g})\boldsymbol{Q}_i(B_{1g})\boldsymbol{Q}_j(B_{1g}) + K_{ij}(B_{2g})\boldsymbol{Q}_i(B_{2g})\boldsymbol{Q}_j(B_{2g})\right)$$

Local (on-site) order parameters

- $\Psi = \langle \hat{S}_{\pm}^{2} \rangle = |\Psi| e^{\pm 2i\varphi}$ is the local superconducting order parameter
- $\langle \boldsymbol{\sigma} \rangle$ is the local spin value
- $n = 1 + \langle S_z \rangle$ is the local hole density
- $1 - \langle S_z^2 \rangle$ is the local spin density
- $\langle P_{\pm\mu} \rangle$ is the hole-metallic Caron-Pratt local order parameter $\rightarrow$ metallic *P*-mode
- $\langle N_{\pm\mu} \rangle$ is the electron-metallic Caron-Pratt local order parameter $\rightarrow$ metallic *N*-mode

d-wave bosonic superconductivity

$$\langle \hat{S}_{\pm}^{2} \rangle = \langle \hat{B}_1 \rangle \pm i \langle \hat{B}_2 \rangle$$

$\langle \hat{B}_1 \rangle \propto d_{x^2-y^2}$ or $\langle \hat{B}_2 \rangle \propto d_{xy}$ - modes are stabilized by the on-site electron-lattice interaction.

Local superconducting d-type symmetry order parameter is nonzero only for the "on-site" electron-hole mixtures! In other words, in the hole-doped cuprates the bosonic superconductivity persists if the electron centers (Cu^{1+}) do exist, while in the electron-doped cuprates the bosonic superconductivity persists if the hole centers (Cu^{3+}) do exist!

Particular phase states of effective spin-pseudospin Hamiltonian

- Single-order-parameter phases or “monophases”:

NO, CDW, AFMI, BS, FL

Atomic limit

$$\hat{H}_{pot} = \sum_i (\Delta S_{iz}^2 - \mu S_{iz}) + \frac{1}{2} \sum_{ij} V_{ij} S_{iz} S_{jz}$$

$$\hat{H}_{ex} = \frac{1}{4} \sum_{i<j} J_{ij} \boldsymbol{\sigma}_i \boldsymbol{\sigma}_j \qquad \hat{\boldsymbol{\sigma}} = 2\hat{P}_0 \hat{\boldsymbol{s}}; \;\; \hat{P}_0 = 1 - \hat{S}_z^2$$

$$\hat{H}_{e-l}^{(A)} = \sum_i \left(a_1 \hat{S}_{iz} + a_2 \hat{S}_{iz}^2\right) Q_i\left(A_{1g}\right)$$

- Charge density (pseudospin) waves (CDW) at large negative Δ
- Antiferromagnetic insulator (AFMI) at large positive Δ
- Spin-pseudospin waves (CDW-AFMI)

Atomic limit

- Two-sublattice approximation
- Nearest-neighbors interaction
- Ising approximation for spin exchange
- MFA+MC+Bethe
- Phase diagrams
- Phase separation
- Critical behavior
- Specific heat
- Susceptibility

- J. Phys.: Conf. Ser. 592, 012076 (2015).
- JSNM 29, 1057 (2016).
- JETP 148, 549 (2015).
- JLTP185, 409 (2016)
- JSNM 29, 1077, (2016)
- J. Low Temp. Phys. 187, 646, (2017)
- JETP Lett. 106, (2017) 440 (2017)
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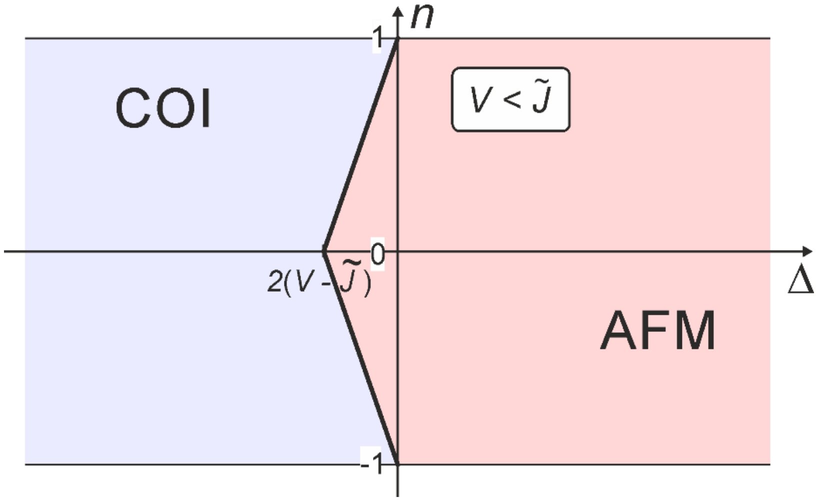
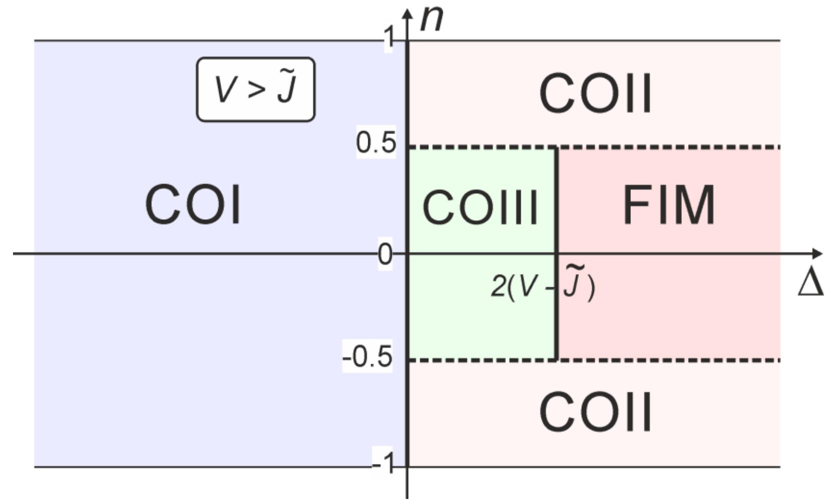
- Acta Physica Polonica A 133, 432 (2018)
- JMMM 477, 162 (2019)
- ФТТ 61, 1676 (2019)
- Acta Physica Polonica A 137, 979 (2020)
- ФТТ 62, 1543 (2020)

Ground state phase diagrams

“Strong” exchange



“Weak” exchange

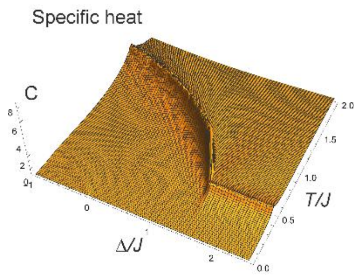


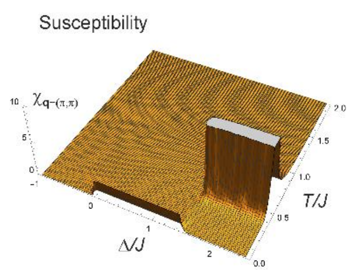
Осн. сост.	$\varepsilon = \langle \mathcal{H} \rangle / N$	$\langle S_z \rangle_j$	$1 - \langle S_z^2 \rangle_j$
COI	$\Delta - 2V(1 - 2\lvert n\rvert)$	$n + (-1)^j (1 - \lvert n\rvert)$	0
COII	$\lvert n\rvert\Delta - 2V(1 - 2\lvert n\rvert)$	$n + (-1)^j (1 - \lvert n\rvert)$	$(1 - \lvert n\rvert)(1 - (-1)^j \operatorname{sgn} n)$
COIII	$(1 - \lvert n\rvert)\Delta - 2V(1 - 2\lvert n\rvert)$	$n + (-1)^j (1 - \lvert n\rvert)$	$\lvert n\rvert - (-1)^j n$
FIM	$\lvert n\rvert\Delta - 2\tilde{J}(1 - 2\lvert n\rvert)$	$n + (-1)^j \lvert n\rvert$	$1 - \lvert n\rvert - (-1)^j n$
AFM	$\lvert n\rvert\Delta - 2\tilde{J}(1 - \lvert n\rvert)^2 + 2n^2 V$	n	$1 - \lvert n\rvert$

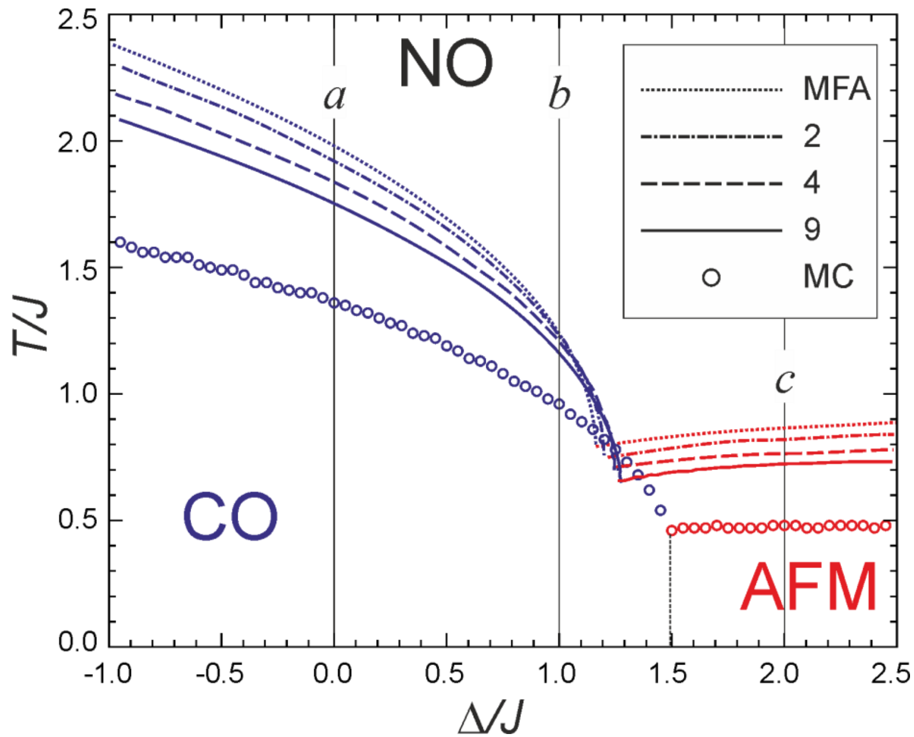
где $j = 0(1)$ для подрешетки A(B).

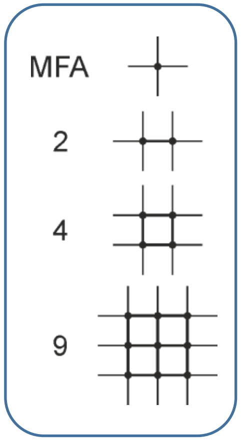
MFA *vs* Monte-Carlo

“Weak” exchange (n=0.1, V/Js^2=4.0)

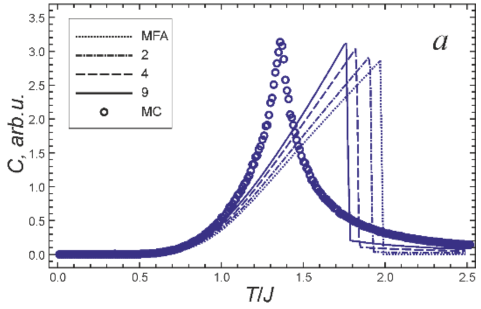


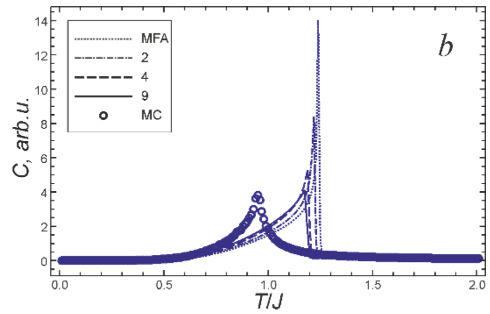


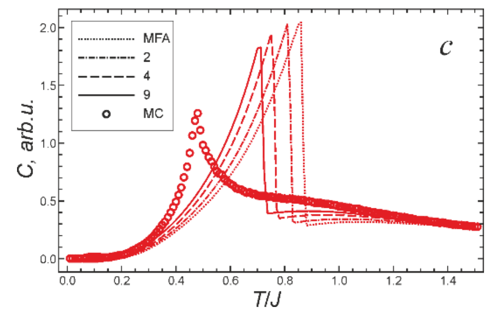




Specific heat

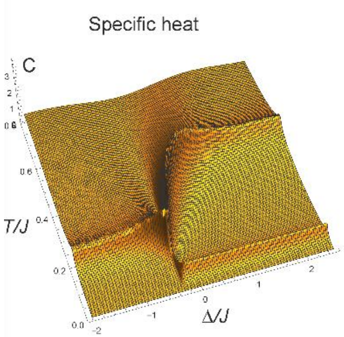


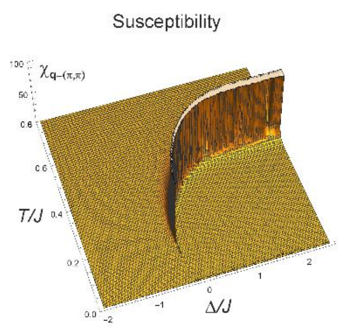


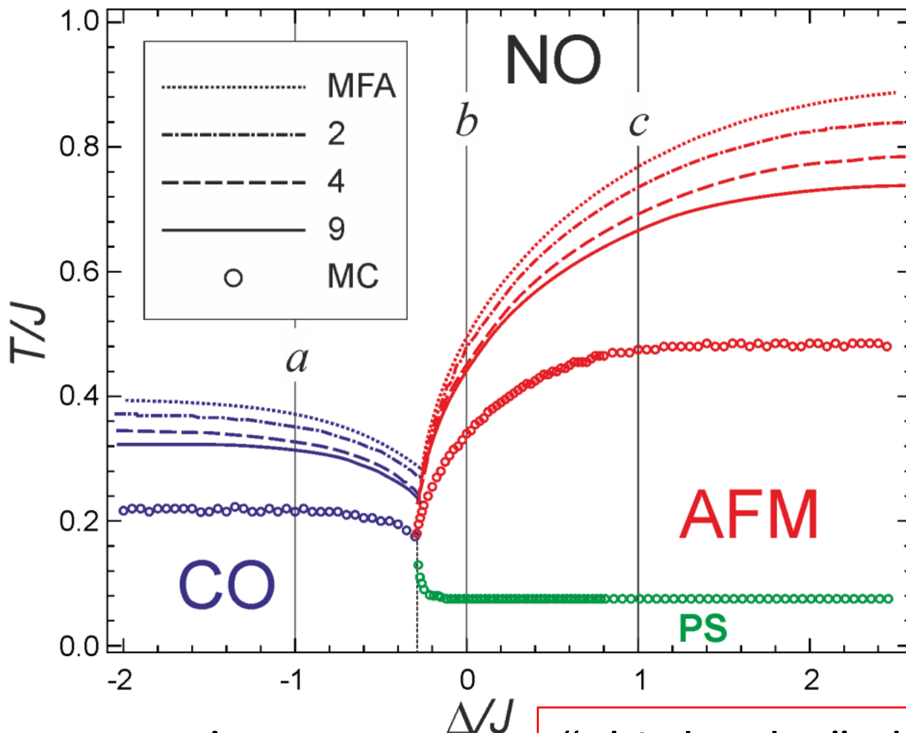


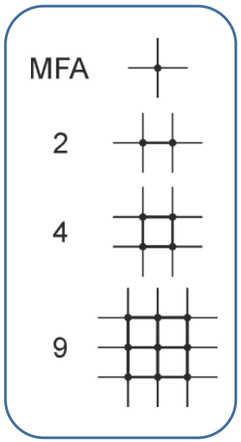
MFA *vs* Monte-Carlo

“Strong” exchange (n=0.1, V/Js^2=0.4)



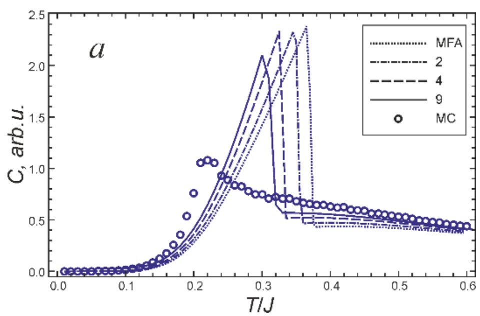


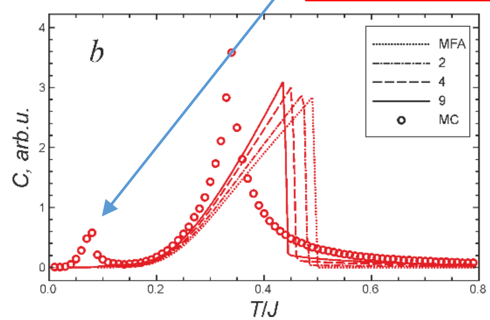


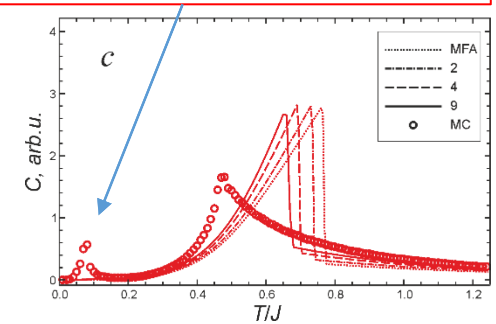


Heat capacity

“Third order” phase transition





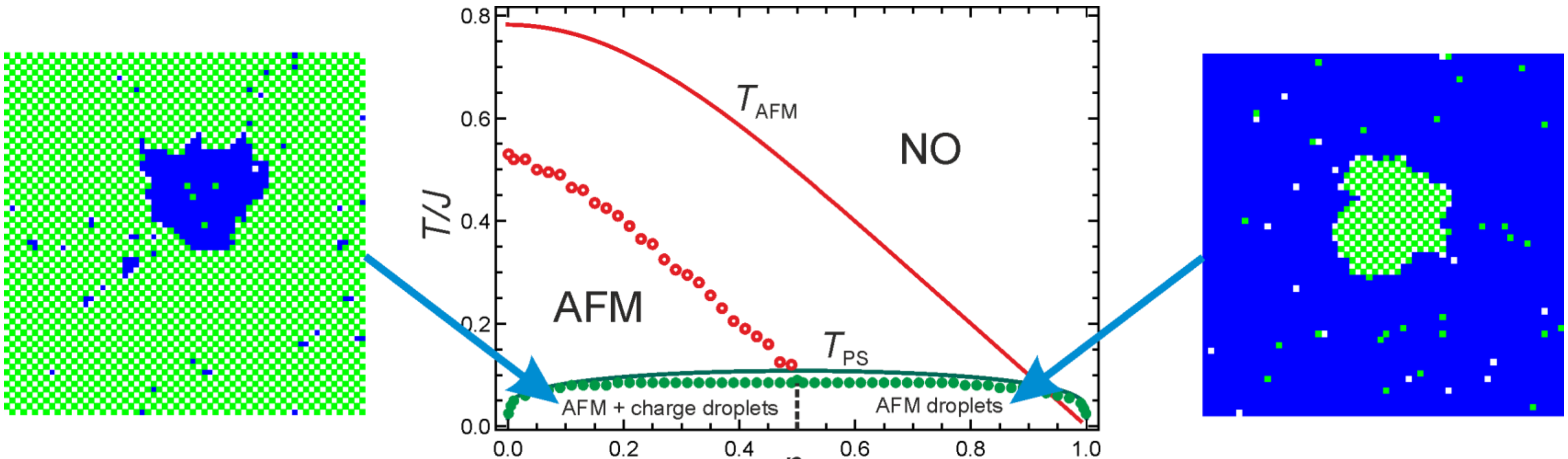


Phase separation (PS)

Maxwell construction: $|n|\, f_C(1) + (1-|n|)\, f_{AFM}(0) = f_{AFM}(n)$

PS temperature: $$T_{PS} = \frac{2|n|\,(1-|n|)\,(V-\tilde{J})}{|n|\ln|n| + (1-|n|)\ln(1-|n|)}$$

The PS exists at n ≠ 0 in the strong exchange limit for all Δ > 0 and T_{PS} does not depend on Δ in agreement with the MC results



Red circles denote the MC results for the maxima of susceptibility due to the AFM ordering, and filled green circles show the maxima of the specific heat at the PS transition. Solid curves show the value of the MFA critical temperature and T_{PS}

Fermi liquid phase of parent and doped cuprate

Half-filled band description for parent cuprate

- Let assume the ground state of the parent cuprate is associated with the half-filled 2D band. In the crudest single-band approximation, the Fermi surface for this band is an array of squares touching at the corners, which can be regarded as containing electrons around Γ-point (0,0) or containing holes around X-point (π, π).

Unconventional Fermi-liquid

- Elementary excitations over the ground state, that is electrons and holes, should be described by Hamiltonian

$$\hat{H}_{FL} = \Delta - \mu \sum_{i\nu} (p_{i\nu} - n_{i\nu}) + \hat{V}_{int} + \hat{H}^{(1)}_{kin}$$

$$\hat{V}_{int} = \sum_{i>j} \sum_{\nu} V_{ij} (p_{i\nu} p_{j\nu} + n_{i\nu} n_{j\nu} - 2 p_{i\nu} n_{j\nu})$$

$$p_{i\nu} = \bar{\hat{P}}^{\nu}_{i+} \hat{P}^{\nu}_{i-} \text{ and } n_{i\nu} = \bar{\hat{N}}^{\nu}_{i-} \hat{N}^{\nu}_{i+}$$

$$\hat{H}^{(1)}_{kin} = -\sum_{i>j} \sum_{\nu} [t^{p}_{ij} \hat{P}^{\nu}_{i+} \hat{P}^{\nu}_{j-} + t^{n}_{ij} \hat{N}^{\nu}_{i+} \hat{N}^{\nu}_{j-} + \frac{1}{2} t^{pn}_{ij} (\hat{P}^{\nu}_{i+} \hat{N}^{\nu}_{j-} + \hat{P}^{\nu}_{i-} \hat{N}^{\nu}_{j+}) + h.c.] ,$$

Unconventional Fermi-liquid

$$\hat{H}^{(1)}_{kin} = \sum_{\mathbf{k}\nu} [\epsilon^{p}_{\mathbf{k}} \hat{P}^{\nu}_{\mathbf{k}+} \hat{P}^{\nu}_{\mathbf{k}-} + \epsilon^{n}_{\mathbf{k}} \hat{N}^{\nu}_{\mathbf{k}+} \hat{N}^{\nu}_{\mathbf{k}-} +$$

$$\frac{1}{2} \epsilon^{pn}_{\mathbf{k}} (\hat{P}^{\nu}_{\mathbf{k}+} \hat{N}^{\nu}_{\mathbf{k}-} + \hat{P}^{\nu}_{\mathbf{k}-} \hat{N}^{\nu}_{\mathbf{k}+}) + h.c.] =$$

$$\sum \hat{\Psi}^{\dagger}_{\mathbf{k}\nu} \hat{H}_{\mathbf{k}} \hat{\Psi}_{\mathbf{k}\nu}$$

$$\epsilon^{p,n,pn}_{\mathbf{k}} = -2t^{p,n,pn}_{1} (\cos k_x + \cos k_y) +$$

$$4t^{p,n,pn}_{2} \cos k_x \cos k_y - 2t^{p,n,pn}_{3} (\cos 2k_x + \cos 2k_y) -$$

$$4t^{p,n,pn}_{4} (\cos 2k_x \cos k_y + \cos 2k_y \cos k_x) \, ,$$

Bosonic hole superconductivity

$$\hat{H}_{pot} = \sum_i (\Delta S_{iz}^2 - \mu S_{iz}) + \frac{1}{2}\sum_{ij} V_{ij} S_{iz} S_{jz}$$

$$\hat{H}_{kin}^{(2)} = -\sum_{i<j} t_{ij}^b (\hat{S}_{i+}^2 \hat{S}_{j-}^2 + \hat{S}_{i-}^2 \hat{S}_{j+}^2)$$

- The Hamiltonian describes a competition of the parent phase ($U=\Delta/2 \to \infty$), charge order and bosonic superconductivity
- BS phase is realized given small positive or negative local correlations

Large-negative-*U* limit: $U=\Delta/2\rightarrow-\infty$

- The system is equivalent to a system of lattice local (hard-core) bosons

$$H_{hc} = -\sum_{\langle ij\rangle} t_{ij}\hat{P}(\hat{b}_i^{\dagger}\hat{b}_j + \hat{b}_j^{\dagger}\hat{b}_i)\hat{P} + \\ + \sum_{\langle ij\rangle} V_{ij} n_i n_j - \mu \sum_i n_i,$$

- The Hamiltonian is equivalent to the Hamiltonian of anisotropic spin s=1/2 magnet in an external field || O_Z

$$H_{hc} = \sum_{\langle ij\rangle} J_{ij}^{xy}(\hat{s}_i^{+}\hat{s}_j^{-} + \hat{s}_j^{+}\hat{s}_i^{-}) + \sum_{\langle ij\rangle} J_{ij}^{z}\hat{s}_i^{z}\hat{s}_j^{z} - \mu\sum_i \hat{s}_i^{z},$$

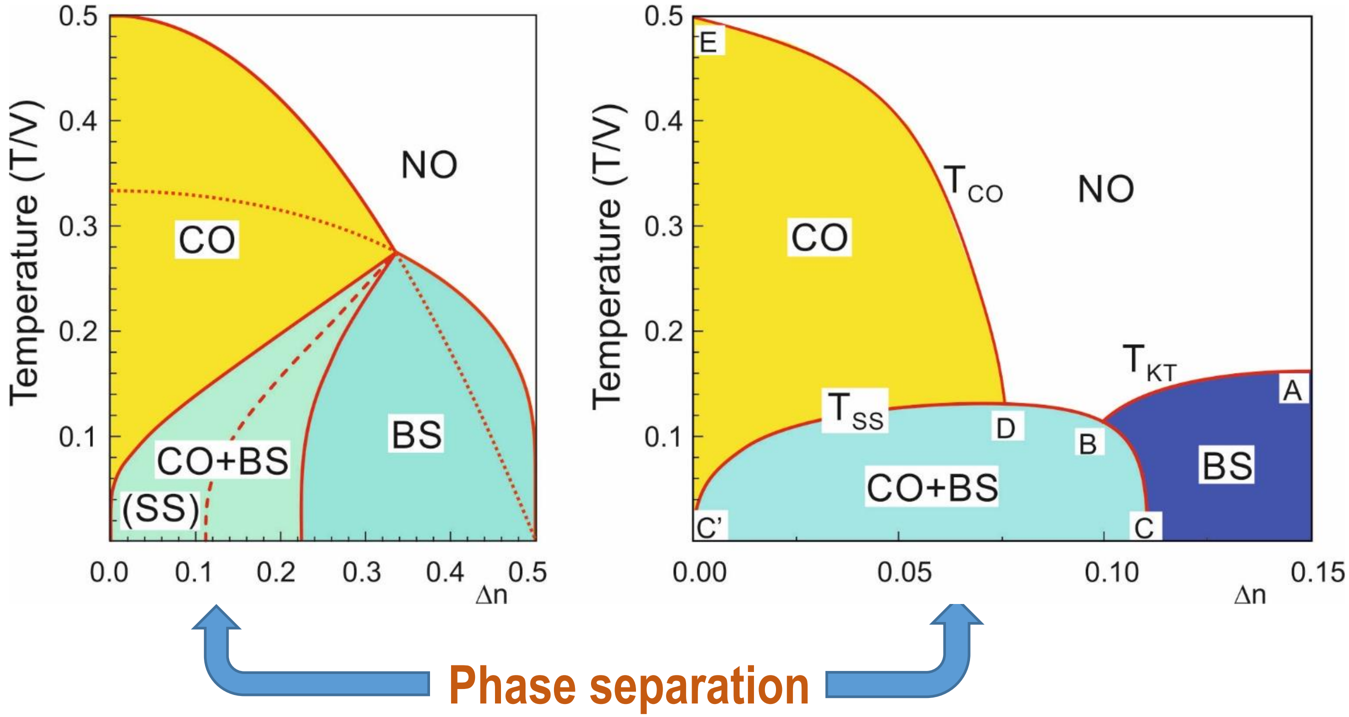
Phase diagram of local (hard-core) bosons (*V=3t*)

MFA

QMC

Micnas et al. RMP, **62**, 1990

Schmid et al. PRL, **88**, 2002



Phase separation turns out to be a typical phenomenon for systems described by particular versions of the model spin-pseudospin Hamiltonian

Effective field theory for spin-pseudospin Hamiltonian

- Nearest neighbors
- Two sublattices (A, B)
- Single-order-parameter phases or "monophases":

NO, CDW, AFMI, BS, FL

- Uniform (14) and staggered (14) order parameters:

$$O_{\pm} = \frac{1}{2}(O_A \pm O_B) = \frac{1}{2\beta}\frac{\partial ln Z_c}{\partial H_{\pm}}$$

$$Z_c = Tr\left(e^{-\beta H_c}\right) = Z_A Z_B$$

Effective field theory for spin-pseudospin Hamiltonian

$$\hat{\mathcal{H}}_0 = \sum_{c=1}^{N/2} \hat{\mathcal{H}}_c, \qquad \hat{\mathcal{H}}_c = \hat{\mathcal{H}}_A + \hat{\mathcal{H}}_B \,,$$

$$\hat{\mathcal{H}}_\alpha = \Delta \hat{S}^2_{z\alpha} - \left(H_z \pm H_z^L\right) \hat{S}_{z\alpha} - \left(\mathrm{h} \pm \mathrm{h}^l\right) \hat{\boldsymbol{\sigma}}_\alpha - \left(\mathrm{h}_b \pm \mathrm{h}_b^L\right) \hat{\mathrm{B}}_\alpha$$
$$- \sum_\nu \left(\mathrm{h}_p^\nu \pm \mathrm{h}_p^{L,\nu}\right) \hat{\mathrm{P}}_\alpha^\nu - \sum_\sigma \left(\mathrm{h}_n^\nu \pm \mathrm{h}_n^{L,\nu}\right) \hat{\mathrm{N}}_\alpha^\nu \,, \quad (46)$$

The variational approach (VA) we employed is based on the Bogolyubov inequality for the grand potential

$$\Omega(H) \leq \Omega(H_0) + (H - H_0)$$

Free energy per site: $f = \frac{\Omega}{N} + \mu n$

$$f = -\frac{1}{2\beta}\ln Z_c + 2V\left(n^2 - L_z^2\right) +$$

$$2Js^2\left(\mathbf{m}^2 - \mathbf{l}^2\right) - t_b\left(\mathbf{B}_0^2 - \mathbf{B}_\pi^2\right) -$$

$$t_p\sum_\nu\left(\mathbf{P}^{\nu\,2} - \mathbf{P}_L^{\nu\,2}\right) - t_n\sum_\nu\left(\mathbf{N}^{\nu\,2} - \mathbf{N}_L^{\nu\,2}\right) -$$

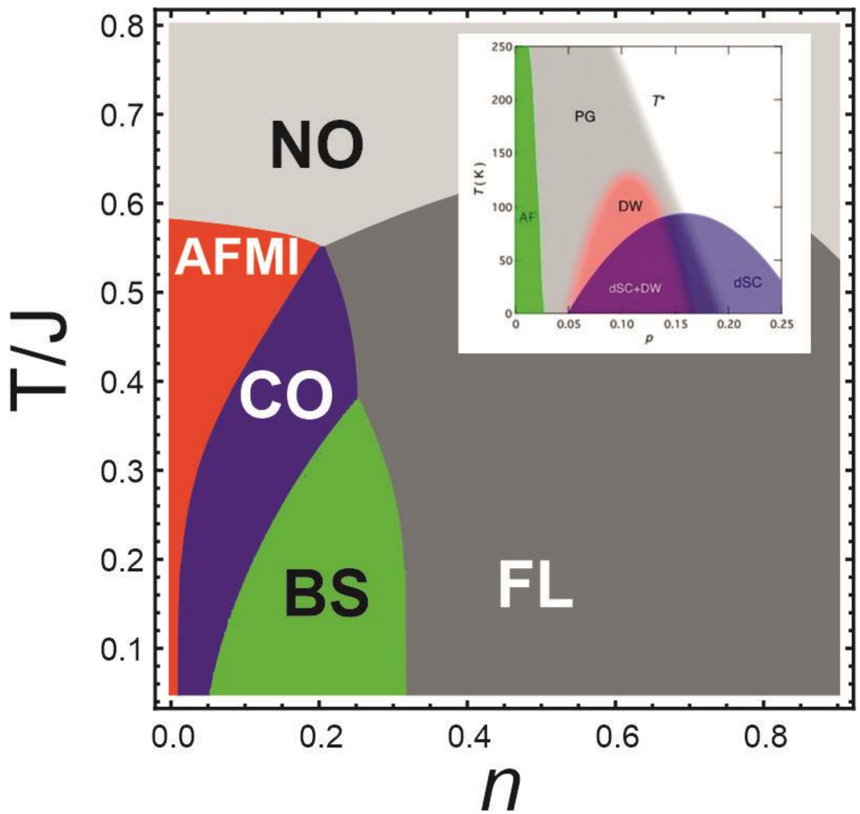
$$t_{pn}\sum_\nu\left(\mathbf{P}^\nu\mathbf{N}^\nu - \mathbf{P}_L^\nu\mathbf{N}_L^\nu\right) +$$

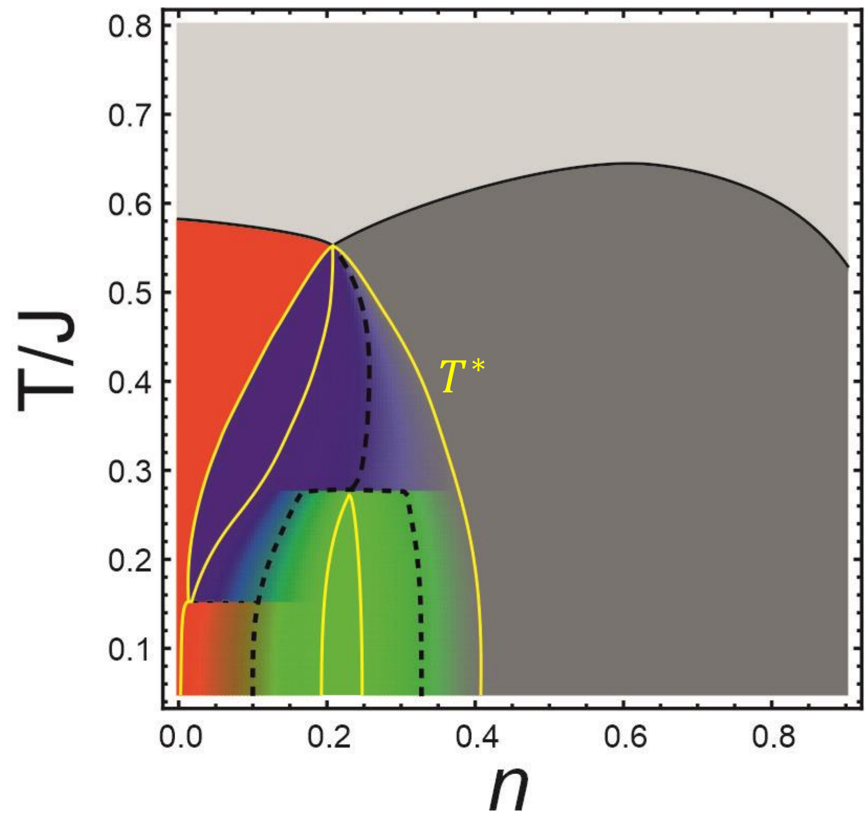
$$H_z n + H_z^L L_z + \mathbf{h}\mathbf{m} + \mathbf{h}^l\mathbf{l} + \mathbf{h}_b\mathbf{B}_0 + \mathbf{h}_b^L\mathbf{B}_\pi +$$

$$\sum_\nu\left(\mathbf{h}_p^\nu\mathbf{P}^\nu + \mathbf{h}_p^{L,\nu}\mathbf{P}_L^\nu + \mathbf{h}_n^\nu\mathbf{N}^\nu + \mathbf{h}_n^{L,\nu}\mathbf{N}_L^\nu\right).$$

By minimizing the free energy, we get a system of site dependent self-consistent VA equations to determine the values of the order parameters

Phase diagram of the model cuprate



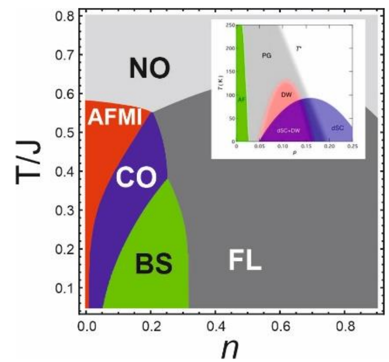


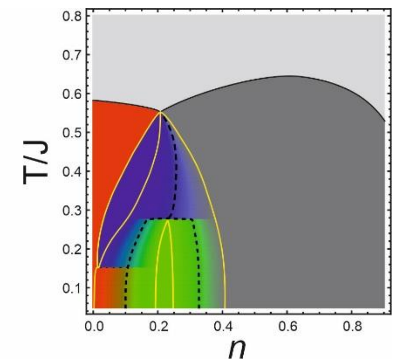
$\Delta = 0.20; V = 0.35;\ t_p = t_n = 0.46;\ t_{pn} = 0.05;\ t_B = 0.65$

(all in units of the exchange integral *J*)

EFT predictions for HTSC cuprates

1. Phase separation: AFMI-BS; CO-BS, CO-FL; BS-FL, T^* but not AFMI-CO
2. T^* is the pseudogap candidate temperature of the third order phase transition which separates the gapless 100% FL phase from the gapped AFMI, CO, and BS phases
3. Pseudogap phase is a phase with static/dynamic phase separation





4. Within the pseudogap phase we predict several characteristic temperatures of the third order and percolation phase transitions

5. Superconducting transition has a percolative nature

Phase separation in HTSC cuprates

SCIENCE ADVANCES | RESEARCH ARTICLE

CONDENSED MATTER PHYSICS

Unusual behavior of cuprates explained by heterogeneous charge localization

D. Pelc[1,2], P. Popčević[3,4], M. Požek[1]*, M. Greven[2]*, N. Barišić[1,2,3]*

Sci. Adv. 2019; **5**: eaau4538

- Pelc et al. argue that the Fermi liquid subsystem in cuprates is responsible for the normal state with angle-resolved photoemission spectra (ARPES), magnetic quantum oscillations, and Fermi arcs, but not for the unconventional superconducting state. In other words, *cuprate superconductivity is not related to the doped hole pairing*, the carriers which exhibit the Fermi liquid behaviour are not the ones that give rise to superconductivity. According to the authors, their model is "comparable to well-known phenomenological approaches in science, such as the Standard Model of particle physics, the Landau theory of phase transitions, and models of population growth". However, the authors could not elucidate the nature of local pairing to be a central point of the cuprate puzzle.

A little bit self-criticism…

- MFA poorly describes quasi-2D systems
- EFT ignores quantum nonlocal correlations
- We limited ourselves to only the nearest neighbors and two sublattices
- We neglected the doping dependent screening for the model parameters
- We took into account only the indirect effect of the electron-lattice coupling
- We neglected the nonuniform potential due to nonisovalent substitution
- We made use of the simplest version of the Caron-Pratt method for the "real-space" description of the single-particle transport
- We considered only single-order-parameter phases
- Etcetera, etcetera …

Summary

- The model of charge triplets provides a self-consistent description of phase diagrams for HTSC cuprates
- HTSC is related with the condensation of **hole on-site composite bosons**, it is not a consequence of pairing of doped holes/electrons
- Main single-order-parameter MFA phases, AFMI, CO, BS, FL coexist in a phase separated state encircled by a third order transition temperature T^* to be a main candidate for the pseudogap temperature
- The Fermi liquid subsystem in cuprates is responsible for the normal state with ARPES, Hall, magnetic quantum oscillations, and Fermi arcs, but not for the unconventional superconducting state.
- However, MFA phases hide a quantum background formed by stable EH-dimers and more complex quantum entities

Thank you for your attention!