Nanoscale Phase-Separation in Magnetic Oxides

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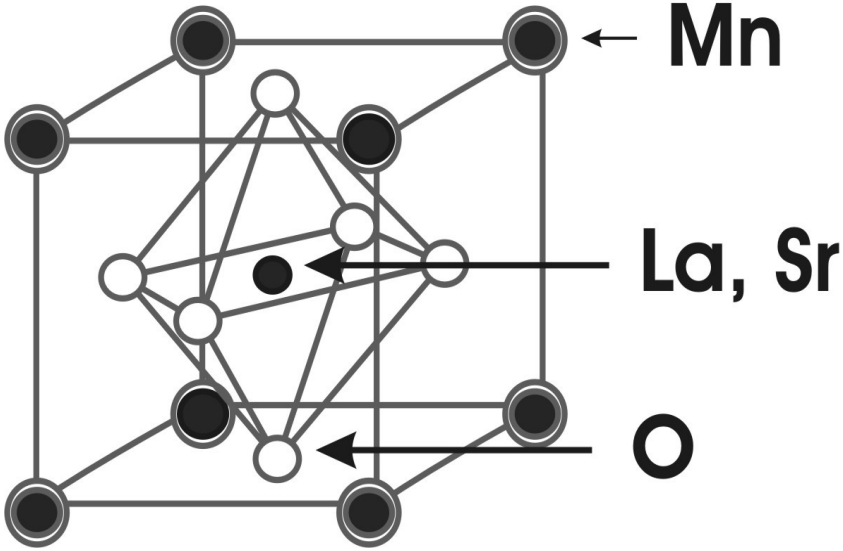
Crystal Structure of Manganites

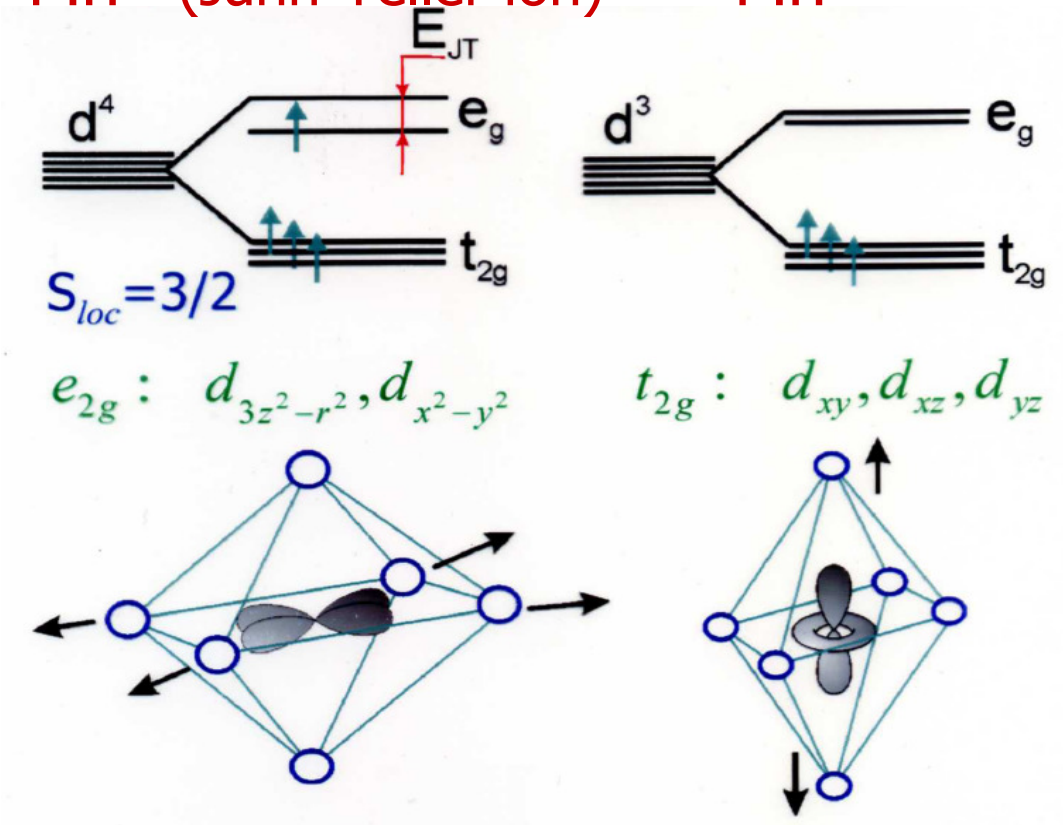
$Ln_{1-x}A_xMnO_3$: Ln = La;Pr;Nd;Sm
A = Ca;Sr;Ba ideal cubic sell



Real structure is slightly orthorombically distorted due to *JT - effect*

Electronic structure

Mn^{3+}(Jahn-Teller ion) Mn^{4+}

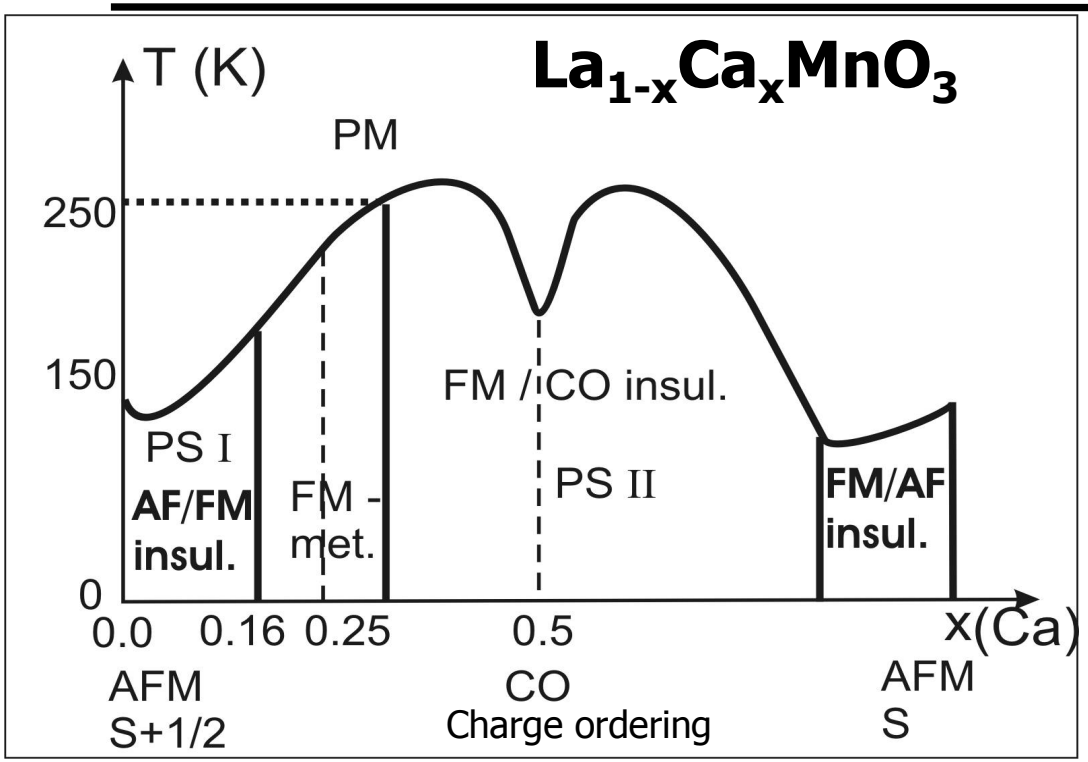


$d_{x^2-y^2}$ octahedra distortion in xy - plane

$d_{3z^2-r^2}$ octahedra distortion along z - axis

As a result Jahn-Teller gap E_{JT} appears.
We assume that E_{JT} is large, so everywhere (except the physics of orbital polaron) only one conduction band is occupied.

Gross Phase-diagram of Manganites



$0 < x < 0.16$ – phase separation (PS) on metallic **FM droplets** inside **AFM** insulating matrix

$x_{opt} = 0.25$ – **FM metal** (CMR)

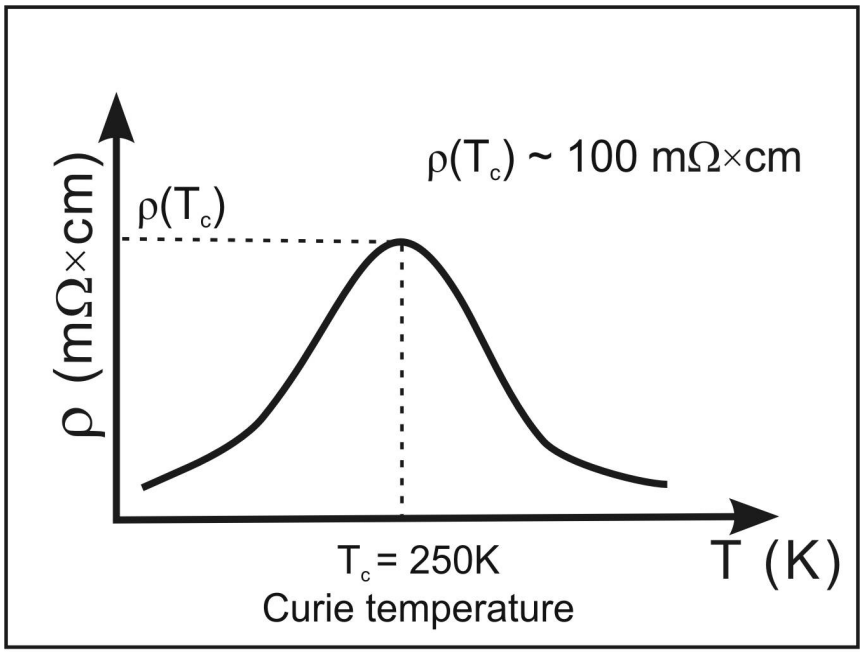
$x = 0.5$ – **charge ordering**

Around $x = 0.5$ - large region of PS on metallic **FM droplets** inside **CO** insulating matrix.

There is also a beautiful physics of orbital ordering which we briefly discuss in this talk for small $x \leq 0.16$.

Resistivity at Optimal Concentration

$x_{opt} = 0.25$ and $T_c = 250K$: **FM → PM transition** *coincides with* **metall → insulator transition**



$$T<T_c:\ \rho \sim \rho_0 + AT^{\beta};\ \ \beta \sim 2.5;\ \ \frac{d\rho}{dT} > 0$$

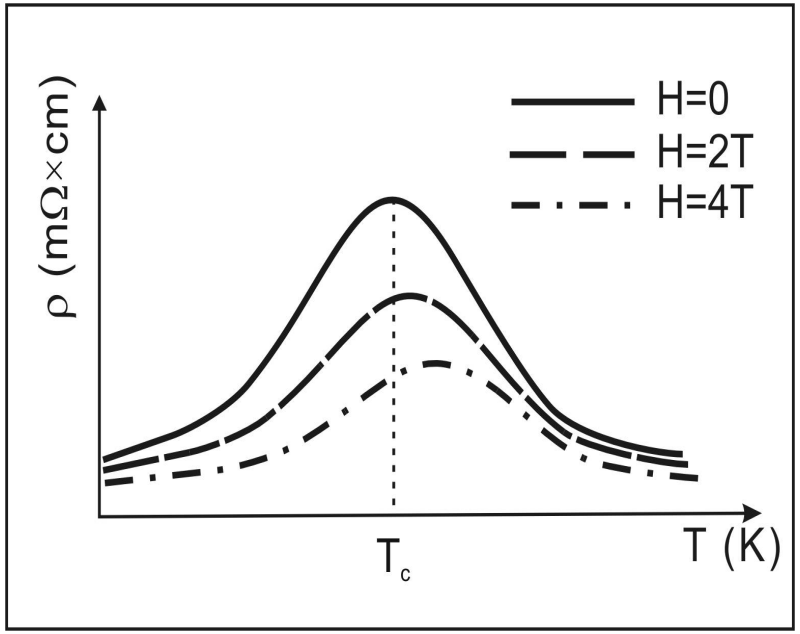
metallic behavior

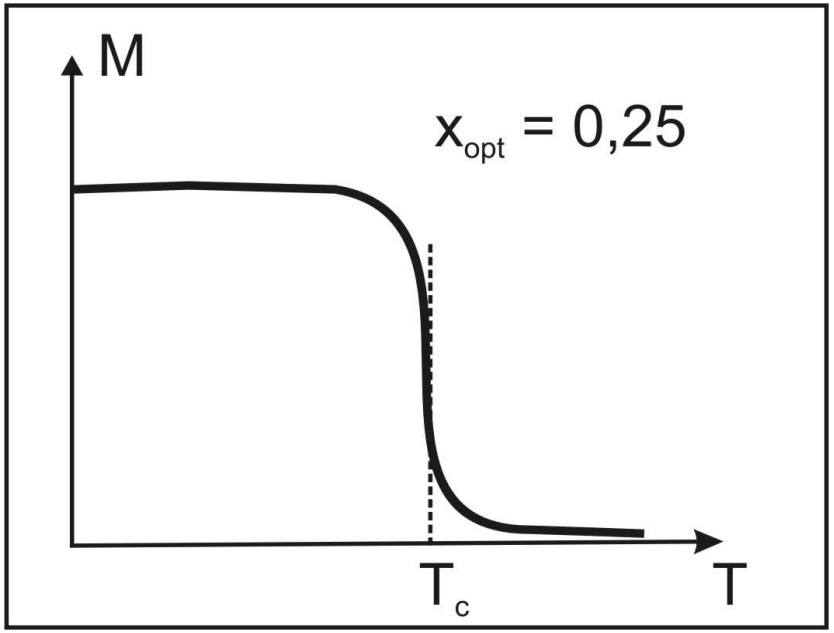
$$T>T_c:\ \rho \sim Be^{A/T};\ \ \frac{d\rho}{dT} < 0$$

Insulating thermoactivative behavior

Colossal Magnetoresistance

(x_{opt} = 0.25)





$$(MR) = -\frac{\Delta R}{R(H)} = \frac{R(0) - R(H)}{R(H)} \approx \frac{R(0)}{R(H)} \sim 10^2 - 10^3$$

giant negative magnetoresistance

S. Jin, T.H. Tiefel et.al., Science ***264****. 413 (1994)*

Theoretical Model

$$\hat{H} = -J_H \sum_i \vec{S}_i \vec{\sigma}_i - t \sum_{<ij>} c^+{}_{i\sigma}\, c_{j\sigma} + J_{ff} \sum_{<ij>} \vec{S}_i \vec{S}_j$$

For one conductivity band we have double exchange model (*De Gennes 1960*) with the hierarchy of the parameters:

$$J_H S >> t >> J_{ff} S^2$$

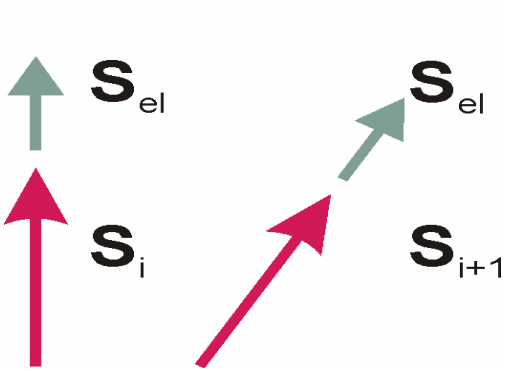
For real magnitudes:

$$J_H S \approx 1\ eV, \quad t \approx 0.3\ eV, \quad J_{ff} S^2 \approx 0.001\ eV$$

Double occupancy is prohibited in this model by large Hund's term.

Homogeneous canting for $x << 1$

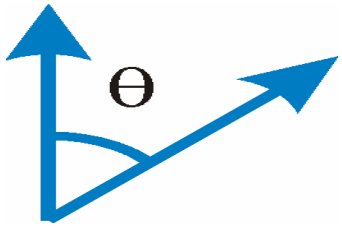
When an electron hops from one site to a neighboring one, it cants the local spins.



$J_H > W \Rightarrow |\mathbf{S}_{tot}| = S + 1/2$

on each site

θ - canting angle



Ψ-function of conduction electrons has a spinor character. Electron hopping results in an effective rotation of the Ψ-function components on the angle $\theta/2$.

$$t_{eff} = t\cos(\theta/2)$$

(*Anderson, Hasegawa 1959; De Gennes 1960*)

Canted State Instability

$E = -zt\cos\frac{\theta}{2}x + zJ_{ff}S^2\cos\theta$ - an energy of a classical canted state of De Gennes

$\frac{dE}{d\cos\frac{\theta}{2}} = 0 \Rightarrow \cos\frac{\theta}{2} = \frac{t}{4J_{ff}S^2}x$ - depends linearly upon doping

$E = -\frac{zt^2}{8J_{ff}S^2}x^2 - zJ_{ff}S^2$

However a canted state has negative compressibility:

$$\kappa^{-1} = \frac{d^2E}{dx^2} = -\frac{zt^2}{4J_{ff}S^2} < 0$$

Negative compressibility reflects an instability of a canted state towards phase – separation.

M. Yu. Kagan, D.I. Khomskii et.al., Eur. Phys. Jour. B ***12****, 217 (1999)*

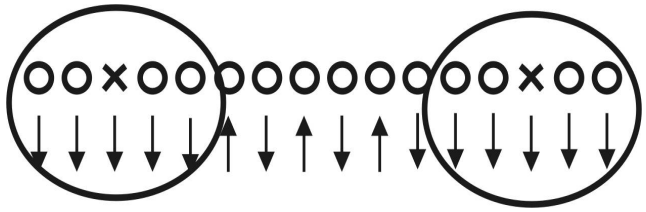
Small FM-polarons inside AFM-matrix

$$E_{pol} = -tx\left(z - \frac{\pi^2 a^2}{R^2}\right) + zJ_{ff}S^2 \frac{4}{3}\pi\left(\frac{R}{a}\right)^3 x - zJ_{ff}S^2\left[1 - \frac{4}{3}\pi\left(\frac{R}{a}\right)^3 x\right]$$

$\Omega = \frac{4}{3}\pi\left(\frac{R}{a}\right)^3$ — volume of a spherical polaron in isotropic 3D case

$-tzx$ — a bottom of the band in an infinite FM – cluster

$$\frac{dE_{pol}}{dR} = 0 \Rightarrow \frac{R_{pol}}{a} = \left(\frac{\pi t}{2zJ_{ff}S^2}\right)^{1/5}$$



E.L. Nagaev 1967, T. Kasuya 1970, N.F. Mott 1971

$$E_{pol} = -tzx + \frac{5}{3}\pi zx(\pi t)^{3/5}\left(2zJ_{ff}S^2\right)^{2/5} - zJ_{ff}S^2$$

The canting angle $\theta = 0$ inside the ferron and $\theta = \pi$ outside the ferron. The boundary of the ferron is rigid: an angle θ changes from 0 to π on a distance of the order of a.

Temperature ferrons

Even at $x \sim x_{opt} - 0.25$ above Curie temperature $T > T_C \approx 250$ K there is a phase – separation on FM – droplets inside PM insulating matrix. The radius of the droplet for hierarchy of the parameters: $z\, J_{ff}\, S^2 \le T_C < T << t$ can be defined form the minimization of the free – energy:

$$\Delta F = -tx\left(z - \frac{\pi^2 a^2}{R^2}\right) + T\ln(2S+1)\frac{4}{3}\pi\left(\frac{R}{a}\right)^3 x,$$

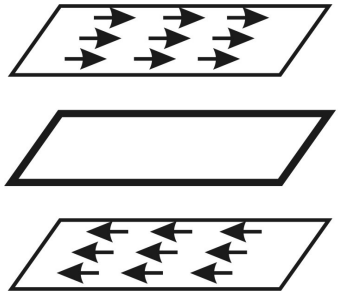
where the second term is the reduction of the spin – entropy inside the ferron.

As a result in 3D case: $$\frac{R_{pol}}{a} = \left[\frac{\pi t}{2T\ln(2S+1)}\right]^{1/5}$$

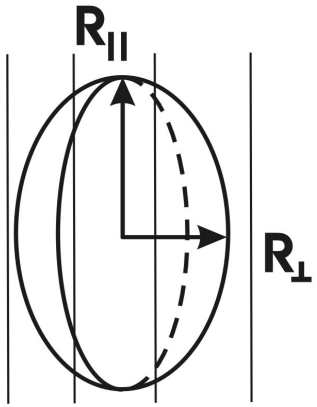
M. Krivoglaz 1972

Polarons in a layered case

$(La, Ca)_{n+1}Mn_nO_{3n+1}$ – layered manganites resemble HTSC - compounds



FM –ordered planes of local spins with alternating moments (A1 – structure)



$$\Omega = \frac{4}{3}\pi\left(\frac{R_{\parallel}}{a}\right)^2 \frac{R_{\perp}}{a}$$

The most favorable in a layered case is an ellipsoidal shape of a ferron

*M.Yu. Kagan, K.I. Kugel Sov. Phys. Uspekhi, **171**, 577 (2001)*

In the general case of 3D anisotropic AFM – lattice the volume of the ellipsoid:

$$\Omega = \frac{4\pi}{3}\left(\frac{\pi\, t_{eff}}{4\vec{J}S^2}\right)^{3/5},$$

where $t_{eff} = (t_x \cdot t_y \cdot t_z)^{1/3}, \quad \bar{J} = (J_x + J_y + J_z)$

Square lattices in 2D

On a square lattice in 2D the optimal shape of a ferron is a circle $\Omega = \pi (R/a)^2$ with a radius:

$$\frac{R_{pol}}{a} = \left(\frac{t \alpha_o^2}{8\pi J_{eff} S^2} \right)^{1/4},$$

where $\alpha_0 \approx 3\pi/4$ is a first zero of the Bessel function $J_0(kR) = 0$ for $kR_0 = \alpha_0$.
For 2D anisotropic AFM – lattice it is an ellipse with a volume:

$$\Omega = \pi \left(\frac{t_{eff} \alpha_0^2}{4\pi \bar{J} S^2} \right)^{1/2}$$

where $t_{eff} = (t_x \cdot t_y)^{1/2}$ and $\bar{J} = (J_x + J_y)$

*M.Yu. Kagan, K.I. Kugel et. al., Jour. of Phys. Cond. Matt., **18**, 102906 (2006)*

This type of phase – separation is typical for a variety of quasi – 2D (layered) cobaltates with low spin (a hole) in the center of a ferron surrounded by high spin in case of hole – doping.

Triangular lattices in 2D

On a frustrated triangular lattice for planar spin configuration it is again a circle with a volume:

$$\frac{\Omega_{triangle}}{\Omega_{square}} = \left(\frac{4}{3}\right)^{1/2} = \left(\frac{m_{triangle}}{m_{square}}\right)^{1/2}$$

M.Yu. Kagan, S.L. Ogarkov et.al, Jour. of Phys. Cond. Matt., ***20****, 425214 (2008)*

Free and bound magnetic polarons

For very small doping concentration conductivity electrons are bound to Sr impurity centrums. Hence ferrons are also localized in this case.
An appearance of the conductivity in Mn – O subsystem and delocalization transition in the system of ferrons correspond to generalized Mott criterion.

*M.Yu. Kagan, A.V. Klaptsov et. al, Jour. of Phys. A: Math. Gen., **36**, 9155 (2003)*

Having in mind that $x_{opt} \sim 15\%$ we conclude that ferrons are delocalized for $x_{Mott} < x < x_{opt}$. For $x < x_{Mott}$ we have bound magnetic polarons. We will show that they have a large intermediate region where a canting angle is changing gradually from almost 0 to almost π.

The existence of such ferrons (behaving effectively as magnetic impurities) was first assumed by *De Gennes* in 1960. We can get them explicitly in a following simple model.

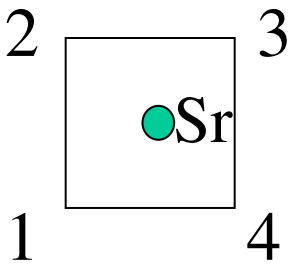
Bound magnetic polarons I

The bound magnetic polarons with extended coat of spin – distortions for $x << x_{Mott}$ are described by the Hamiltonian:

$$\hat{H} = -J_H \sum_i \mathbf{S}_i \boldsymbol{\sigma}_i - t \sum_{\langle i,j \rangle} c^+_{i\sigma} c_{j\sigma} + J_{ff} \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j$$

$$+ V_{imp} \sum \frac{c^+_{i\sigma} c_{j\sigma}}{|\vec{n}_i - \vec{n}_0|} - K \sum_i (S_{ix})^2$$

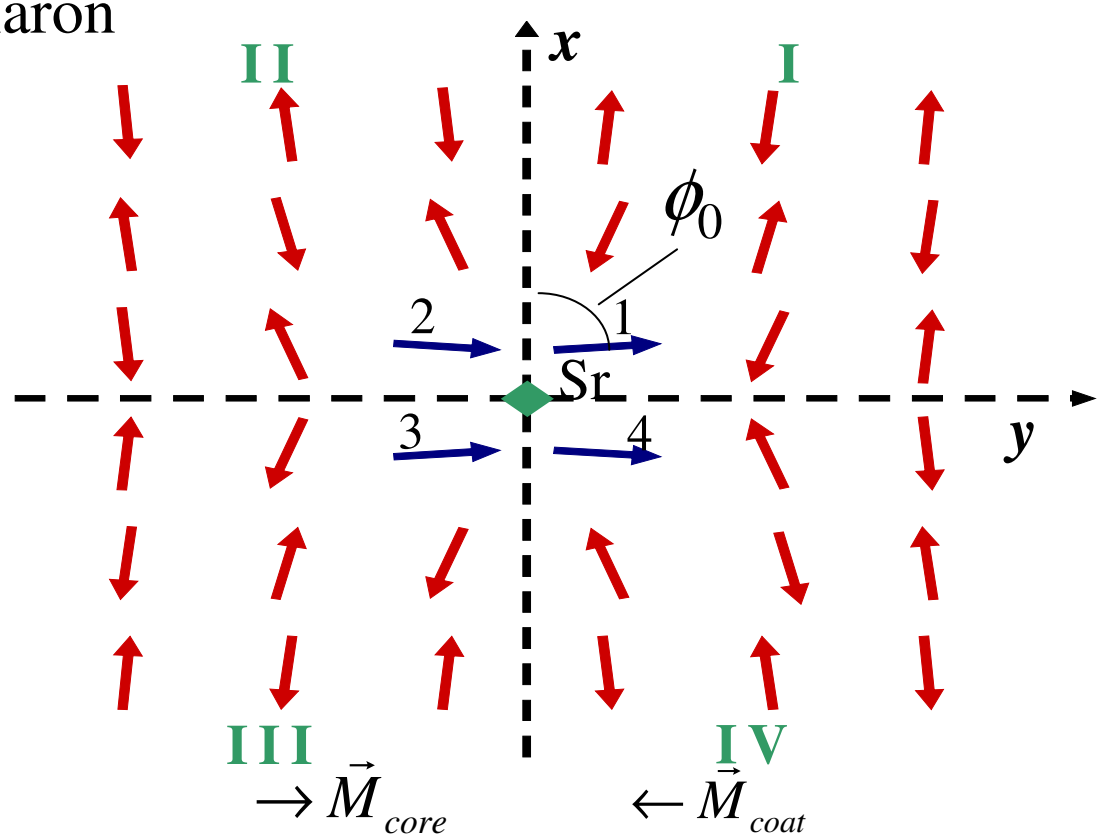
double exchange model with Coulomb interaction between conductivity electrons and Sr impurity, as well as with one – site anisotropy. Sr impurity is situated in the middle of elementary lattice cell. $(J_H\, S \sim V_{\text{imp}}) >> t >> J_{ff} S^2 >> K$ – the hierarchy of parameters.



S.L. Ogarkov, M.Yu. Kagan, et.al. Phys. Rev. B ***74****, 014436 (2006)*

Bound magnetic polarons II

After minimization procedure we get the following picture for coated magnetic polaron



The magnetic moment of the FM–core is less than a saturation value. The coat has a magnetic moment antiparallel to the core. The canting angle ϕ_0 with anisotropy axis OX $\phi_0 < \pi/2$ for spins of the FM–core.

Bound magnetic polarons III

Analytically in the continuous limit we have the FM – core with radius $R_f \sim a$ (and $\phi_0 < \pi/2$ inside the core) and an extended coat of spin – distortions decaying in a power-law fashion at intermediate distances:

$R_f < r < r_0$, where $r_0 = a\sqrt{\frac{J_{ff} S^2}{2K}} >> a$

For cubic lattice in 3D: $\phi \sim R_f^4/r^4$

For quadratic lattice in 2D: $\phi \sim R_f^2/r^2$

For frustrated triangular lattice and planar spin configuration: $\phi \sim R_f/r$

*M.Yu. Kagan, S.L. Ogarkov et.al., J. Phys.: Cond. Matt., **20**, 425214 (2008)*

Finally for $r > r_0$: $\phi \sim exp\{- r /r_0\}$ we have exponential decay of a canting angle ϕ.

Generalized Mott criterion

We consider that x_{Mott} can be qualitatively defined via the radius r_0 of the coat extension for bound magnetic polaron.

In 3D the coats overlap at:

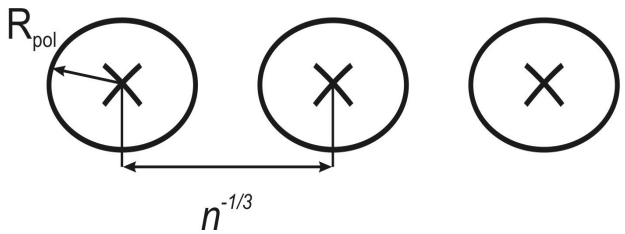
$$x_{Mott} \sim \frac{3}{4\pi}\left(\frac{a}{r_0}\right)^3$$

So $x_{Mott} \sim (0.1 \div 0.2)\%$ for typical $r_0 \sim (5 \div 6)a$.

In 2D: $x_{Mott} \sim \frac{1}{\pi}\left(\frac{a}{r_0}\right)^2 \sim (0.5 \div 1)\%$

The Role of Coulomb Interaction between conductivity electrons I

I. Small electron density



$$a << R_{pol} << n^{-1/3}$$

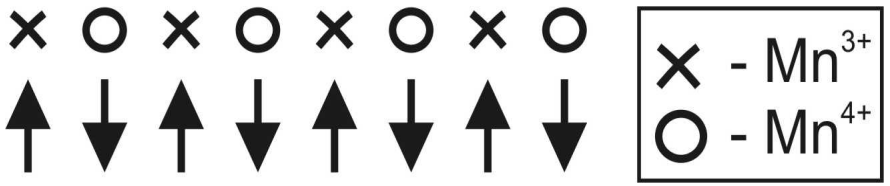
Coulomb energy is the **same** for homogeneous and polaron state.

II. Theoretical model

$$\hat{H} = -J_H \sum_i \vec{S}_i \vec{\sigma}_i - t \sum_{<i,j>} c^+_{i\sigma} c_{j\sigma} + J_{ff} \sum_{<i,j>} \vec{S}_i \vec{S}_j + V \sum_{<i,j>} n_i n_j$$

Kondo – lattice model with Coulomb interaction on neighboring sites

III. Exact case $n = 0{,}5$



Verwey localization: checkboard distribution of electrons and holes.

The Role of Coulomb Interaction between conductivity electrons II

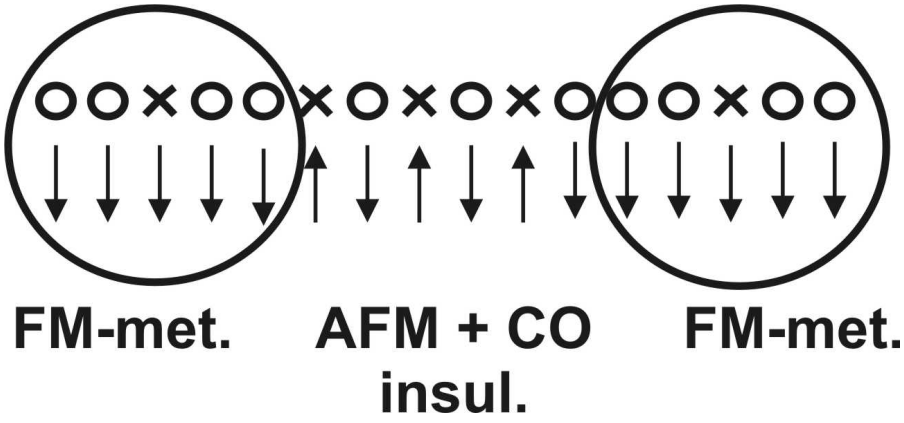
So we have:

$x < x_c$: AFM/FM insulator

$x > x_c$: FM metal

$x = 0.5$: AFM + CO insulator

$\underline{x_c < x < 0.5}$



FM – polarons with **one electron inside**, and a lot of electrons **outside in CO state**

*M.Yu. Kagan, K.I. Kugel, Sov. Phys. Uspekhi **171**, 577 (2001)*

Heisenberg – like orbital interaction

After canonical transformation of the two – band Hubbard model for $U >> t$ and $x \leq 0.16$ we get on 2D square lattice with e_g electrons on $|x^2 - y^2\rangle$ and $|2z^2 - x^2 - y^2\rangle$ orbitals:

$$\hat{H} = -\sum_{\substack{\langle n,m\rangle \\ \alpha,\beta,\sigma}} \left(t_{nm}^{\alpha\beta} P_{n\alpha\sigma}^{+} a_{n\alpha\sigma}^{+} a_{n\alpha\sigma} P_{m\beta\sigma} + h.c. \right) + J \sum_{\langle n,m\rangle} \vec{\tau}_n \vec{\tau}_m$$

S. Ishibara, J. Inoue et. al., Phys. Rev. B ***55****, 8280 (1997)*

- an orbital $t - J$ model, $J \sim t^2/U \sim 900$ K is superexchange interaction of AFM – type ($J > 0$) between two orbitals. $P_{n\beta\sigma}$ are projection operators, excluding double occupation of sites. Pseudospin operators $\vec{\tau}_n = \{\tau_n^x, \tau_n^z\}$, $\tau_n^{x,z} = \sum_{\alpha,\beta,\sigma} a_{n\alpha\sigma}^{+} (\sigma_{\alpha\beta}{}^{x,z}) a_{n\beta\sigma}$ describe an orbital state.

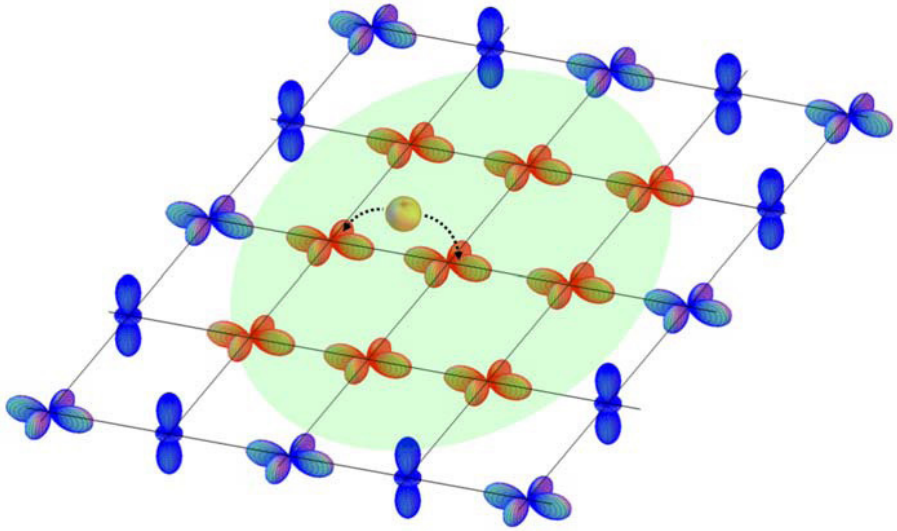
K.I. Kugel, D.I. Khomskii, Sov. Phys. Uspekhi ***136****, 621 (1982)*

$$t_{nm}^{\alpha\beta} = \frac{t_0}{4} \begin{pmatrix} 3 & \mp\sqrt{3} \\ \mp\sqrt{3} & 1 \end{pmatrix}$$

- minus (plus) sign corresponds to $n - m$ bond parallel to x (y) axis

Orbital ferrons

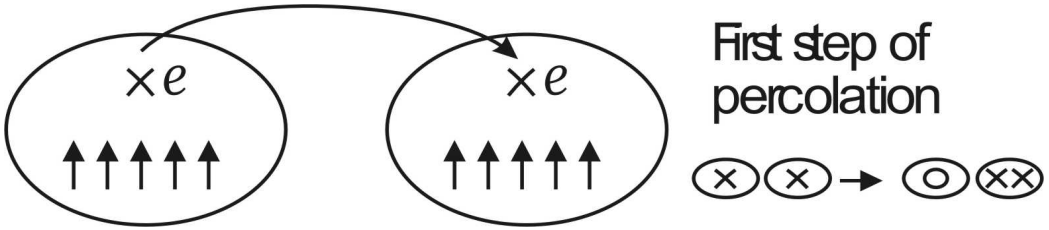
Metallic orbital ferrons inside insulating AFM orbital matrix



Characteristic radius of the droplet: $\frac{R_f}{a} = \left(\frac{t_0 \alpha_0^2}{12JS^2} \right)^{1/4}$ in 2D case

K.I. Kugel, A.L. Rakhmanov et.al., Phys. Rev. B ***78****, 155113 (2008)*

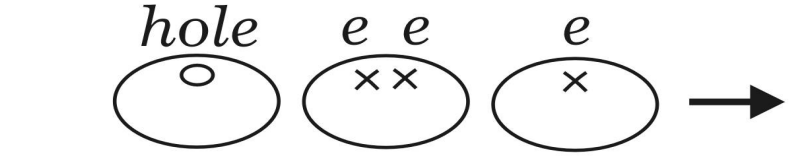
Transport properties in phase-separated states

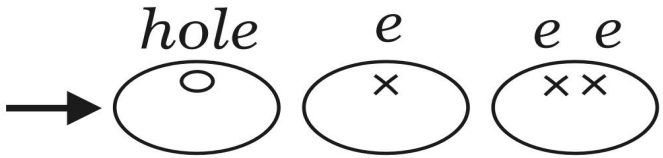


First step of percolation

$$A = E_2 + E_0 - 2E_1$$

$$A \propto \frac{e^2}{\varepsilon_0 R_{pol}} \propto 0{,}1\,\text{eV} \text{ - Coulomb barier}$$





Second step of percolation

This mechanism of electron transport is valid for $\exp\left(-\frac{A}{2T}\right) << \frac{x}{x_c} < 1$

A.L. Rakhmanov, K.I. Kugel et.al., Phys. Rev. B ***63****, 174424 (2001)*

Tunneling Conductivity

For low temperature T and small voltage V a tunneling time reads:

$$\gamma = \frac{1}{\tau_{1,2}} \sim w_0 \exp\left\{-\frac{R}{2R_{pol}} - \frac{A}{2T}\right\},$$

where $w_0 \sim \varepsilon_f \sim 300$ K is a frequency of depolarization of spins.

As a result:

for $A/T >> \frac{1}{n^{1/3} R_{pol}} > 1$ in analogy with the physics of Coulomb blockade in mesoscopics

$$\rho = \frac{1}{\sigma} = B \frac{1}{\sigma_{\min}} \left(\frac{T}{w_0}\right) \exp\left(\frac{A}{2T}\right),$$

where $\sigma_{\min} = e^2 n^{1/3}$

$B \sim \exp\left(\frac{0{,}8}{n^{1/3} R_{pol}}\right)$ - smaller percolation exponent of Efros-Shklovski type

Experimental confirmation of nano-scale phase separation

1. Our results are confirmed by NMR – exp. of *Allodi* and *Jakubovskii* (RPL 1997; 2000) – two resonant frequencies instead of one.

2. Exp. on neutron scattering (*Hennion* et al PRL 2000; 2001; *Morimoto* PRB 1999). Elastic scattering yields lorenzian shape of intensity $I(q)$ with $1/q_0 \sim R_{pol} \sim 10$ Å. Inelastic scattering yields two distinct branches of FM and AFM spin waves.

3. The most recent results of *Hennion* are in favor of FM – polarons inside a canted matrix. In the layered case they also confirmed an anisotropic shape of a polaron.

4. Exp. of *Fisher* et al on hysteresis of magnetization (centre of the hysteresis loop shifts from $H = 0$ to $H = 4 \div 6$ Tesla).

5. Exp. of *Babushkina et al* on strong nonlinear $I - V$ characteristics in manganites with $x \sim 0.2$ (in favor of percolative picture).

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I.V. Brodsky, A.V. Klaptsov, S.L. Ogarkov,
Kapitza Institute for Physical Problems, Moscow

Concluding Remarks

1. ***Phase-separation and charge ordering is typical*** for a large variety of strongly correlated systems including CMR – systems.
2. We considered mainly the most physically transparent limit of ***nano-scale phase separation***.
3. Simple picture of nano – scale phase – separation can naturally explain ***the transport properties of CMR – systems*** at low doping regime.
4. When we study the transport properties of phase – separated manganites we create ***the bridge between strongly correlated electron systems and mesoscopics.***

Magnetoresistance

$$R_{pol} \sim a\left(\frac{\pi t}{zJ_{ff}S^2}\right)^{1/5}; \qquad \mathrm{J} \sim 100\mathrm{K}\ \ \mathrm{S} = 3/2$$

$$J(H)S^2 = J(0)S^2 - g\mu_B HS$$

$$\rho(0) \sim \exp\frac{A(0)}{2T}; \qquad A = \frac{e^2}{\varepsilon_0 R_{pol}}$$

$$A(H) = \frac{e^2}{\varepsilon_0 R_{pol}(H)} = [1 - bH]A(0)$$ - change of the droplet radius; $b = 1/5\,\frac{g\mu_B}{J(0)S}$

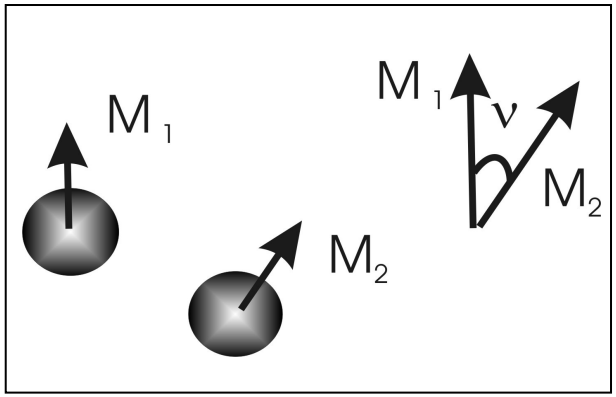
$$\mathbf{MR} = \frac{\rho(0) - \rho(H)}{\rho(H)} = \exp\left(bHA/2T\right) - 1$$

For $T \leq A$: $MR >> 1$ for $H \sim 10$ Tesla

*M.Yu. Kagan, K.I. Kugel, Sov. Phys. Uspekhi **171**, 577 (2001)*

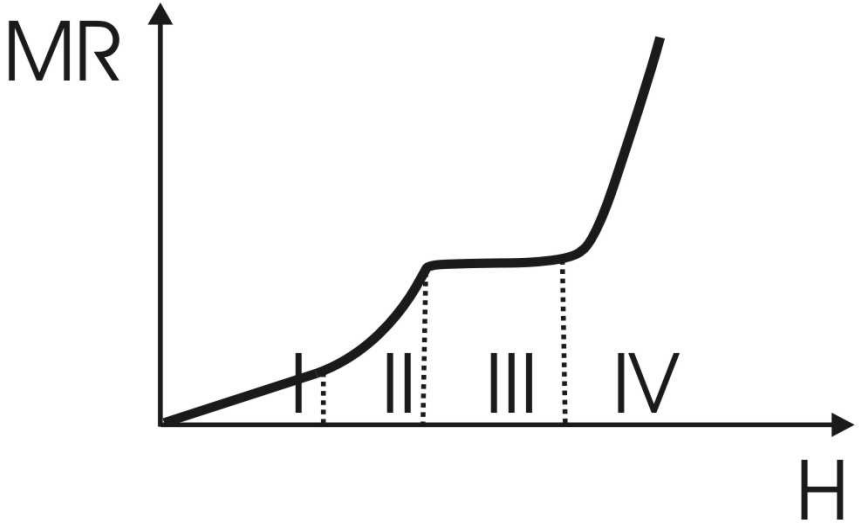
Spin Assistant Tunneling

Effect of a spin assistant tunneling yields nontrivial preexponential factor:



$$\gamma(H) = \gamma(H = 0)\exp\left(-\frac{\sigma\mu_B H_{mol}\cos v - \sigma\mu_B H_{mol}}{kT}\right)$$

- a tunneling time in the presence of a magnetic field



I. H^2/T^2 – in the absence of anisotropy; $H^2 H_a / T^5$ – in strongly anisotropic case, H_a is a field of magnetic anisotropy
II. H^2/T
III. plateau
IV. $\exp(bH_a/2T)$

A.O. Sboychakov, A.L. Rakhmanov et. al., J. Phys.: Cond. Matt., ***15****, 1705 (2003)*

Experimental confirmation

The result $H^2 H_a / T^5$ for a tunneling magnetoresistance was experimentally confirmed by recent studies of magnetically anisotropic manganites $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$, carried out by the group of *Babushkina* (Kurchatov Institute, Moscow), and layered manganites $(La_{0.4}Pr_{0.6})_{1.2}Sr_{1.8}Mn_2O_7$, carried out by the group of *Moshchalkov* (Leuven, Belgium).

K.I. Kugel, A.L. Rakhmanov et al., Sov. Phys. JETP ***125****, 684 (2004)*

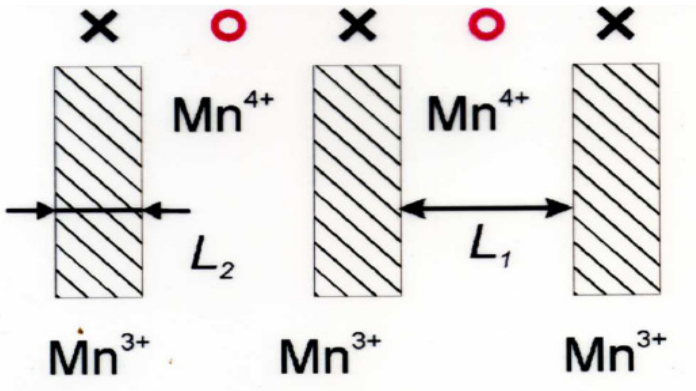
Experiments on large scale phase separation

1. STM – experiments of *Mydosh et. al.*, – direct visualization of metallic and insulating regions for $x \sim 0.16$.

2. Experiments of *Cheong et. al.*, – electron diffraction at $x = 0.5$ confirms checkerboard CO – structure.

   Dark image electron microscopy for $x = 0.4$ shows coexistence of CO and FM domains.

3. Stripes for $x > 0.5$ – Mori et al (Nature 1998) experiments on electron diffraction.



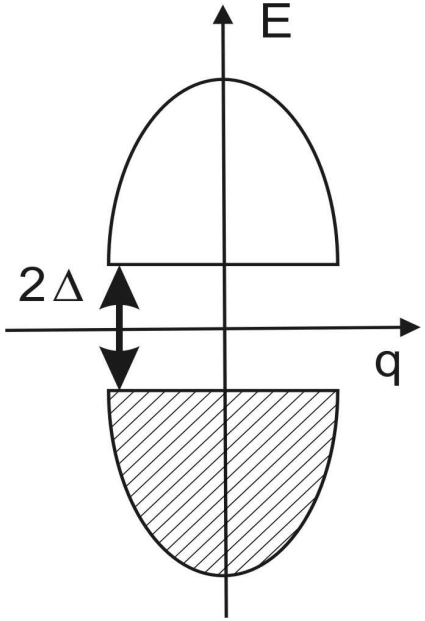
$L_1 \approx 3\ L_2$ – incommensurate charge ordering stripes and static in manganites due to JT effect.

Theoretical confirmation of the instability of CO state

at $x = 0.5$

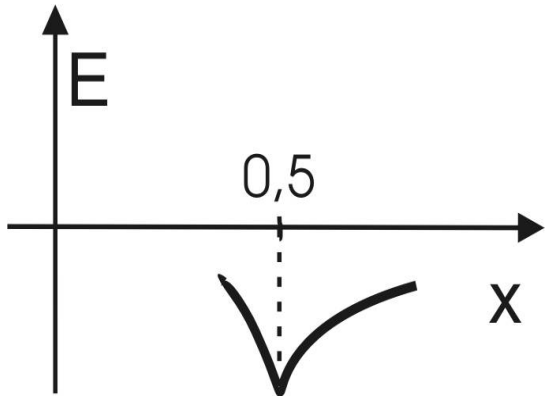
$$E_{CO} - E_N = -\frac{W^2}{6V\,z}$$

$2\Delta = Vz$ - a gap in CO - state



for $x \neq 0.5$ an energy of CO – state has a **cusp:**

$$\kappa^{-1} = \frac{d^2E}{dx^2} < 0$$



CO state is **unstable** for x ≠ 0.5 towards phase – separation

FM Polaron in CO-matrix

$$E_{pol} = -tn_d\left(z - \frac{\pi^2 a^2}{R^2}\right) + zJS^2\frac{4}{3}\pi\left(\frac{R}{a}\right)^3 n_d - \left(zJS^2 + \frac{2zt^2}{3V}\right)\left[1 - \frac{4}{3}\pi\left(\frac{R}{a}\right)^3 n_d\right]$$

n_d - number of polarons (FM = droplets)

Minimization with respect to radius yields: $\frac{R_{pol}}{a} \sim \frac{1}{\left(t/V + J_{ff}S^2/t\right)^{1/5}}$

So finally: *M.Yu. Kagan, K.I. Kugel et.al., Sov. Phys. JETP, **93**, 415 (2001)*

$0 < x < x_{Mott}$ – bound magnetic polarons

$x_{Mott} < x < (J_{ff}S^2/t)^{3/5}$ – AFM/FM

$(J_{ff}S^2/t)^{3/5} < x < (t/V + J_{ff}S^2/t)^{3/5}$ – FM metall

$(t/V + J_{ff}S^2/t)^{3/5} < x < ½$ – FM/CO

In fact a two – band character of e_{2g} – orbitals is important for conductivity electrons.

Two-band Hubbard model

We use two – band Hubbard Hamiltonian to describe orbital ordering:

$$\hat{H} = \sum_{<nm>\alpha\beta} t_{nm}^{\alpha\beta} a_{n\alpha\sigma}^{+} a_{m\beta\sigma} + \varepsilon \sum_{n\sigma} n_{n\beta\sigma} - \mu \sum_{n\alpha\sigma} n_{n\beta\sigma}$$

$$+\frac{1}{2} \sum_{n\alpha\sigma\bar{\sigma}} U^{\alpha} n_{n\alpha\sigma} n_{n\alpha\bar{\sigma}} + \frac{1}{2} U' \sum_{\substack{n\sigma\sigma' \\ \alpha\neq\beta}} n_{n\alpha\sigma} n_{n\beta\sigma'}$$

where μ is the chemical potential, ε is the energy – shift between the centers of the bands. In our case ε = E_{JT}.

Assumptions:

without loss of generality $U_1 = U_2 = U' + 2J_H = U$,

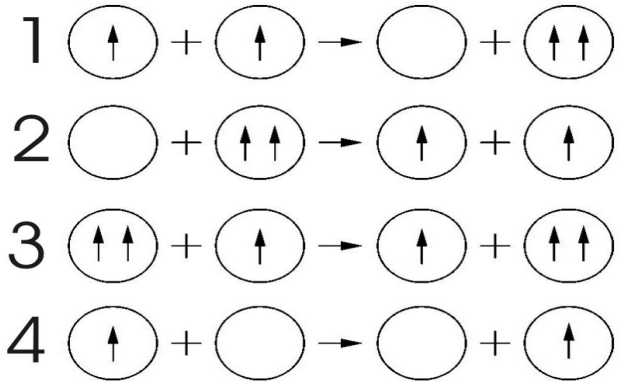
strong on – site Coulomb repulsion $U \sim 10$ eV >> J_H $S \sim 1$ eV >> t,

the total number of electrons per site $n_{tot} = 1 - x$, where $x \leq 0.16$.

Tunneling Conductivity I

- Carriers could jump only on the droplets
- Droplet number $N = N_{el}$

$N = N_0 + N_{1,+1/2} + N_{1,-1/2} + N_2$



$$j = en_{1,2}^{i}\left\langle \sum_{l} v_{1,2}^{l} \right\rangle \qquad \left\langle \sum_{l} v_{1,2}^{l} \right\rangle = \left\langle \sum_{l} \frac{r^{l}\cos\Theta^{l}}{\tau_{1,2}(r^{l},\Theta^{l})} \right\rangle$$

Where $\langle .. \rangle$ means averaging over random droplets location;

τ – characteristic transition time;

r, Θ – the distance between droplets and an angle with respect to the applied electric field.

Quantum canting

In a more sophisticated quantum canting approach there are two bands, instead of one, corresponding respectively to
$S_{tot} = S + ½$, but $S^z_{tot} = S \pm ½$.
Their spectra read:

$$t_{\pm}(\theta) = \frac{t}{2S+1}\left[\sqrt{2S+1+S^2\cos^2\frac{\theta}{2}} \pm S\cos\frac{\theta}{2}\right]$$

$$\text{for } \theta \to 0 \quad (\text{FM - case}) \quad t_+ = t, \quad t_- = \frac{t}{2S+1}$$

$$\text{for } \theta \to \pi \quad (\text{AFM - case}) \quad t_+ = t_- = \frac{t}{\sqrt{2S+1}}$$

The classical one – band canting of De Gennes corresponds for $S >> 1$ to the region of small angles where

$$S^2\cos^2\frac{\theta}{2} >> 2S+1 \quad \text{and} \quad t_+ \approx t\cos\frac{\theta}{2}$$

Compromise between quantum canting and FM-polaron

An energy functional with the normalization condition in the case of quantum canting reads for continuum model:

$$F = -\int dV \left[t(\theta)\left(z|\Psi|^2 + \Psi^* \Delta\Psi \right) - z J_{ff} S^2 \cos^2 \frac{\theta}{2} - \beta |\Psi|^2 \right]$$

A hopping integral for quantum canting:

$$t_+ = t(\theta) = \frac{t}{2S+1}\left[\sqrt{2S+1+S^2\cos^2\frac{\theta}{2}} + S\cos\frac{\theta}{2} \right]$$

at small densities only a lower band t_+ is occupied

for $\theta = 0$ (FM - case) $t(\theta = 0) = t$

for $\theta = \pi$ (AFM - case) $t(\theta = \pi) = \dfrac{t}{\sqrt{2S+1}}$

$$\frac{\delta F}{\delta \Psi^*} = 0: \; t(\theta)(2z\Psi + \Delta\Psi) + \Delta[t(\theta)\Psi] - 2\beta\Psi = 0$$

$$\frac{\delta F}{\delta \theta} = 0: \left[\left(z|\Psi|^2 + \Psi^* \Delta\Psi \right) \frac{d\, t(\theta)}{d\cos\theta/2} - 2 z J_{ff} S^2 \cos\frac{\theta}{2} \right] \sin\frac{\theta}{2} = 0$$

Electronic wave function and the function of the canting angle

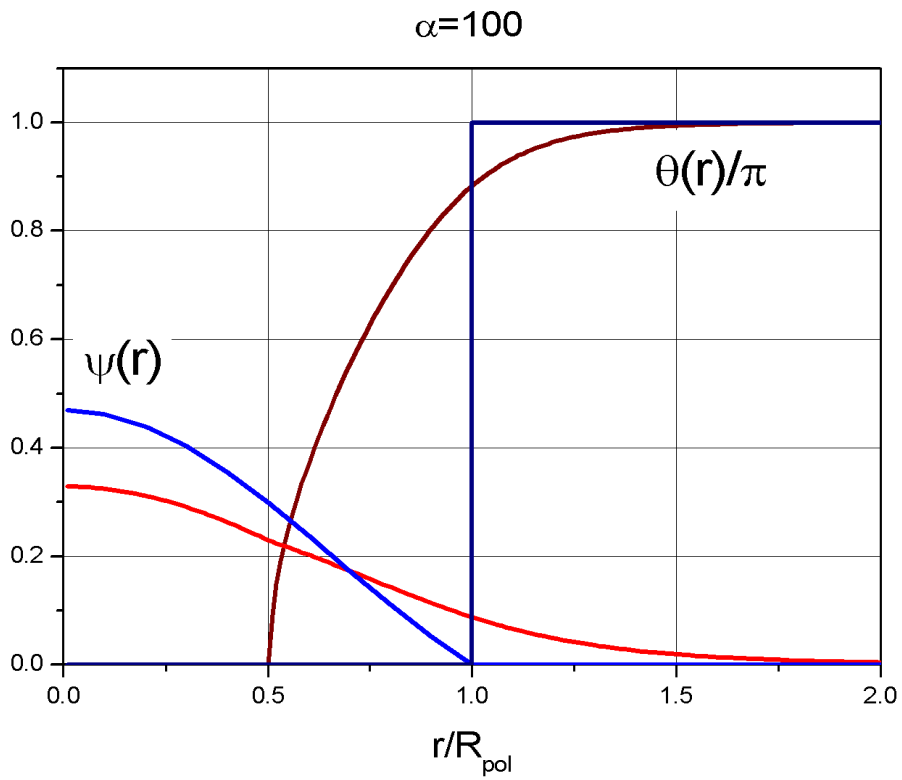
The normalized electronic wave function $\Psi(r)$ and the function of the canting angle $\theta(r)$ were calculated by the method proposed by

S. Pathak and S. Satpathy, Phys. Rev. B ***63****, 214413 (2001)*

for 1D ferrons.

$$\alpha = \frac{t}{J_{ff} S^2} = 100,$$

$$R_{pol} = a\left(\frac{\pi\alpha}{2z}\right)^{1/5}$$ - radius of Nagaev - Mott ferron



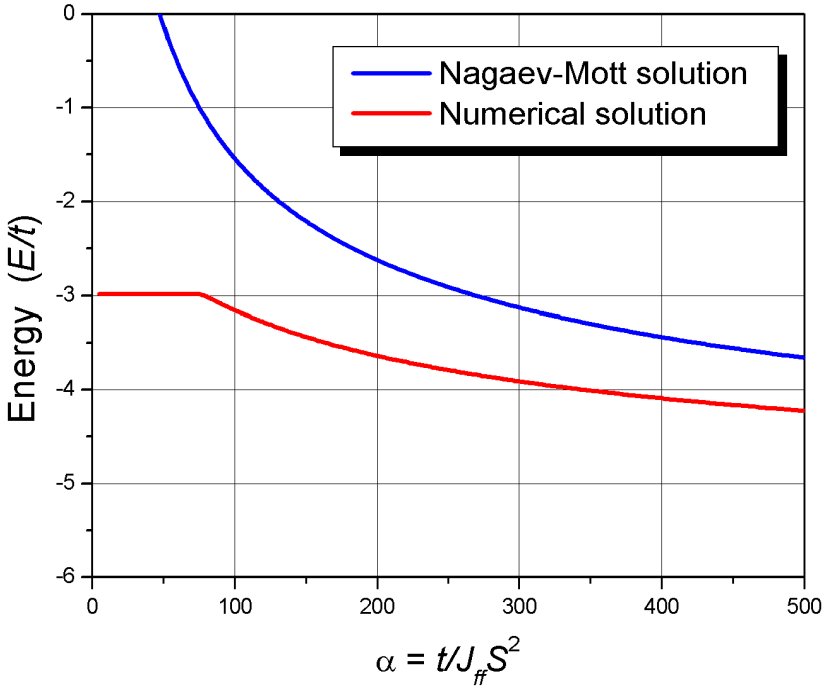
Comparison of Nagaev-Mott and exact solution

Dependence of Nagaev – Mott energy and energy of the exact solution on the parameter α:

$$\frac{E}{t} = -z + \frac{5}{3}\pi^2 \left(\frac{2z}{\pi\alpha}\right)^{2/5}$$

- Nagaev – Mott energy, where

$$E = E_{AFM} = -\frac{zt}{\sqrt{2S+1}}$$



- a bound state disappears and an electron freely moves through AFM – media. The bound state exists when $\alpha = \frac{t}{JS^2} > \alpha_c \approx 75$ for $S = \frac{3}{2}$.

*M.Yu. Kagan, A.V. Klaptsov et.al., J. of Phys. A: Math. Gen., **36**, 9155 (2003)*

1/*f*– noise in a percolative regime I

Using a droplet model it is also possible to get 1/f noise in phase separated state and to explain recent experiments of *Podzorov et. al.*

$$\frac{\langle \delta U^2 \rangle_\omega}{U_{dc}^2} \sim \frac{\langle \delta \sigma^2 \rangle_\omega}{\sigma^2} \sim \frac{\langle \delta n^2 \rangle_\omega}{\bar{n}^2} \sim \frac{1}{x \mathrm{V}_{samp}} \left\langle \frac{\tau(r)}{1+\omega^2\tau^2(r)} \right\rangle$$

$$\tau(r) \sim \frac{1}{\omega_0} \exp\left\{ \frac{r}{2R_{pol}} + \frac{A}{2T} \right\}, \quad \langle f \rangle = 4\pi \int f(r) r^2 dr$$

As a result:

$$\frac{\langle \delta U^2 \rangle_\omega}{U_{dc}^2} \sim \frac{\alpha}{x \mathrm{V}_{samp}} \frac{1}{\omega},$$

where $\alpha \sim \ln^2\left(\frac{\omega}{\omega_0}\right) \sim 10^3$ for $\omega = (1 \div 10^3)\mathrm{Hz}$,

$\mathrm{V}_{samp} = L_1 L_2 L_3$ – sample volume

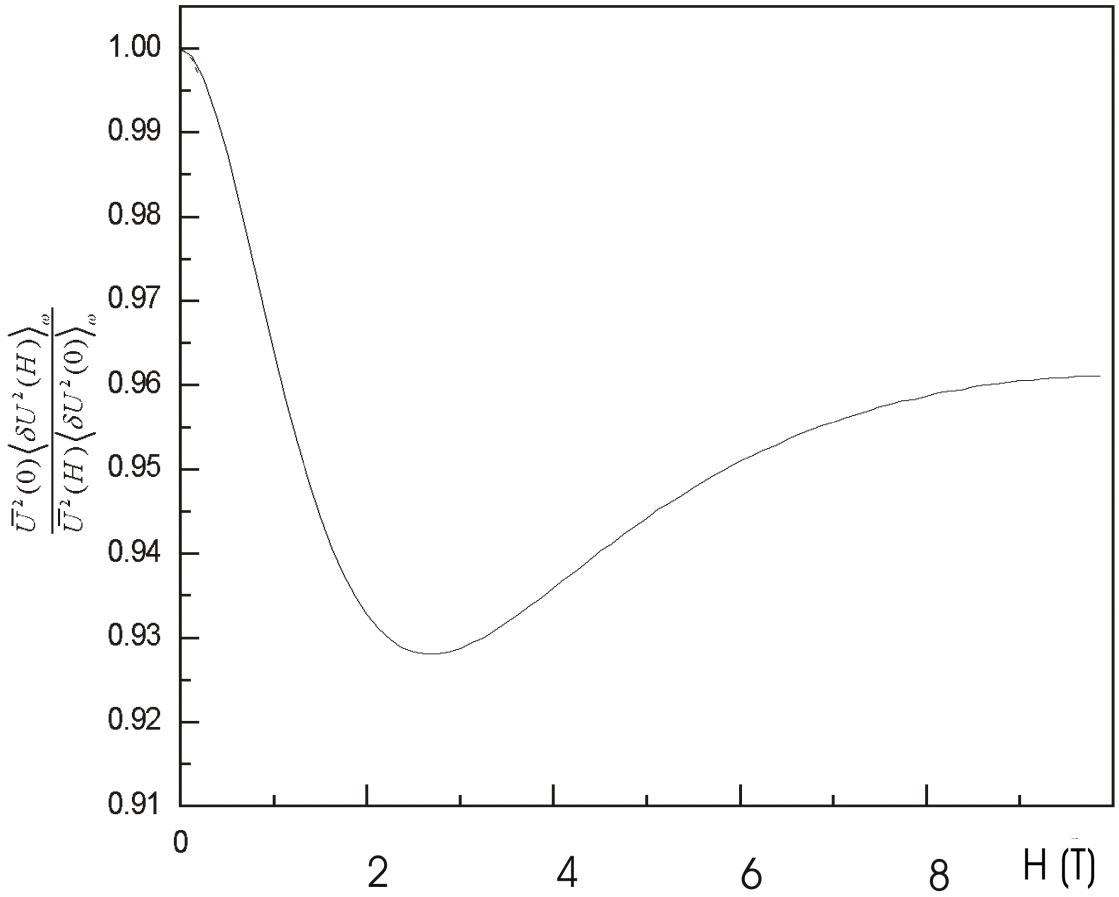
$1/f$– noise in a percolative regime II

$1/f$ - noise exists in a very broad frequency range:

$$\omega_0 \exp(-L/R_{pol}) < \omega < \omega_0 \exp(A/2T).$$

So we get a very large coefficient α. It is 10^6 times larger than in usual homogeneous metals and within factor of 10 coincides with experimental results of *Podzorov*.

1/*f*– noise in a magnetic field



The magnetic field dependence of normalized spectral noise power

There is a pronounced minimum for $H \sim 2T$ on this curve

One-particle Green functions

$$G_\alpha(\omega,k)=\frac{g_\alpha}{\omega+\mu+\varepsilon^\alpha-g_\alpha w^\alpha(k)},$$

$$g \;=1-\frac{n_\alpha}{2}-n_{\bar{\alpha}}$$

Simple cubic lattice, tight- binding model:

$$w^\alpha(\boldsymbol{k}) = -\;\; 6t^\alpha(\cos k^1+\cos k^2+\cos k^3)$$

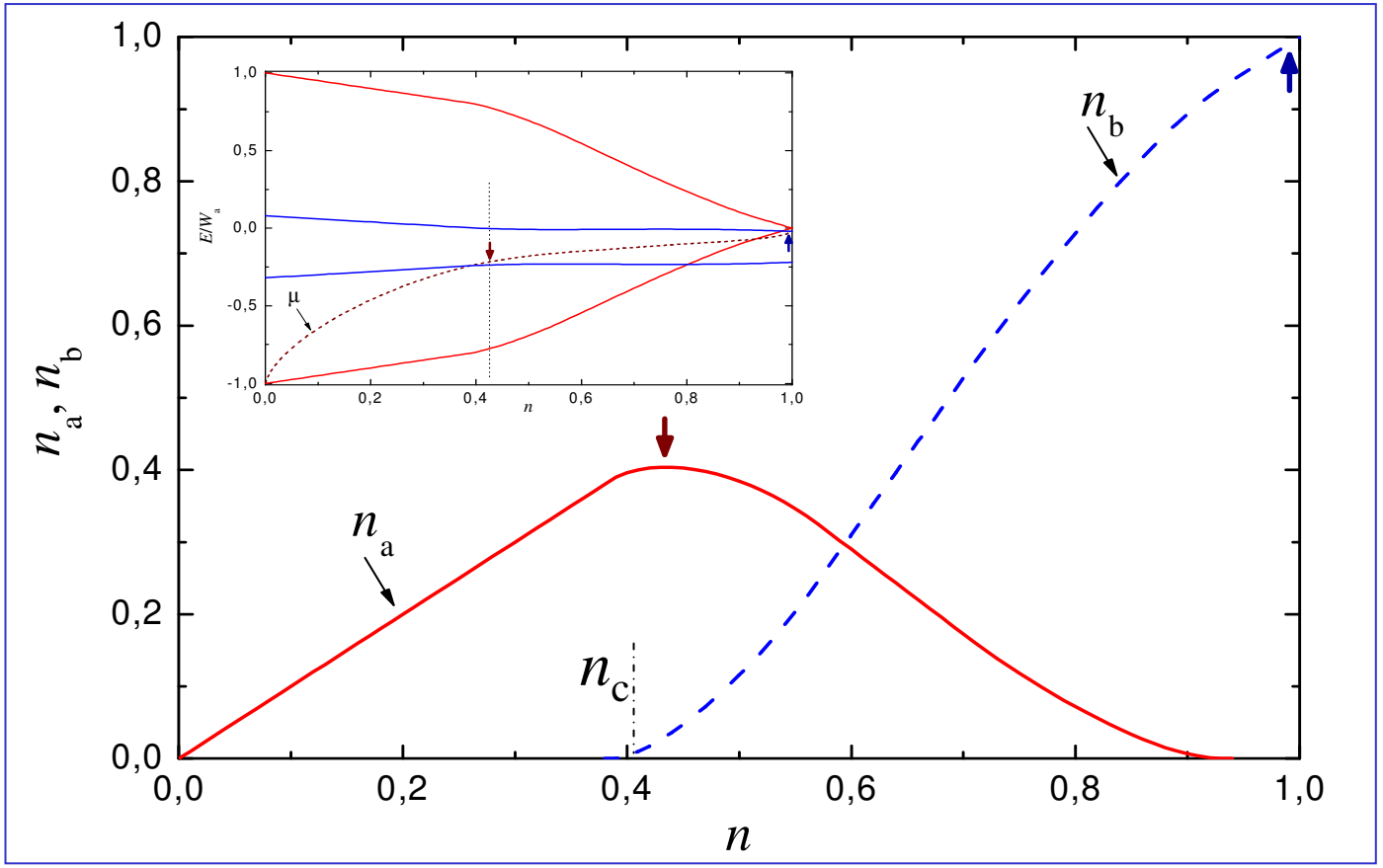
The equations:

$$n_\alpha(\mu)=-2i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\int\frac{dk}{(2\pi)^3}G_\alpha(\omega,k)\,e^{i\omega_0},$$

$$n=\sum_{\alpha=a,b}n_\alpha(\mu)$$

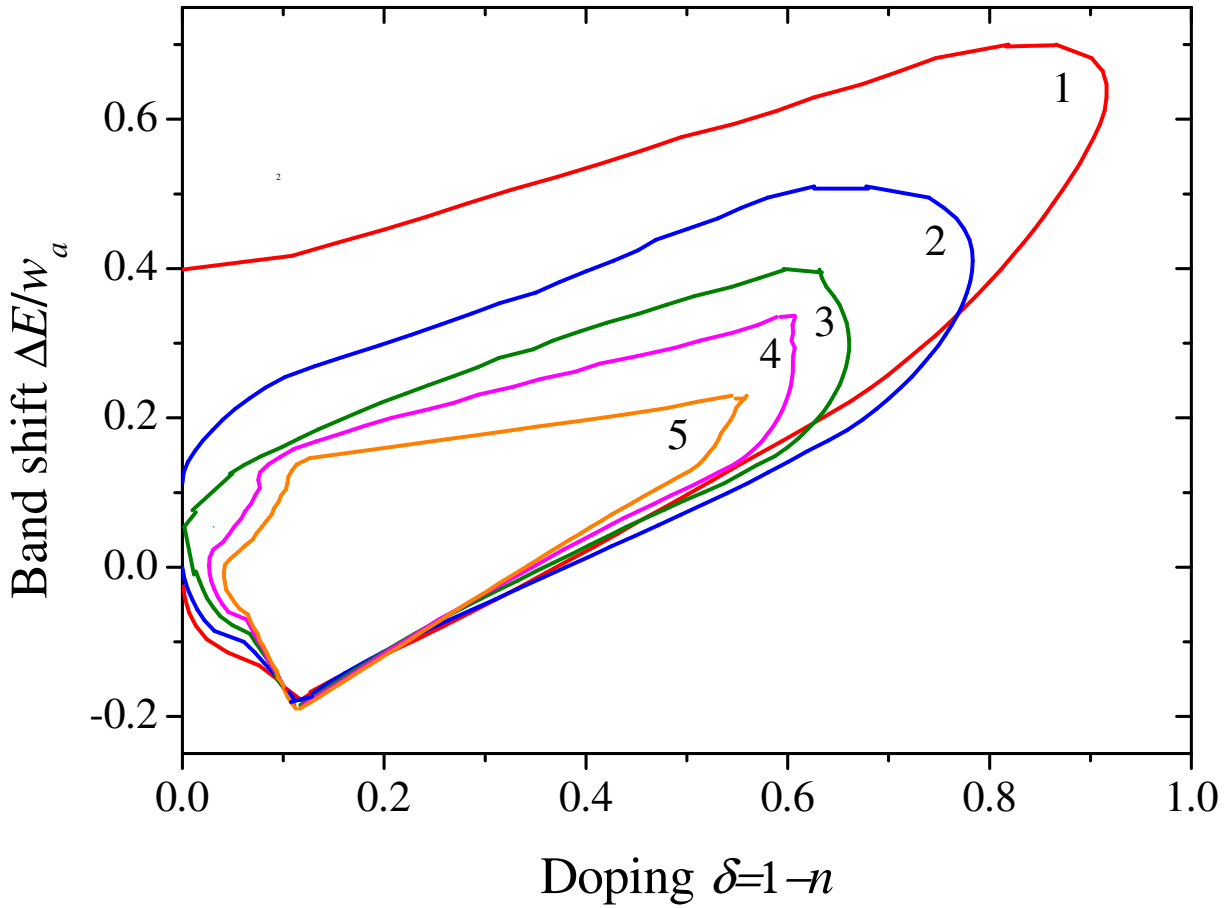
define the number of electrons in each band n_a, n_b depending on doping n.

One-particle Green functions



At low doping, there exist only *a* electrons until the chemical potential reaches the bottom of the *b* band at some value n_C of doping. At $n > n_C$, the *b* electrons appear in the system, and the effective width of *a* band, $w^a = 6t^a g_a$, starts to decrease faster with n.

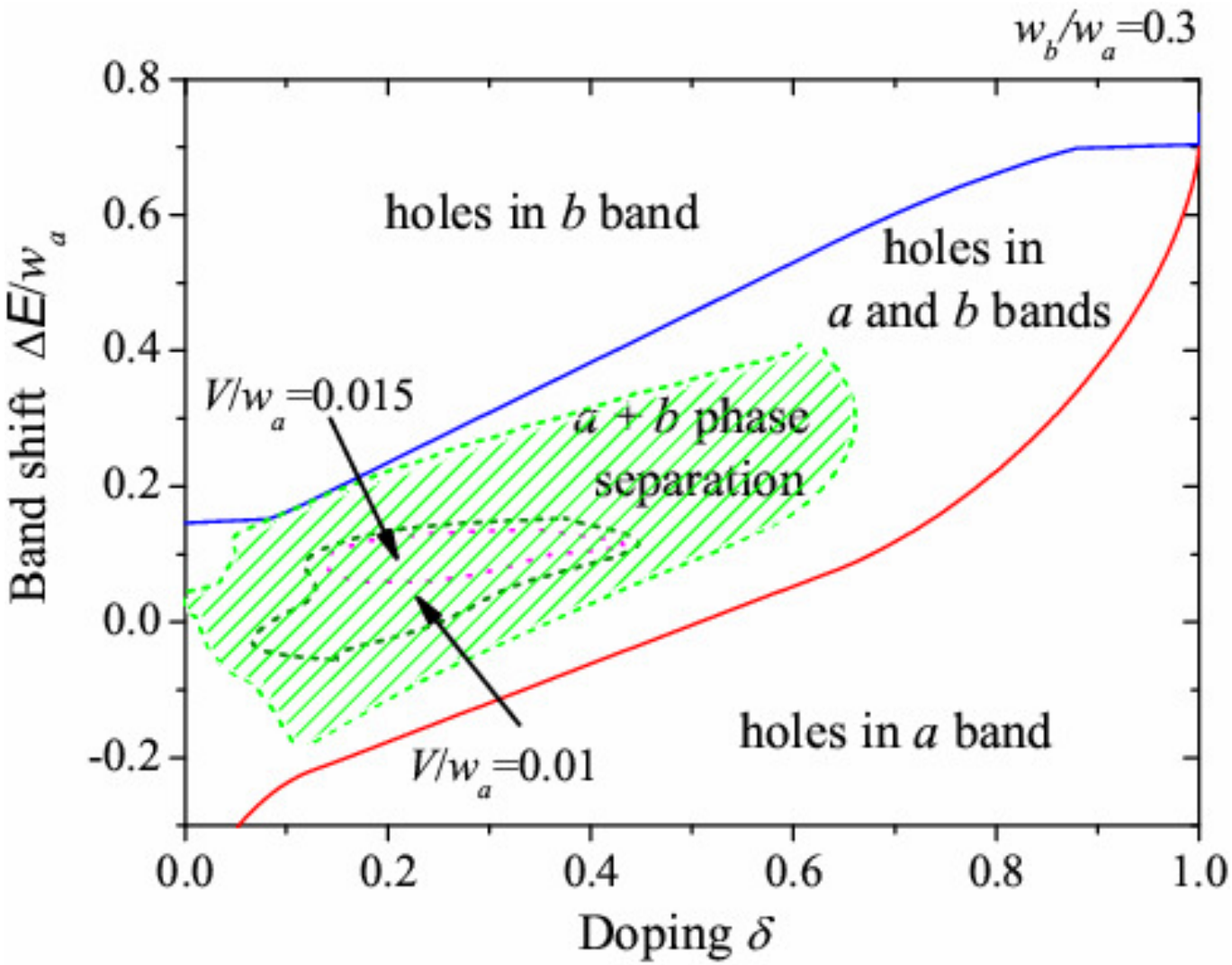
Phase separation at different values of bandwidth ratio



Bandwidth ratio
w_b/w_a =
0.1 (1)
0.2 (2)
0.3 (3)
0.35 (4)
0.4 (5)

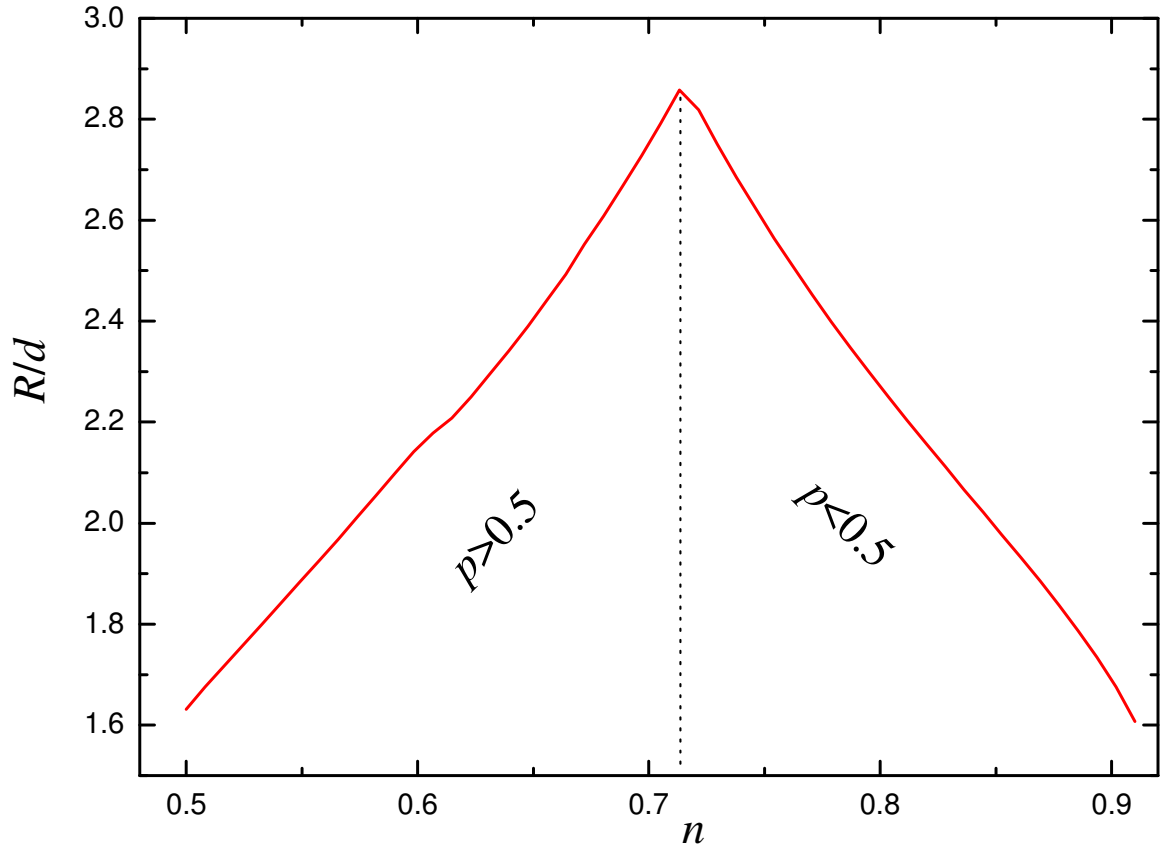
At w_b/w_a >0.4, the phase separation is unfavorable in energy.

Phase diagram at $w_b/w_a = 0.3$



Radius of a droplet

$$R = d\left(\frac{15\sigma(n_1, n_2)}{4\pi V_0^2 (n_1 - n_2)^2 (2 - 3p^{1/3} + p)}\right)^{1/3}$$

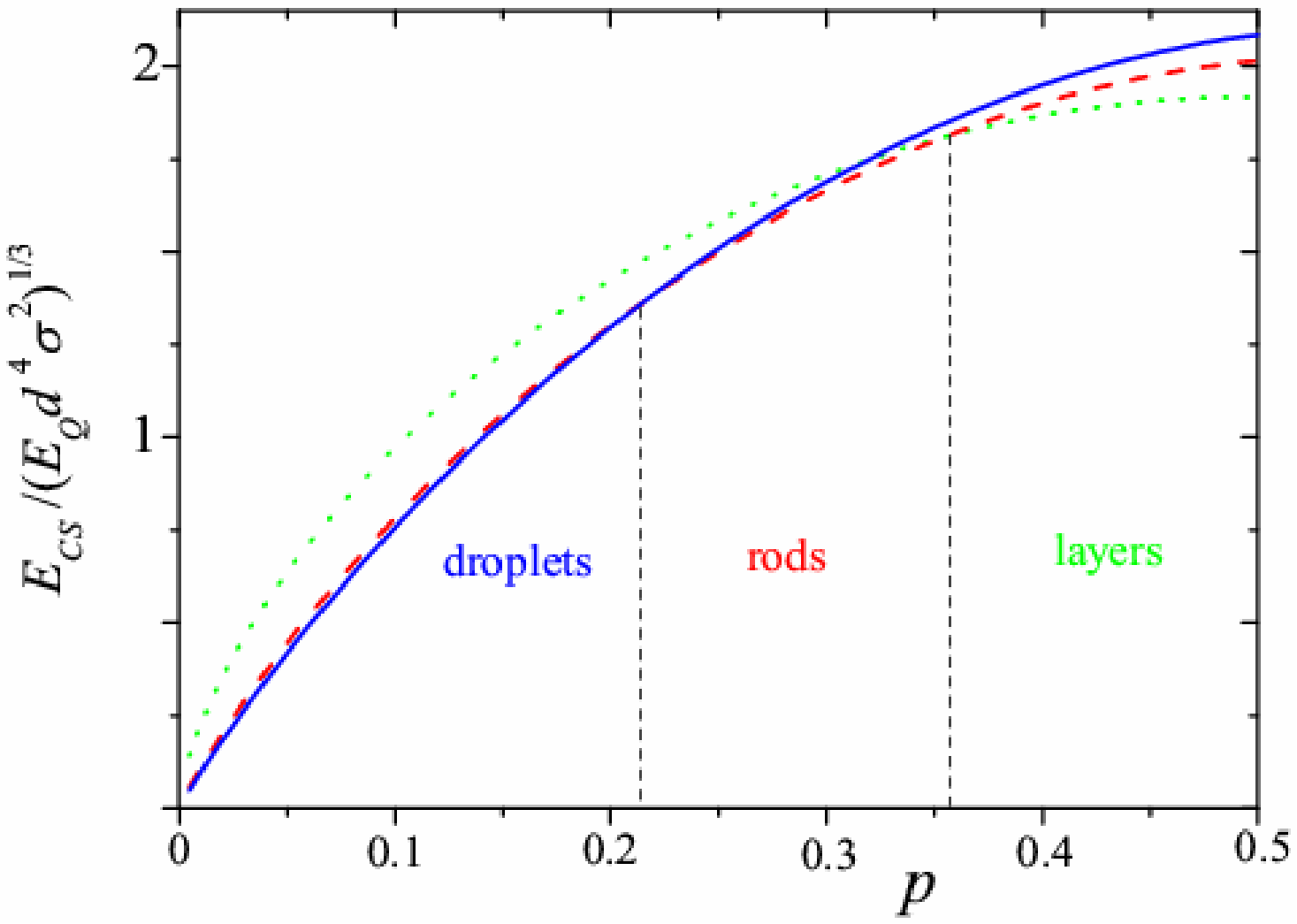


$w_d/w_b = 5$

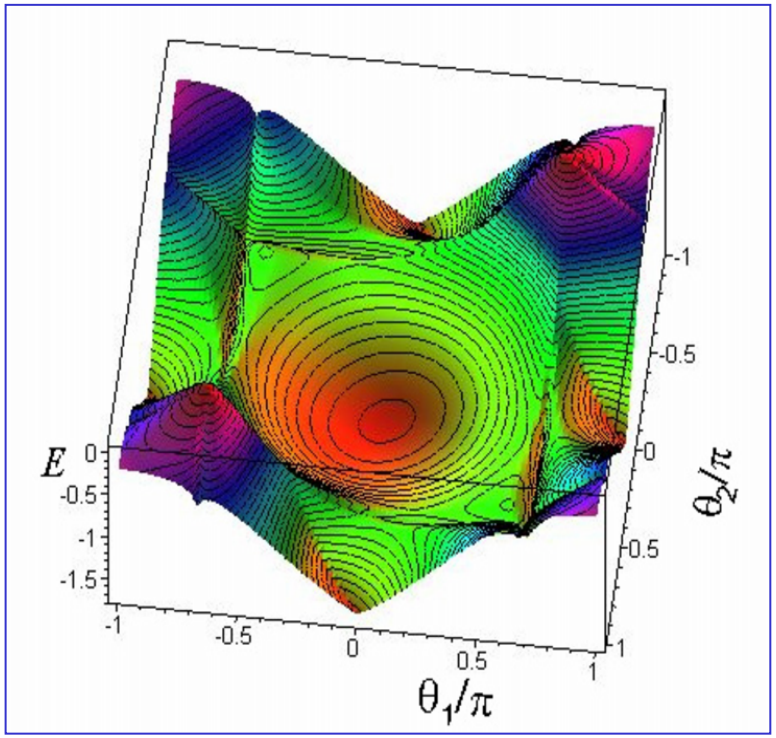
$\varepsilon/w_a = 0.12$

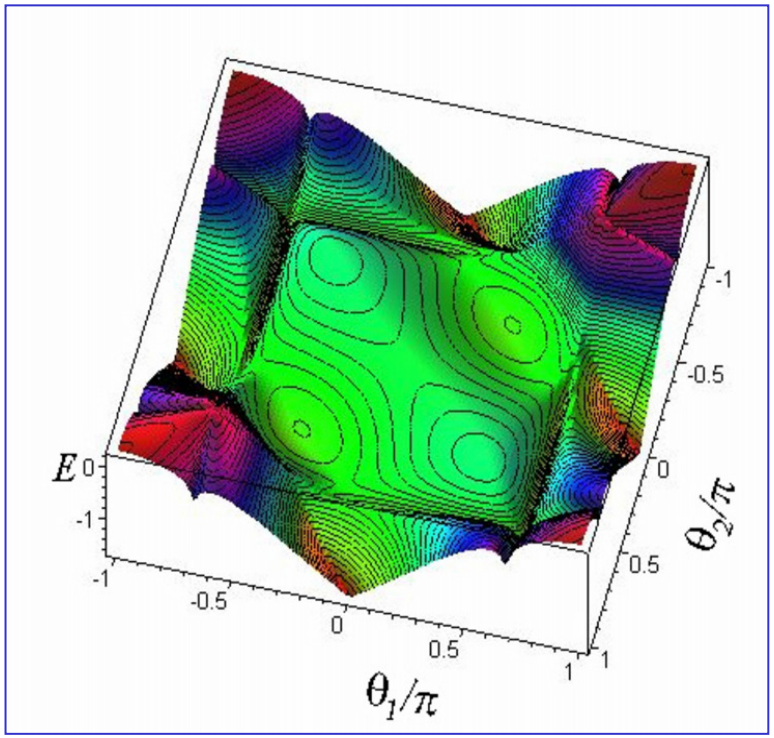
$V_0/w_a = 0.02$

Possible shapes of inhomogeneities



Energy $E(\theta_1,\theta_2)$ has one ($\theta_1 = \theta_2 = 0$; left panel) or four ($\theta_1 = \pm \pi/3$, $\theta_2 = \pm 2\pi/3$ and $\theta_1 \leftrightarrow \theta_2$; right figure) lowest minima depending on J/t_0.



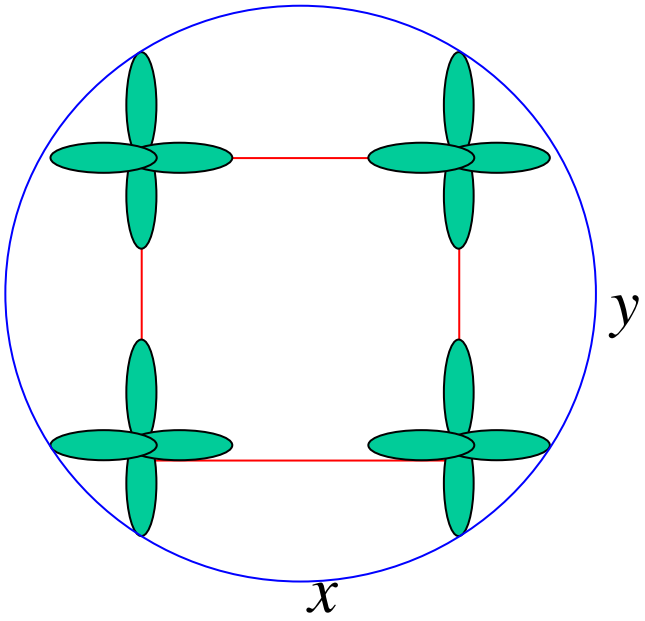


$J < J_{cr}$ ($\cong 0.0075t_0$). $\theta_1 = \theta_2 = 0$: circular ferro – OO droplets with $|x^2\text{-}y^2\rangle$ orbitals.

$J > J_{cr}$. $\theta_1 = \pm \pi/3$, $\theta_2 = \pm 2\pi/3$:1D chains of alternating $|x^2\text{-}z^2\rangle$, $|2y^2\text{-}x^2\text{-}z^2\rangle$ or $|y^2\text{-}z^2\rangle$, $|2x^2\text{-}y^2\text{-}z^2\rangle$ orbitals stretched along y or x axis.

Inhomogeneities in orbitally ordered structures I

A hole introduced by doping becomes self- trapped, forming a ferro – OO region with occupied |θ> orbitals



$d_{x^2-y^2}$ orbitals, $\theta = \pi$

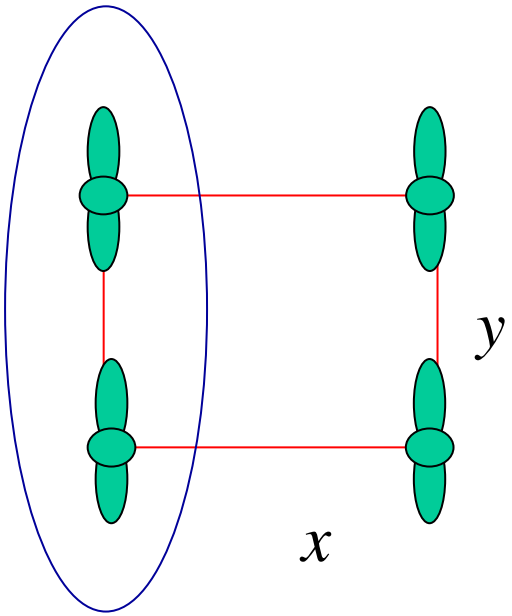
configuration with the highest gain in kinetic energy

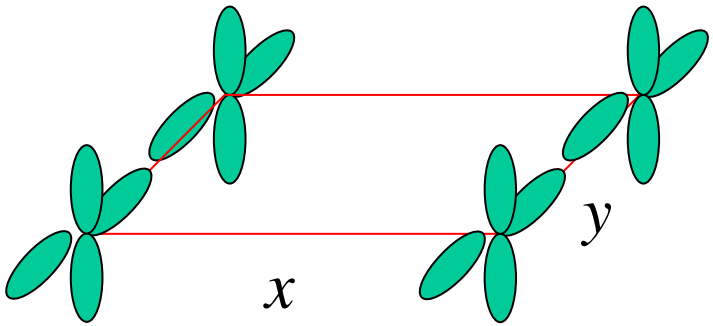
circular droplet

Inhomogeneities in orbitally ordered structures II

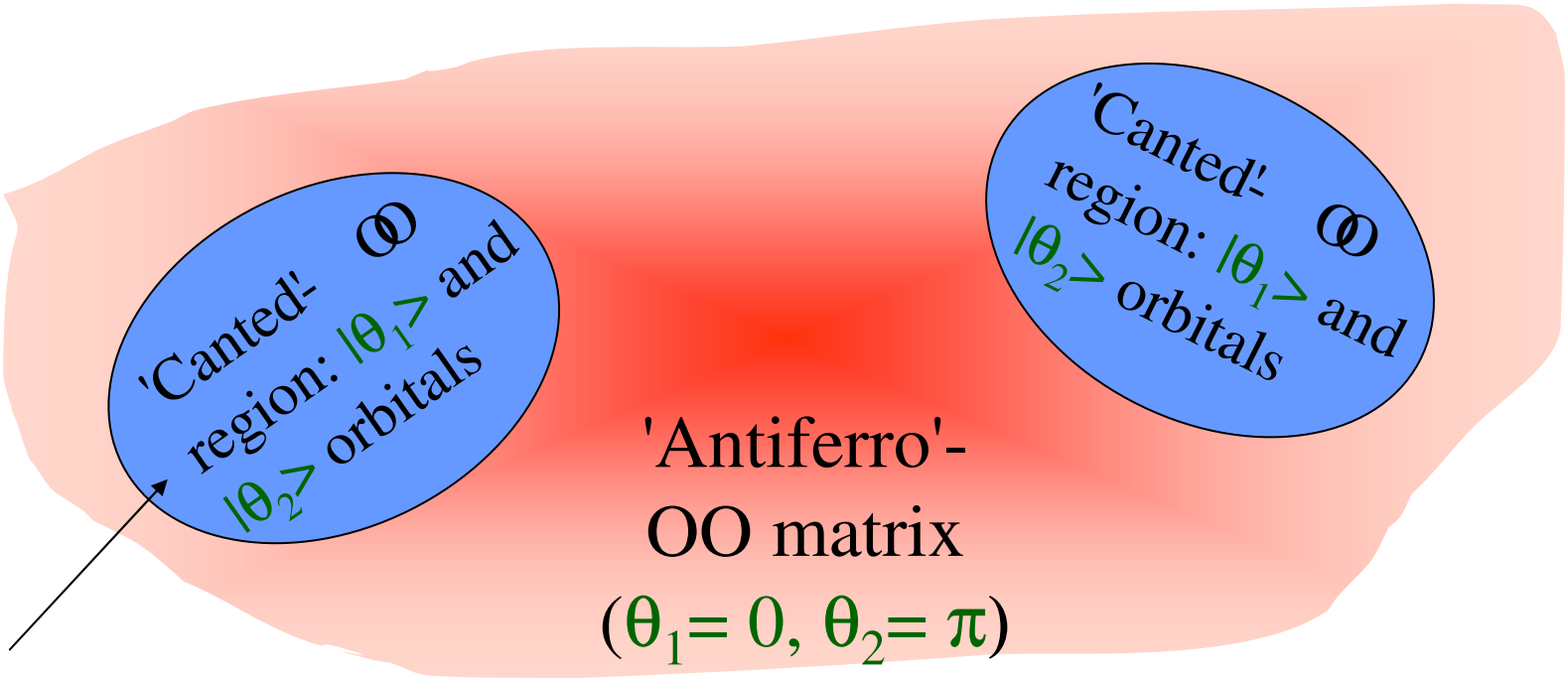
$d_{z^2-y^2}$ orbitals, $\theta = \pi/3$ configuration with a lower loss in the energy of AF – OO background

Needle – like droplet





Inhomogeneous OO states: orbital polarons



Each hole is trapped in an ellipse, forming an OO structure with alternating $|\theta_1\rangle$ and $|\theta_2\rangle$ orbitals.

Effective Hamiltonian of a hole:

$$H^{eff} = -t_0\left[A_x(\theta_1,\theta_2)+A_y(\theta_1,\theta_2)\right]+\frac{t_0}{2}\left[A_x(\theta_1,\theta_2)\frac{\partial^2}{\partial x^2}+A_y(\theta_1,\theta_2)\frac{\partial^2}{\partial y^2}\right]$$

Solving the Schrödinger equation within an ellipse with semiaxes $A_x^{1/2} r_0$, $A_y^{1/2} r_0$, we get the **energy of a OO droplet**:

$$E = \left[-t_0 \left(A_x + A_y \right) + \frac{t_0 j_{0,1}^2}{2\rho_0^2} \right] + 4\pi\rho_0^2 J \sqrt{A_x A_y} \cos^2\left(\frac{\theta_1 - \theta_2}{2} \right), \qquad j_{0,1} \approx 2.405$$

Kinetic energy gain

The cost in the energy of orbital ordering

Minimization of E with respect to r_0 yields:

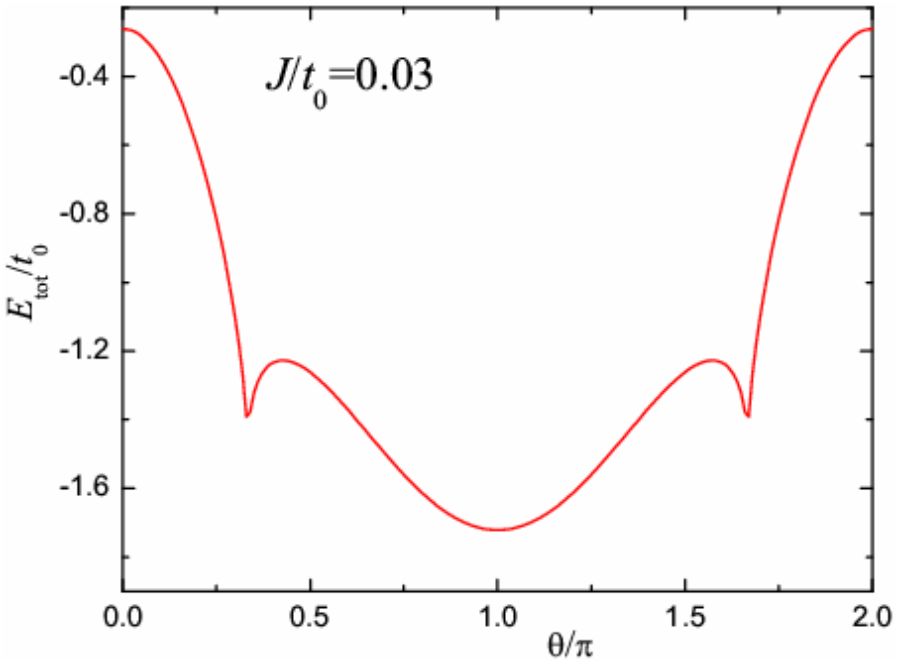
$$E(\theta_1, \theta_2) = -t_0 \left(A_x + A_y \right) + j_{0,1} \left(8\pi t_0 J \sqrt{A_x A_y} \right)^{1/2} \left| \cos\left(\frac{\theta_1 - \theta_2}{2} \right) \right|$$

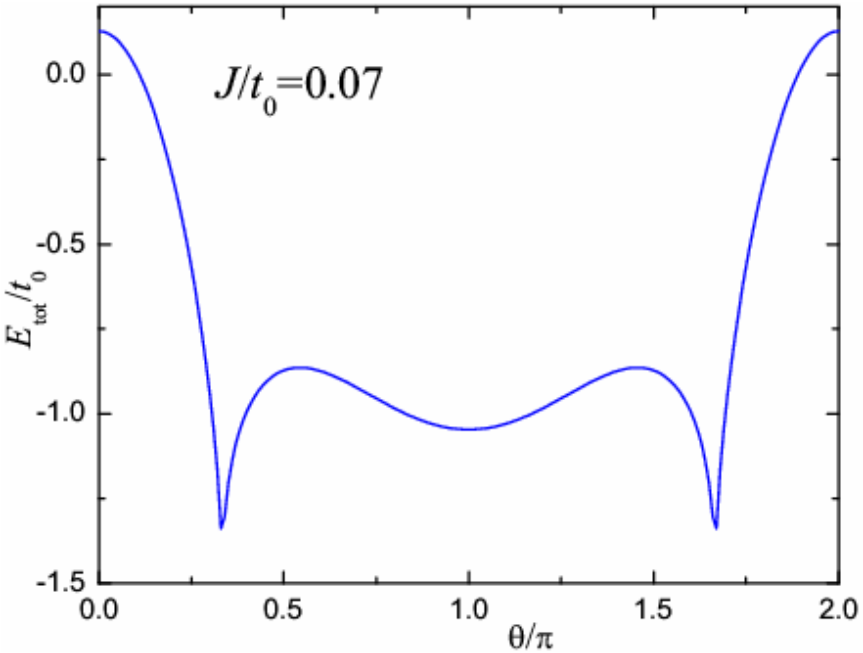
Energy of ferro – OO droplet *vs* angle θ

J: energy loss of AF O background (per site) due to the formation of ferro – OO droplet

$J_c/t_0 \approx 0.05$

t_0: characteristic hopping integral





$J < J_c$ $d_{x^2-y^2}$ orbitals, $\theta = \pi$

$J > J_c$ $d_{z^2-y^2}$ orbitals, $\theta = \pi/3$