Quantum Criticality in Polar Materials II :

A Flavor for Two Current Research Projects

P. Chandra
(Rutgers)

How can systems that have classical first-order transitions display quantum criticality ??

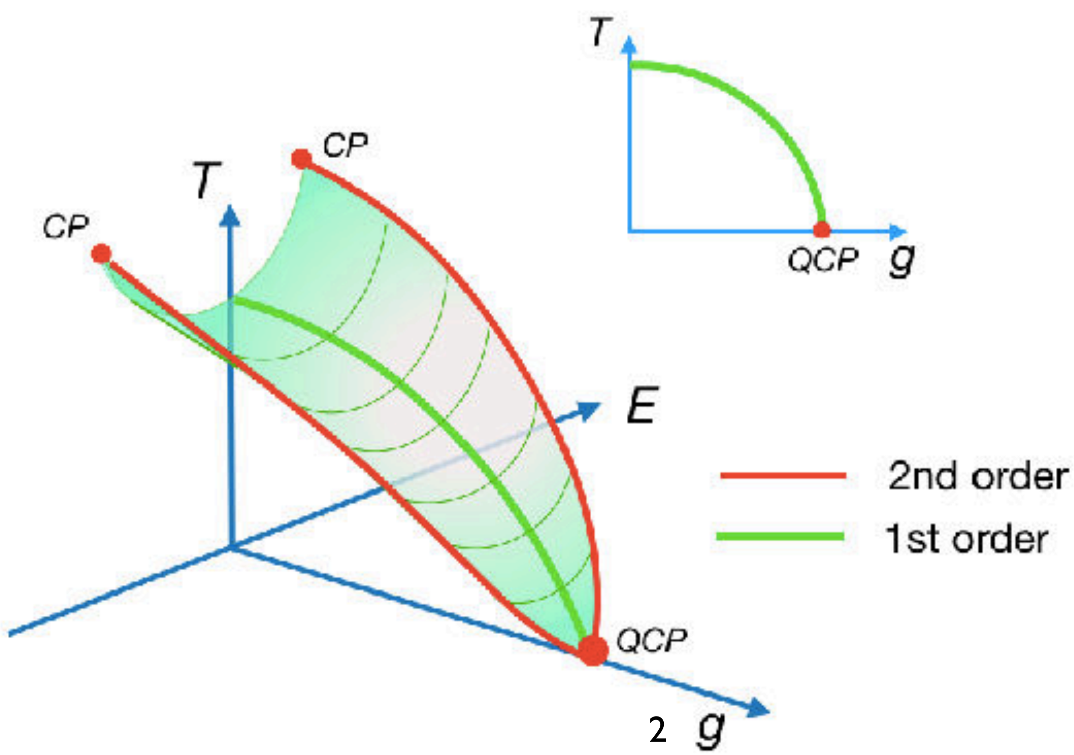
Can metals near polar quantum critical points host novel strongly correlated phases ??

Many more questions for future research

Interplay of Quantum Criticality with First Order Phase Transitions?

P. Coleman (Rutgers)
M. Continentino (CBPF)
G. Lonzarich (Cambridge)

Quantum Annealed Criticality



arXiv 1805.11771

Interplay of Quantum Criticality with First Order Phase Transitions?

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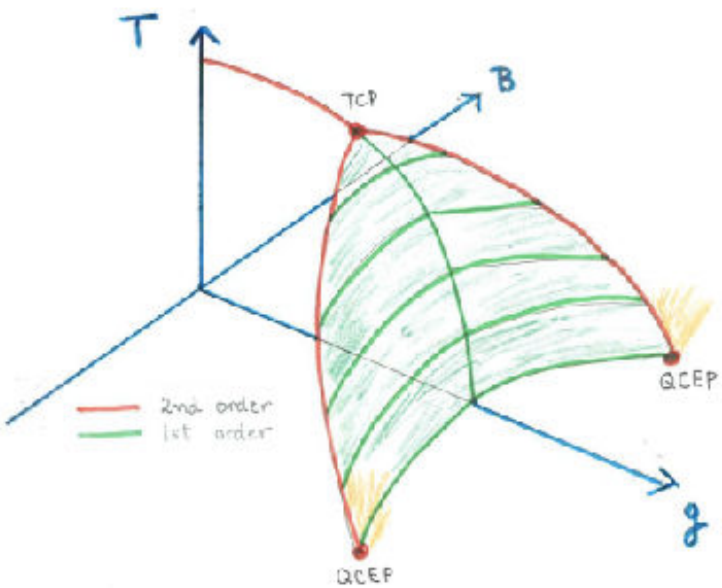
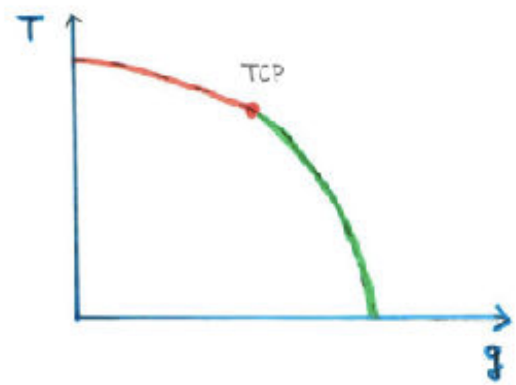
Quantum Critical Endpoints





Grigera et al. Science (2001)
Brando et al. RMP (2016)

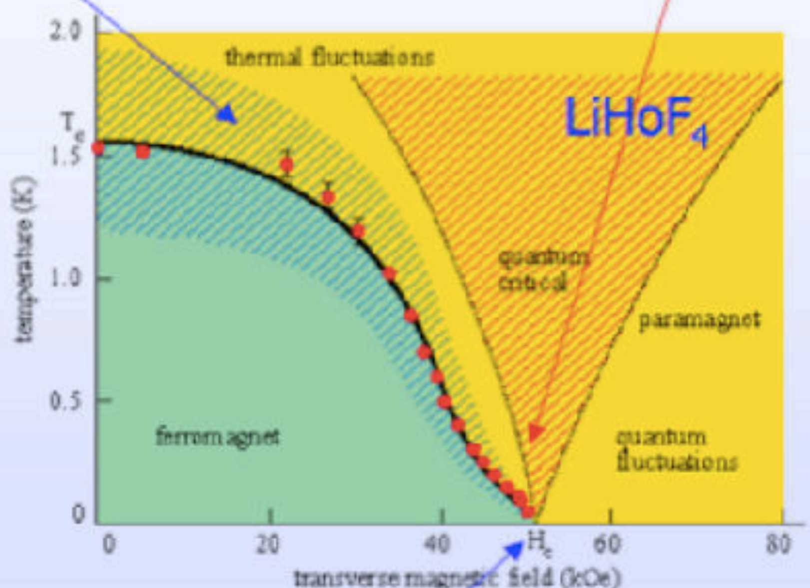
Classical and Quantum Phase Transitions

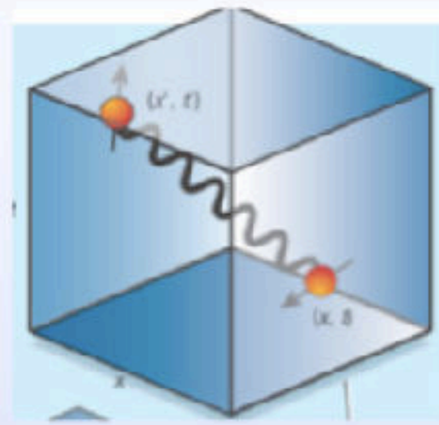
classical phase transition

$\xi \propto (T - T_c)^{-\nu_c}$ $(T >> J)$

quantum critical regime

$\xi(T) \propto T^{-\frac{1}{z}}$ $(T << J)$





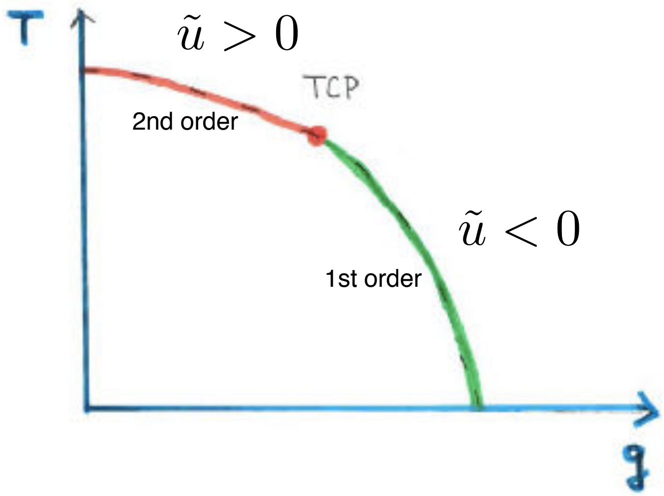
$d_{eff} = d + z$

D. Bitko et al., Phys. Rev. Lett. **77,** 940 (1996)

2nd order quantum phase transition

$$\xi(T = 0) \propto (g - g_c)^{-\nu}$$

Quantum Critical Endpoints



$$\tilde{u} \quad = \quad -u_0 \quad + \quad \Delta u$$

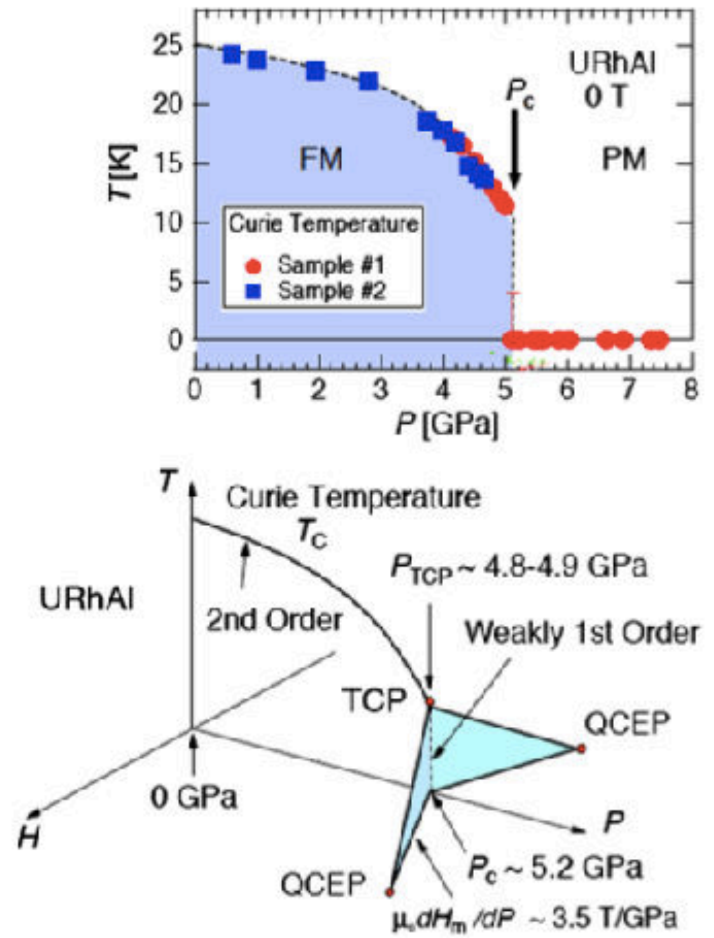
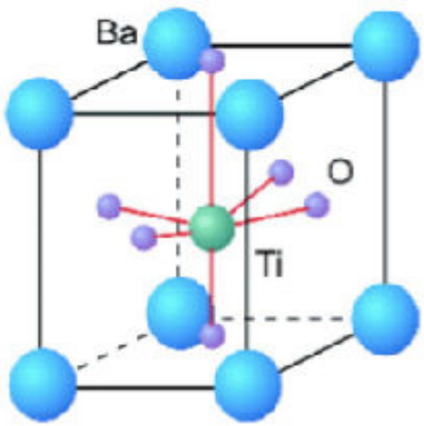


FIG. 11. Upper panel: Temperature-pressure phase diagram of URhAl in zero field determined from resistivity measurements. Lower panel: Temperature-pressure-field diagram inferred from metamagnetic behavior observed in an external field. From Shimizu *et al.*, 2015b.

Grigera et al. Science (2001)

Brando et al. RMP (2016)

Experimental Motivation: Ferroelectrics



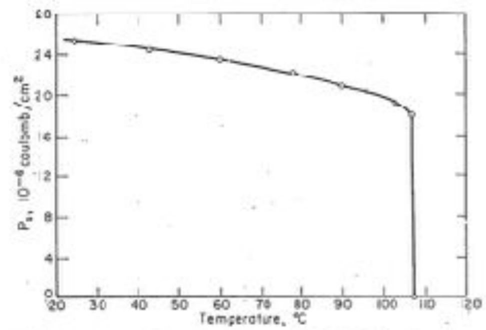
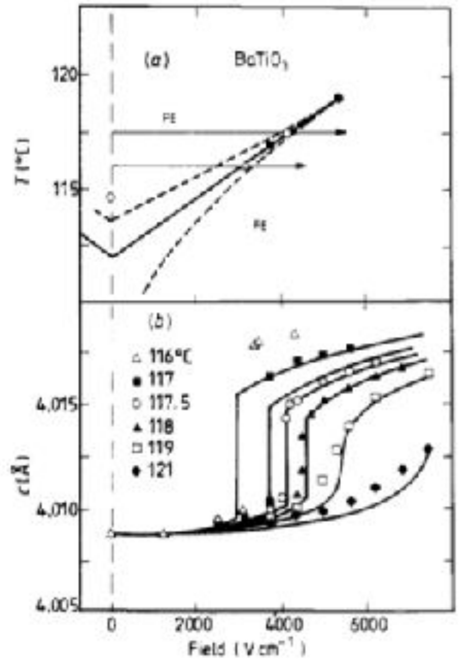


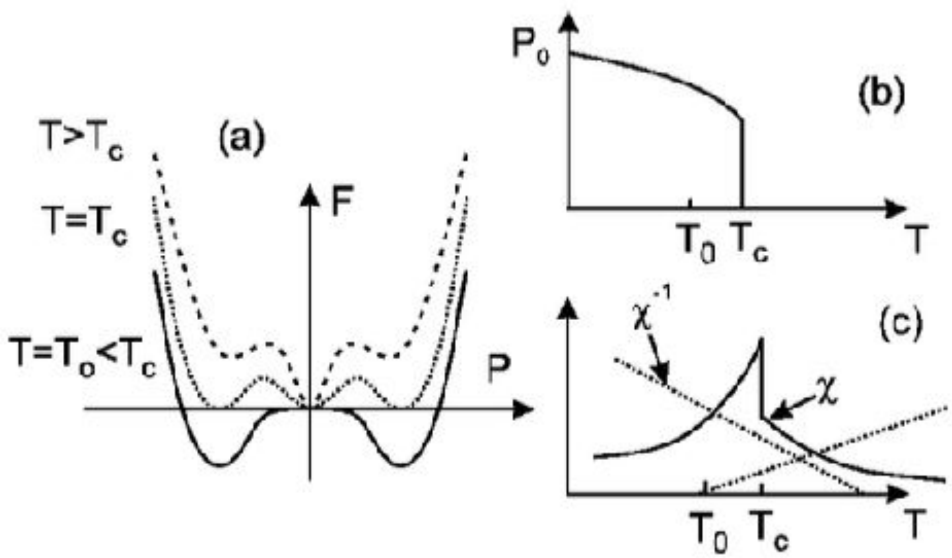
FIG. IV-. Spontaneous polarization of tetragonal $BaTiO_3$ as a function of temperature (according to Merz (M 21)).

Jona and Shirane, FE Crystals (1962)

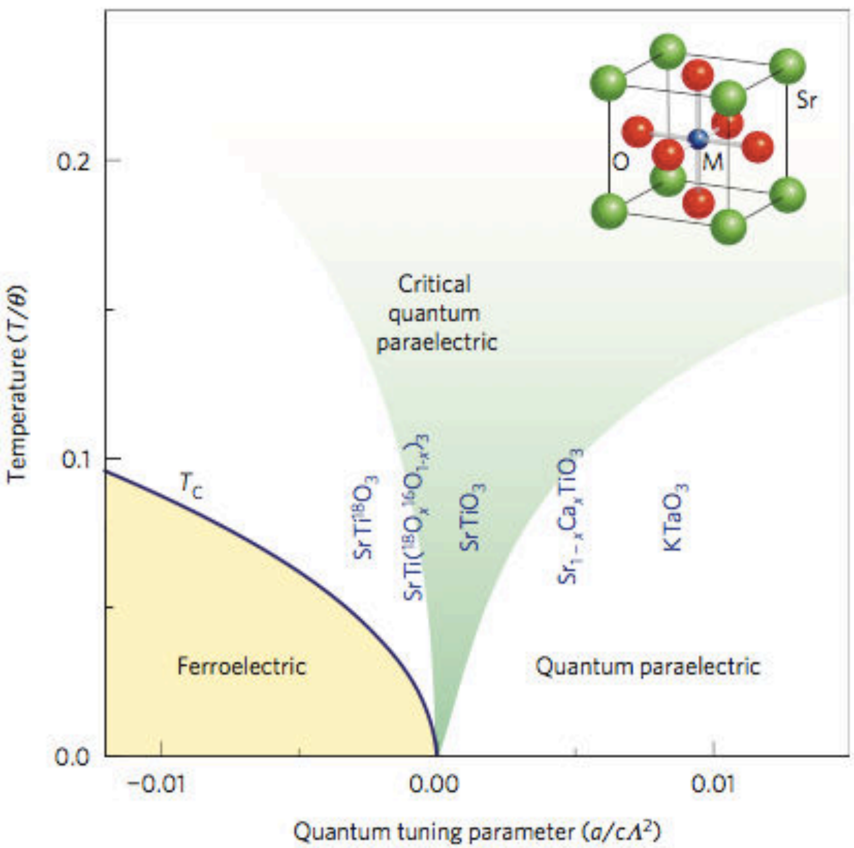


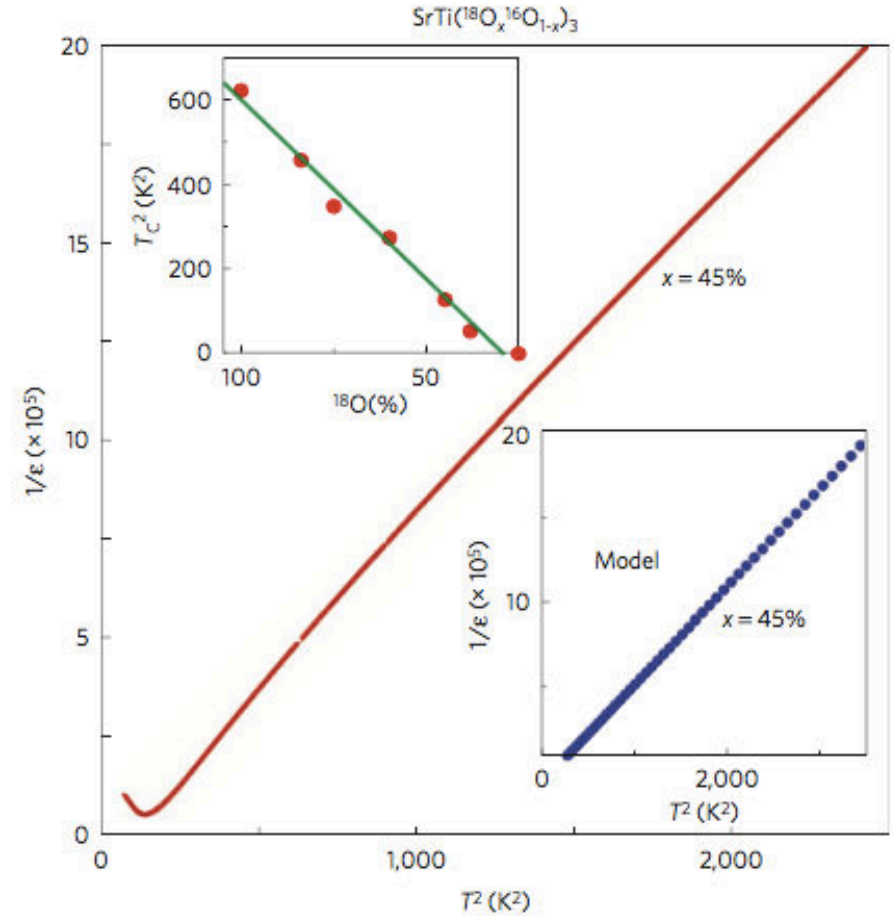
McWhan et al., J.Phys. C (1985)

Figure 1. (*a*) Phase diagram of $BaTiO_3$ showing line of first-order transitions terminating at a critical point (full circle). (*b*) Lattice constant against electric field at different temperatures. Full and broken curves in 1(*a*) and 1(*b*) are calculated by minimising the free energy and they correspond to the equilibrium and spinodal boundaries.



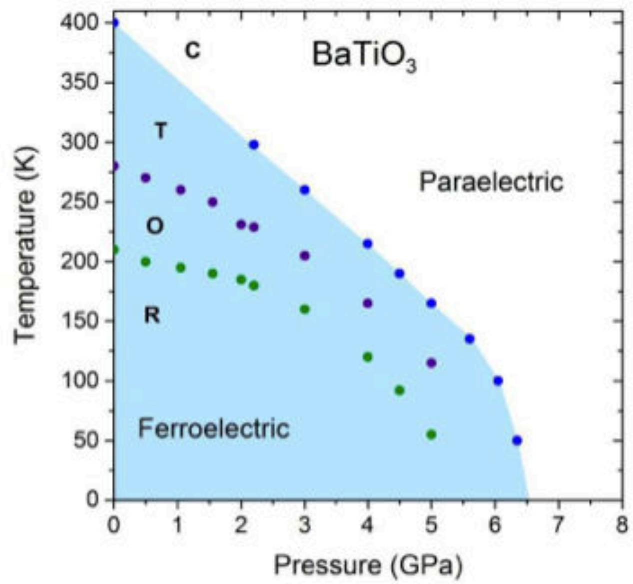
Classically First-Order !

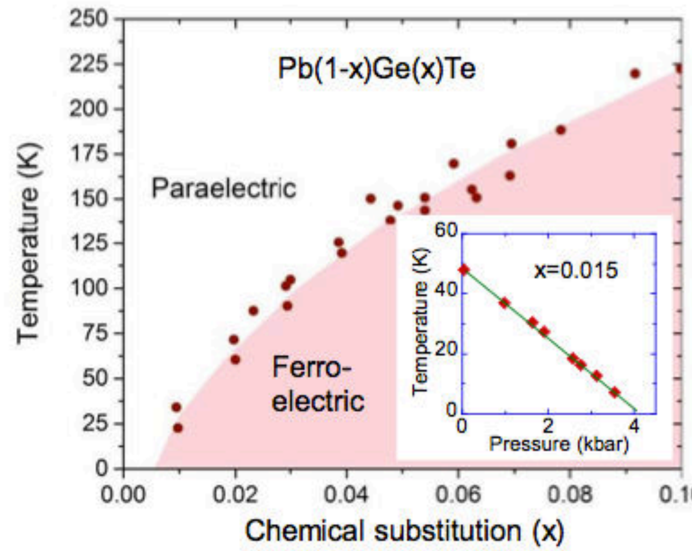


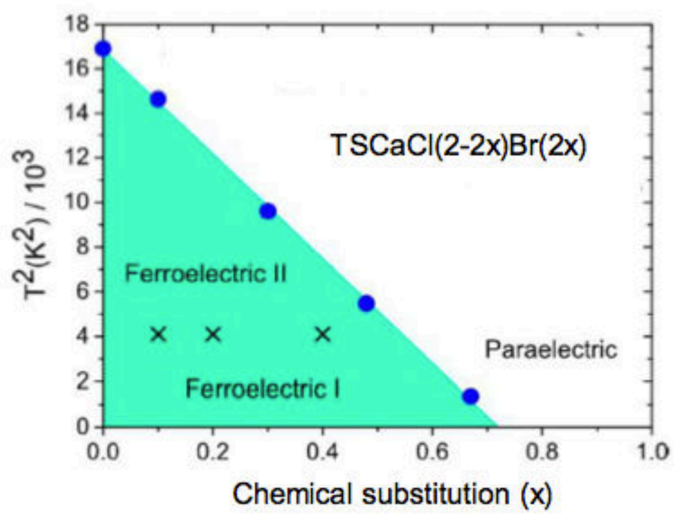


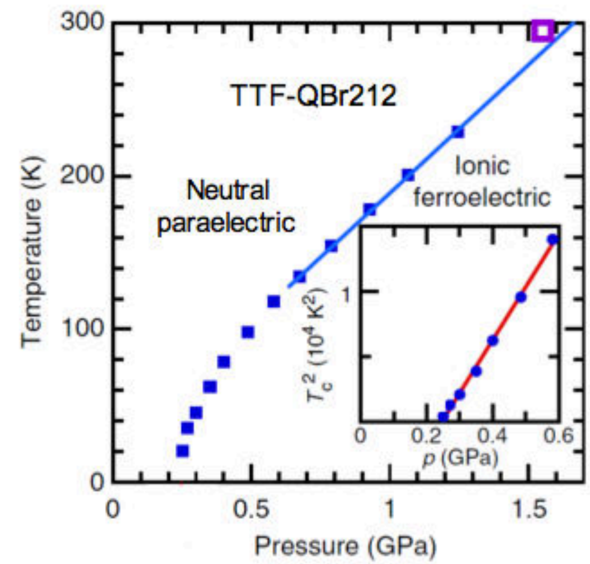
S. Rowley, L. Spalek, R. Smith, M. Dean, M. Itoh, J.F. Scott, G.G. Lonzarich and S. Saxena, Nature Physics 10, 367-72 (2014)

Quantum Criticality with Classical First-Order Transitions ?









PC, Lonzarich, Rowley and Scott, ROPP (2017)

(Classical) Larkin-Pikin Mechanism

(A. I. Larkin and S. Pikin, Sov. Phys. JETP 29, 891 (1969))

Interaction of strain with fluctuating critical order parameter

Diverging Specific Heat in a Clamped System

$\downarrow$

1st Order Transition in the Unclamped System

LP Criterion for 1st Order Transition

$$\kappa < \frac{\Delta C_V}{T_c}\left(\frac{dT_c}{d\ln V}\right)^2$$

$$\kappa^{-1} = K^{-1} - (K + \frac{4}{3}\mu)^{-1}$$

$$\kappa \sim K\frac{c_L^2}{c_T^2}$$

Shear Strain Crucial

Coupling of the uniform strain to the energy density

$\downarrow$

Macroscopic Instability of the Critical Point

$\downarrow$

Discontinuous Phase Transition

Generalization for the Quantum Case ???

Overview of the Classical Larkin-Pikin Mechanism

Simplest case: Isotropic elasticity and scalar order parameter
Compressible system where order parameter $\psi(\vec{x})$ is coupled to the volumetric strain

$$\mathcal{S}[\psi, u] = \mathcal{S}_A + \mathcal{S}_B + \mathcal{S}_I = \frac{1}{T}\int d^3x(\mathcal{L}_A[\psi] + \mathcal{L}_B[u] + \mathcal{L}_I[\psi, e]).$$

$$\mathcal{L}_A[\psi, a, b] = \frac{1}{2}(\partial_\mu\psi)^2 + \frac{a}{2}\psi^2 + \frac{b}{4!}\psi^4,$$

Physics of the Order Parameter

$$a \propto \frac{T - T_c}{T_c} \text{ and } b > 0$$

Sole Contribution for the Clamped Case

Overview of the Classical Larkin-Pikin Mechanism

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$$\mathcal{S}[\psi, u] = \mathcal{S}_A + \mathcal{S}_B + \mathcal{S}_I = \frac{1}{T}\int d^3x(\mathcal{L}_A[\psi] + \mathcal{L}_B[u] + \mathcal{L}_I[\psi, e]).$$

$$\mathcal{L}_B[u] = \frac{1}{2}\left[\left(K - \frac{2}{3}\mu\right)e_{ll}^2 + 2\mu e_{ab}^2\right] - \sigma_{ab}e_{ab}$$

Describes Elastic Degrees of Freedom

σ_{ab} External Stress

$u_a(\vec{x})$ Local Atomic Displacement

$$e_{ab}(\vec{x}) = \frac{1}{2}\left(\frac{\partial u_a}{\partial x_b} + \frac{\partial u_b}{\partial x_a}\right)$$ Strain Tensor

$$e_{ll}(x) = \mathrm{Tr}[e(\vec{x})]$$ Volumetric Strain

Overview of the Classical Larkin-Pikin Mechanism

Simplest case: Isotropic elasticity and scalar order parameter
Compressible system where order parameter $\psi(\vec{x})$ is coupled to the volumetric strain

$$\mathcal{S}[\psi, u] = \mathcal{S}_A + \mathcal{S}_B + \mathcal{S}_I = \frac{1}{T}\int d^3x(\mathcal{L}_A[\psi] + \mathcal{L}_B[u] + \mathcal{L}_I[\psi, e]).$$

$$\mathcal{L}_I[\psi, e] = \lambda e_{ll}\psi^2$$

Interaction between the Volumetric Strain and the Squared Amplitude of the Order Parameter

$$\lambda = \left(\frac{dT_c}{d\ln V}\right)$$

Coupling Constant Associated with the Strain-Dependence of T_c

ψ^2 “Energy Density” of the Order Parameter

Overview of the Classical Larkin-Pikin Mechanism

Simplest case: Isotropic elasticity and scalar order parameter
Compressible system where order parameter $\psi(\vec{x})$ is coupled to the volumetric strain

$$\mathcal{S}[\psi, u] = \mathcal{S}_A + \mathcal{S}_B + \mathcal{S}_I = \frac{1}{T}\int d^3x(\mathcal{L}_A[\psi] + \mathcal{L}_B[u] + \mathcal{L}_I[\psi, e]).$$

Physics of the Order Parameter

Strain -“Energy Density” Coupling

Describes Elastic Degrees of Freedom

Key Idea: Integrate out Gaussian Elastic Degrees of Freedom

$$Z = \int \mathcal{D}[\psi] \int \mathcal{D}[u]\ e^{-\mathcal{S}[\psi,u]} \qquad \longrightarrow \qquad Z = \int \mathcal{D}[\psi] e^{-S[\psi]}$$

Elastic Degrees of Freedom Gaussian, but Integration Must be Performed Carefully

Special Role of Boundary Normal Modes
(Wavelength Comparable to System Size)

$$(\lambda \sim L)$$

“Elastic Anomaly”: Integration over Boundary Modes Generates a Non-Local Order Parameter Interaction in the Bulk Action

Destroys Locality of Original Theory and Paradoxically is Independent of Detailed Boundary Conditions (as a Bulk Term in the Action)

Elastic Degrees of Freedom Gaussian, but Integration Must be Performed Carefully

In a system with Periodic Boundary Conditions (Larkin-Pikin choice)

$$e_{ab}(\vec{x}) = e_{ab} + \frac{1}{V}\sum_{\vec{q}\neq 0}\frac{i}{2}[q_a u_b(\vec{q}) + q_b u_a(\vec{q})]e^{i\vec{q}\cdot\vec{x}},$$

Boundary Mode

Fluctuating Atomic Displacements

$$\{a,b\} \in [1,3] \qquad V = L^3$$

$u_a(q)$ Fourier Transform of $u_a(x)$

$$\vec{q} = \frac{2\pi}{L}(l,m,n)$$

l, m, n Integers

Elastic Degrees of Freedom Gaussian, but Integration Must be Performed Carefully

In a system with Periodic Boundary Conditions (Larkin-Pikin choice)

$$e_{ab}(\vec{x}) = e_{ab} + \frac{1}{V}\sum_{\vec{q}\neq 0}\frac{i}{2}[q_a u_b(\vec{q}) + q_b u_a(\vec{q})]e^{i\vec{q}\cdot\vec{x}},$$

Boundary Mode

Fluctuating Atomic Displacements

Formally solid forms a 3-torus

$$\oint e_{ab}(x)dx_b = e_{ab}\oint dx_b = b_a$$

Burger's vector of the enclosed defects

Boundary Modes of the Strain have a Topological Character

Integration over the Strain Fields

Correction to the Action of the Order Parameter

$$S[\psi] = S_A[\psi, a, b] + \Delta S[\psi]$$

where

$$e^{-\Delta S[\psi]} = \int \mathcal{D}[u] e^{-(S_B + S_I)}$$

The resulting action

$$S[\psi] = S_A[\psi, a, b^*] - \frac{\lambda^2 V}{2T}\left(\frac{1}{K} - \frac{1}{K + \frac{4}{3}\mu}\right)\left[\frac{1}{V^2}\int d^3x \int d^3x' \ \psi^2(x)\ \psi^2(x')\right]$$

$$b^* = b - \frac{12\lambda^2}{K + \frac{4}{3}\mu}$$

Perturbative $O(\lambda^2)$
Renormalization of
the Short-Range Interaction

Distance-Independent Interaction
Between the Energy Densities of
the Order Parameter

This term drives a non-perturbative
first order transition at arbitrarily
small coupling λ

The resulting action

Prefactor Only Nonzero for Finite Shear Modulus $\mu \neq 0$
(Solids but not Liquids)

$$S[\psi] = S_A[\psi, a, b^*] - \frac{\lambda^2 V}{2T} \overbrace{\left(\frac{1}{K} - \frac{1}{K + \frac{4}{3}\mu}\right)}^{\kappa^{-1}} \left[\frac{1}{V^2} \int d^3x \int d^3x' \; \psi^2(x) \; \psi^2(x')\right]$$

q = 0 Strain

Only Present for the Clamped System

Subtly from finite q elastic fluctuations. Residual repulsion due to "boson hole" in the longitudinal interactions

Present for Clamped System

Distance-Independent Interaction Between the Energy Densities of the Order Parameter

This term drives a non-perturbative first order transition at arbitrarily small coupling λ

The resulting action

$$S[\psi] = S_A[\psi, a, b^*] - \frac{\lambda^2 V}{2T}\left(\frac{1}{K} - \frac{1}{K+\frac{4}{3}\mu}\right)\left[\frac{1}{V^2}\int d^3x \int d^3x' \; \psi^2(x)\; \psi^2(x')\right]$$

$$S[\psi] = S_A - \frac{\lambda^2 V}{2T\kappa}(\Psi^2)^2$$

$$\Psi^2 \equiv \left[\frac{1}{V}\int d^3x \; \psi^2(x)\right]$$

Volume Average of the Energy Density

Intensive Variable

$$\langle(\delta\Psi^2)\rangle \sim O\left(\frac{1}{V}\right)$$

$$\delta\Psi^2 = \Psi^2 - \langle\Psi^2\rangle$$

The resulting action

$$S[\psi] = S_A[\psi, a, b^*] - \frac{\lambda^2 V}{2T}\left(\frac{1}{K} - \frac{1}{K + \frac{4}{3}\mu}\right)\left[\frac{1}{V^2}\int d^3x \int d^3x' \; \psi^2(x)\; \psi^2(x')\right]$$

$$\downarrow$$

$$S[\psi] = S_A - \frac{\lambda^2 V}{2T\kappa}(\Psi^2)^2$$

$$\left(\Psi^2\right)^2 = \left(\langle\Psi^2\rangle + \delta\Psi^2\right)\right)^2 = 2\Psi^2\langle\Psi^2\rangle - \langle\Psi^2\rangle^2 + O(1/V)$$

Set of Self-Consistent Equations

$$S[\psi] = \frac{1}{T}\int d^3x \left[\mathcal{L}_A(\psi,a) - \frac{\lambda^2}{\kappa}\langle\Psi^2\rangle\ \psi^2(x)\right] + \frac{\lambda^2 V}{2\kappa}\langle\Psi^2\rangle^2$$

$$\langle\Psi^2\rangle = \frac{\int d\psi\ \Psi^2\ e^{-S_A[\psi]}}{\int d\psi\ e^{-S_A[\psi]}}.$$

Introduce Auxiliary "Strain" Variable $\phi = -\frac{\lambda\langle\Psi^2\rangle}{\kappa}$

$$e^{-\frac{\tilde{F}(\phi)}{T}} = \int \mathcal{D}\psi\ e^{-S[\psi,\phi]}$$

$$S[\psi,\phi] = \frac{1}{T}\int d^3x \left[\mathcal{L}_A(\psi,a) + \lambda\phi\psi^2 + \frac{\kappa}{2}\phi^2\right]$$

Self-Consistency Imposed by Stationarity of the Free Energy

$$\frac{\partial\tilde{F}[\phi]}{\partial\phi} = 0 \quad\Longrightarrow\quad \left[\lambda\langle\Psi^2\rangle + \kappa\phi\right] V = 0.$$

Set of Self-Consistent Equations

$$S[\psi] = \frac{1}{T}\int d^3x \left[\mathcal{L}_A(\psi,a) - \frac{\lambda^2}{\kappa}\langle\Psi^2\rangle\ \psi^2(x)\right] + \frac{\lambda^2 V}{2\kappa}\langle\Psi^2\rangle^2$$

$$\langle\Psi^2\rangle = \frac{\int d\psi\ \Psi^2\ e^{-S_A[\psi]}}{\int d\psi\ e^{-S_A[\psi]}}.$$

Introduce Auxiliary "Strain" Variable $\phi = -\frac{\lambda\langle\Psi^2\rangle}{\kappa}$

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$$S[\psi,\phi] = \frac{1}{T}\int d^3x \left[\mathcal{L}_A(\psi,a) + \lambda\phi\psi^2 + \frac{\kappa}{2}\phi^2\right]$$

Integration out of order parameter fluctuations $\longrightarrow$ $\tilde{\kappa} = \kappa - \Delta\kappa$

Integration out of elasticity variable ϕ

Review of the Original Larkin-Pikin argument

$$S[\psi, \phi] = \frac{1}{T} \int d^3x \, [\mathcal{L}_A(\psi, a + 2\lambda\phi)] + \frac{\kappa V}{2} \phi^2$$

$$a \to x = a + 2\lambda\phi$$

Free energy of the clamped system

$$e^{-\frac{F(a)}{T}} = \int \mathcal{D}[\psi] \; e^{-\mathcal{S}_A[\psi, a]}$$

Free energy of the unclamped system

$$\tilde{F}[\phi, a] = F[x] + \frac{\kappa V}{2} \phi^2$$

$$x = a + 2\lambda\phi$$

Shift of tuning parameter due to energy fluctuations

$$\frac{1}{V}\frac{\partial F}{\partial x} = \frac{\langle \Psi^2 \rangle}{2}$$

$$\phi = -\frac{\lambda \langle \Psi^2 \rangle}{\kappa} = -\frac{2\lambda}{V\kappa}\left(\frac{\partial F}{\partial x}\right) \equiv -\frac{2\lambda}{V\kappa} F'[x]$$

$$\tilde{f} \equiv \frac{2\lambda}{V\kappa}\tilde{F}\ , \qquad f \equiv \frac{2\lambda}{V\kappa} F$$

$$\downarrow$$

Two equations describing the unclamped system

$$\tilde{f} = f[x] + \lambda \left(f'[x]\right)^2$$

$$a = x + 2\lambda f'[x]$$

$$\left(a \propto \frac{T - T_c}{T_c} \equiv t\right)$$

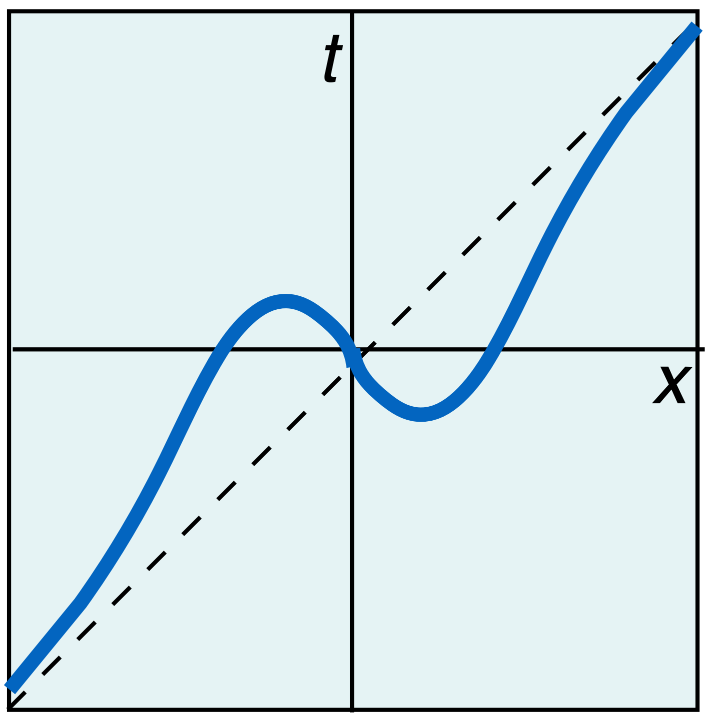
that must be solved self-consistently

Continuous Transition in the Clamped System

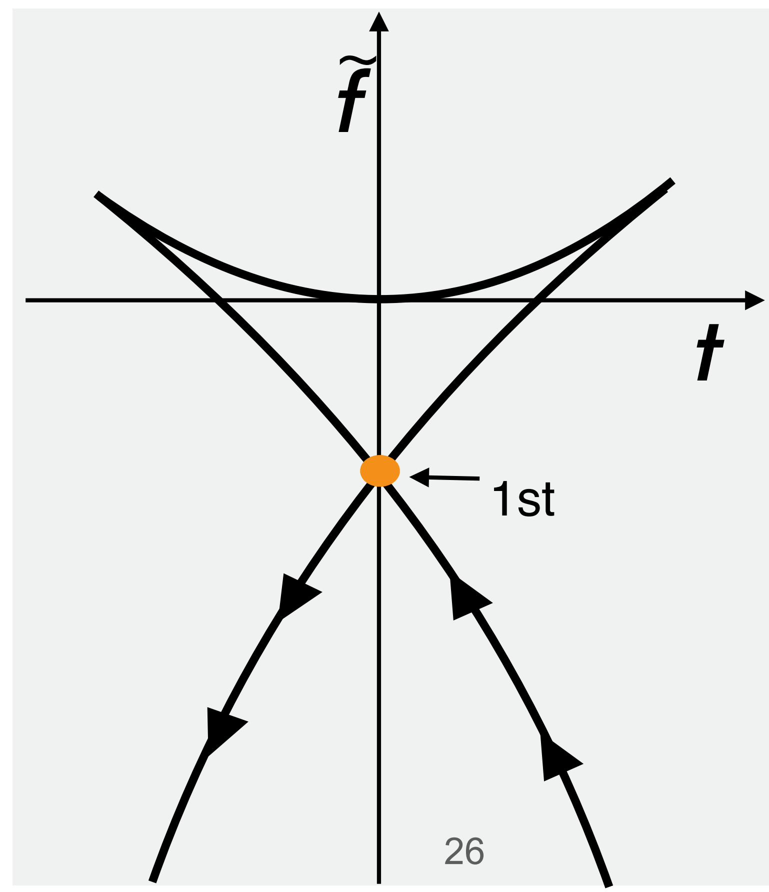
$$\boxed{f \propto -|t|^{2-\alpha} \qquad (\alpha > 0)}$$

$$t = x + 2\lambda f'[x]$$
$$= x - 2\lambda(2-\alpha)|x|^{1-\alpha}\mathrm{sgn}(x)$$

Non-Monotonic



1st Order Phase Transition
for the Unclamped System !!



T = 0 case $(d = d_{space} + z)$ $d > 4$ $\alpha = 0$

$$f \propto -|x|^2$$

$$t = x + 2\lambda f' = x(1 - 4\lambda)$$

Monotonic

Continuous

Marginal Case $d = 4 - \epsilon$

$$f_{sing} = \frac{1}{2} A x^2 \ln x$$

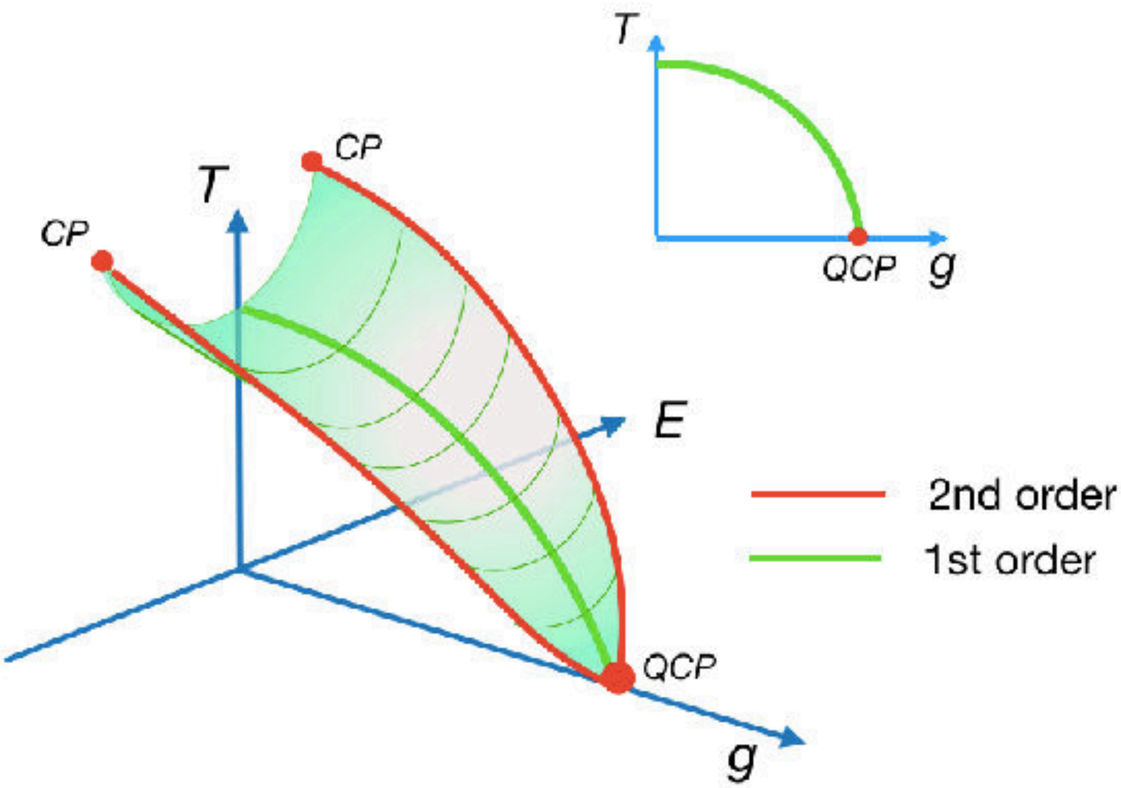
$$t = x + 2\lambda A x \ \ln x \ \sqrt{e}$$

Weakly Non-Monotonic

$$t = 0 \qquad \Delta f \equiv f_2(x = |x^+|) - f_1(x = 0) \propto e^{-\frac{1}{\lambda}}$$

Very Weak First Order Transition

Generalized Larkin-Pikin Results



Experimental Signatures

New Lattice-Sensitive

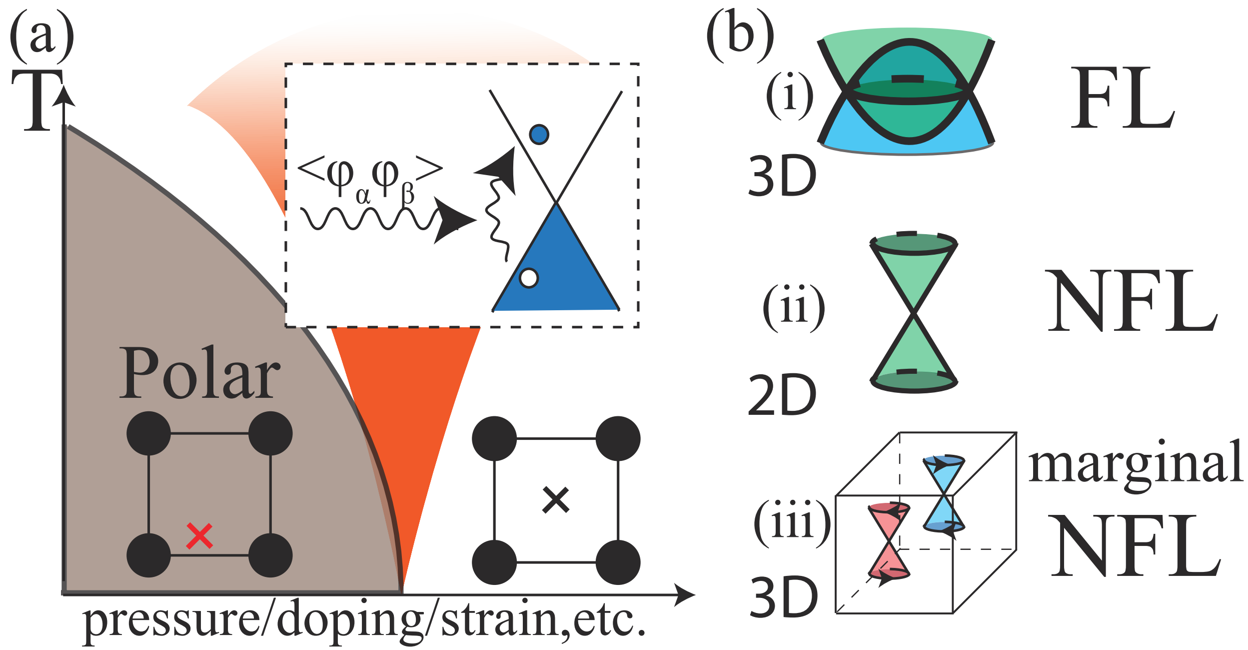
Settings for Exploration

of Exotic Quantum Phases

Elastic Anisotropy ??
Domain Dynamics??
Disorder ??
Metallic Systems ??

PC, P. Coleman, M.A. Continentino and G.G. Lonzarich, arXiv 1805.11771

Multiband Quantum Criticality of Polar Metals

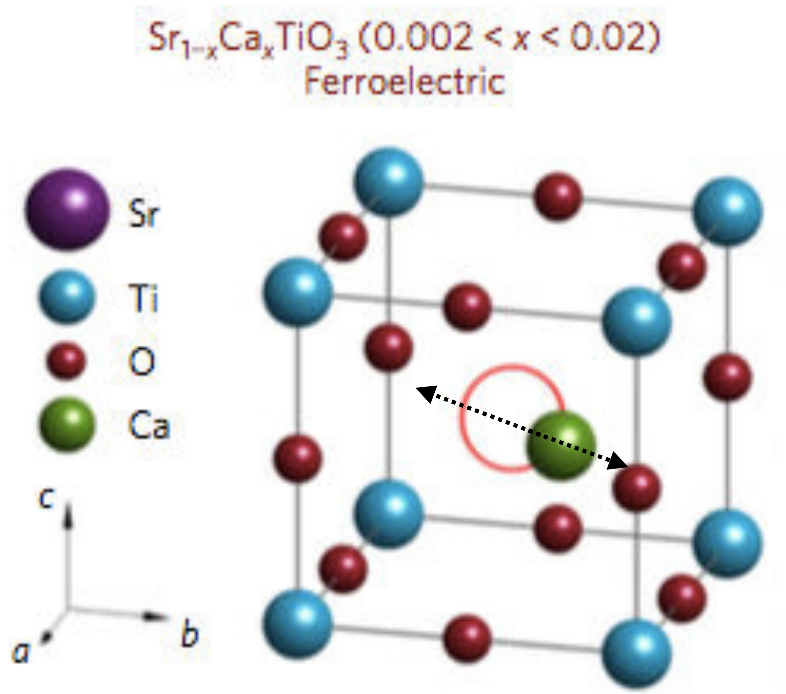


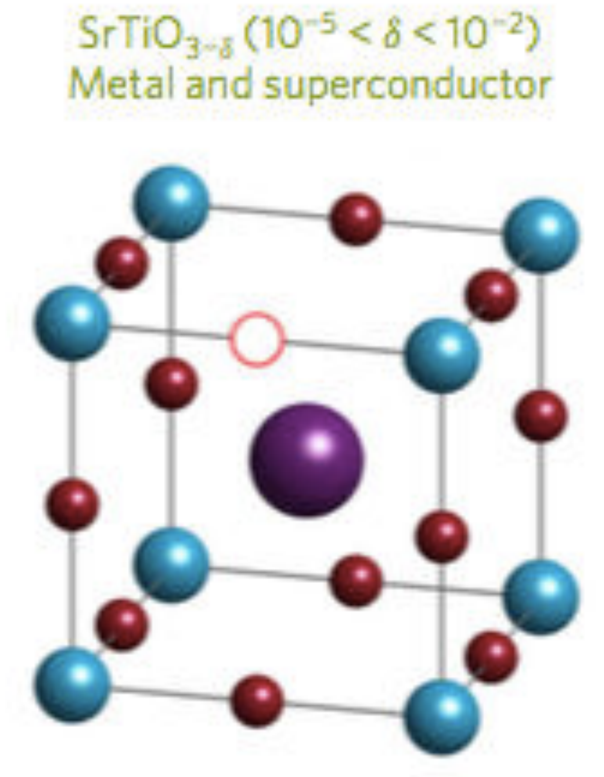
Pavel Volkov (Rutgers)

Novel phases in quantum critical polar metals ??

P.A. Volkov and PC, PRL 124, 237601 (2020)

Polar Metal ?





Critical boson = Transverse Optical Phonon

$$\mathbf{q} \approx 0$$

Rischau et al., Nature Physics 134: 643 (2017)

Polar Metal ?

Doped Ferroelectric

Screening of Dipole Moments

Inversion Symmetry-Breaking Transition Remains

(Anderson and Blount PRL 12, 217 (1965)

Polar Metal ?

Intrinsic and "Engineered
Polar Metals Exist

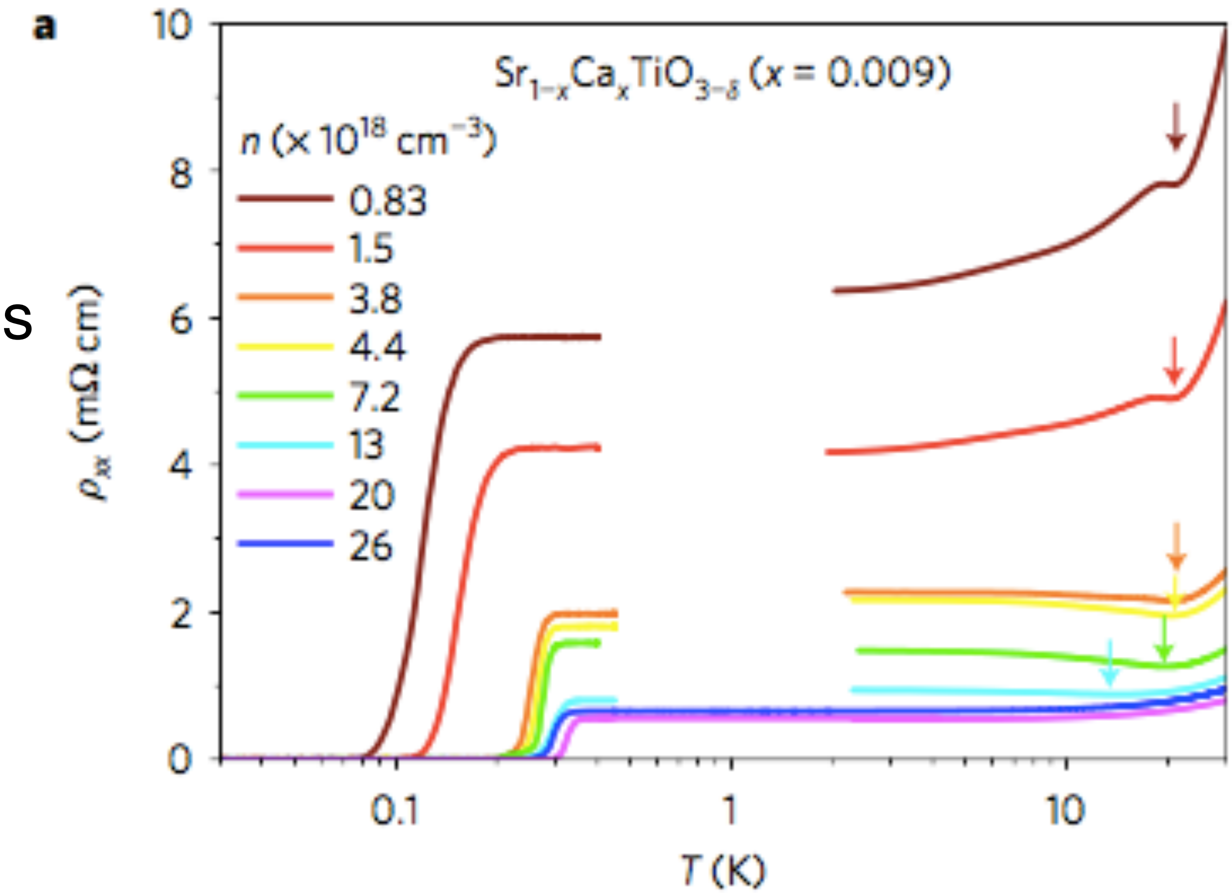
Search for Weyl semimetals

↓

Polar Semimetals

Chemical Tuning of Tc

Novel Metallic Quantum
Criticality ???



Rischau et al., Nature Physics 134: 643 (2017)

Challenge: Strong Electronic Coupling to the Critical Polar Mode ?

Coulomb Interactions
(in weak screening limit lead to LO/TO splitting)

Yukawa Coupling

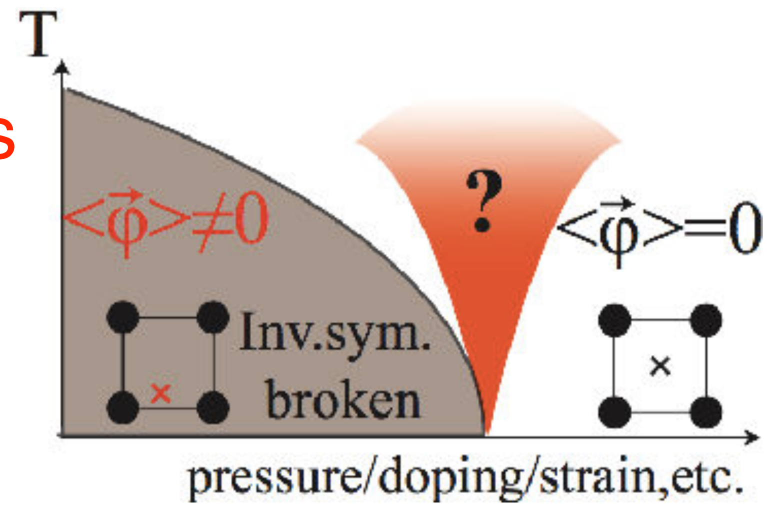
$$H_Y = \lambda \int d\mathbf{r}\varphi(\mathbf{r})c^\dagger(\mathbf{r})c(\mathbf{r}$$

known to produce strong correlations for other QCPs

Polar QCP ??

Yukawa Coupling to the Polar Mode

How do the electrons couple to an inversion symmetry-breaking field?



Wanted: Fermionic bilinear that breaks Inversion Symmetry (but not Time-Reversal Symmetry)

$$H_{coupling} = \lambda \int d\mathbf{k}\ \varphi(\mathbf{k})\ \hat{O}^i(\mathbf{k})$$

Single Conduction Band (without SOC)

$$\hat{O}(\mathbf{k}) = \hat{c}^\dagger_{\mathbf{k}} f_0(\mathbf{k}) \hat{c}_{\mathbf{k}} \qquad\qquad \mathcal{P}, \mathcal{T} \ \rightarrow \ f_0 \quad \text{even}$$

No ISB without TRSB !!

Yukawa Coupling to the Polar Mode

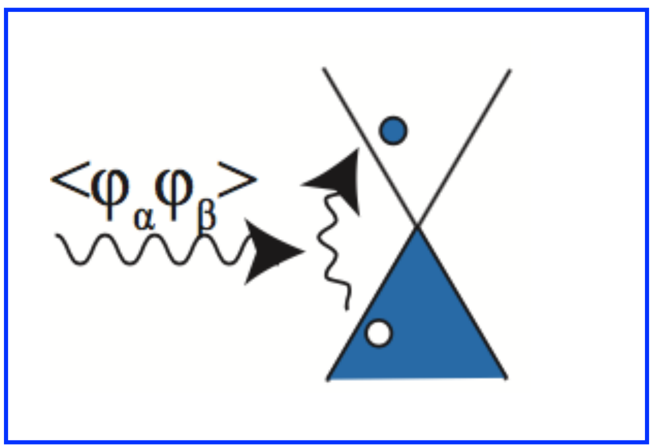
Polar Mode Couples to an Interband Bilinear
(no SOC required)

$$H^{(a)}_{coupl} = \lambda \sum_{i,\mathbf{q},\mathbf{k}} f^i_a(\mathbf{k}) \varphi^i_{\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}/2} \sigma_1 c_{\mathbf{k}-\mathbf{q}/2}, \qquad \mathcal{P} \sim \sigma_3$$

(different parity bands)

$$H^{(b)}_{coupl} = \lambda \sum_{i,\mathbf{q},\mathbf{k}} f^i_b(\mathbf{k}) \varphi^i_{\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q}/2} \sigma_2 c_{\mathbf{k}-\mathbf{q}/2}, \qquad \mathcal{P} \sim \sigma_0$$

(same parity bands)



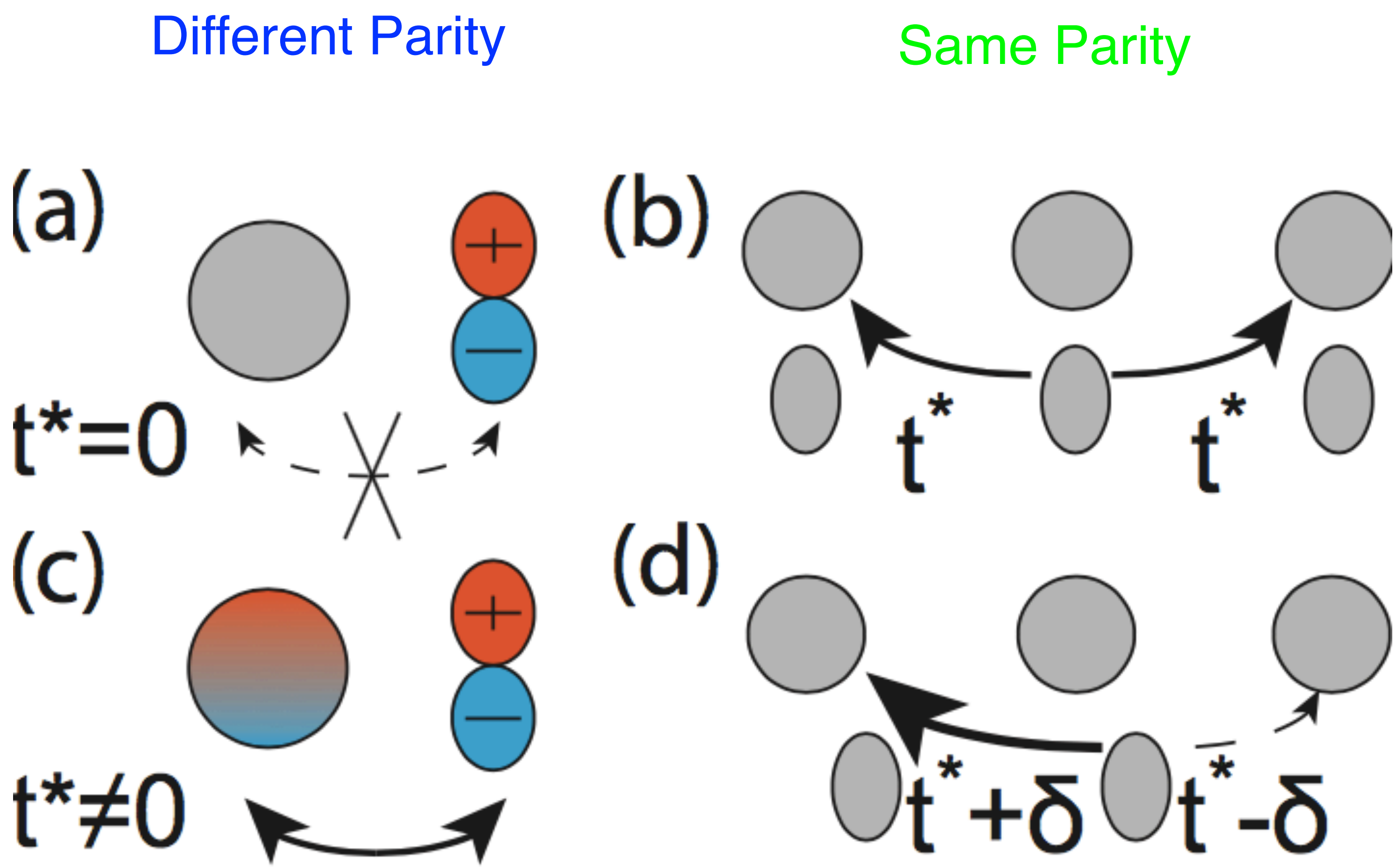
$f^i_{a(b)}(\mathbf{k})$ even (odd) $\mathbf{k}$

Yukawa Coupling to the Polar Mode: Physical Mechanism

(assuming bands arise from two distinct orbitals)

$\varphi^i = 0$

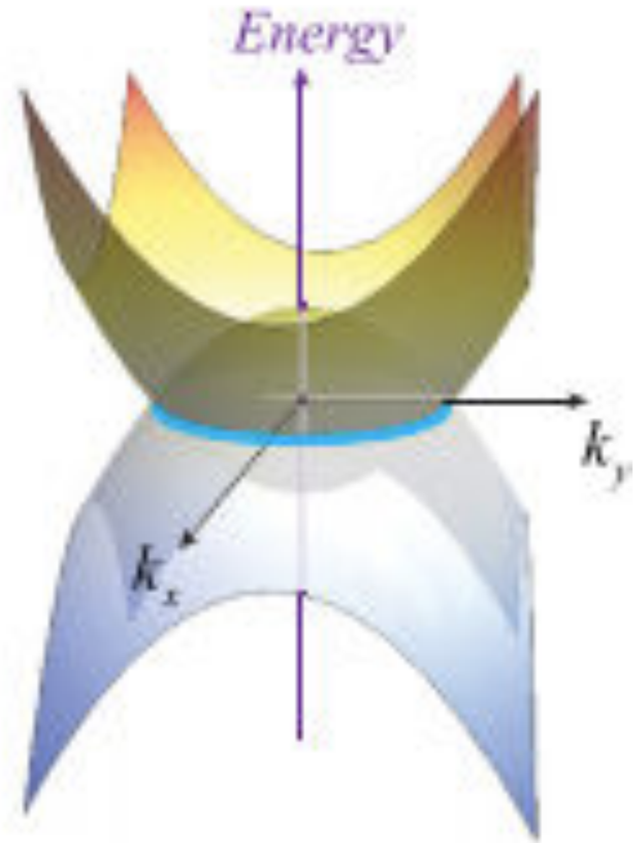
$\varphi^i \neq 0$



Interorbital Hopping Changes in Both Cases !!

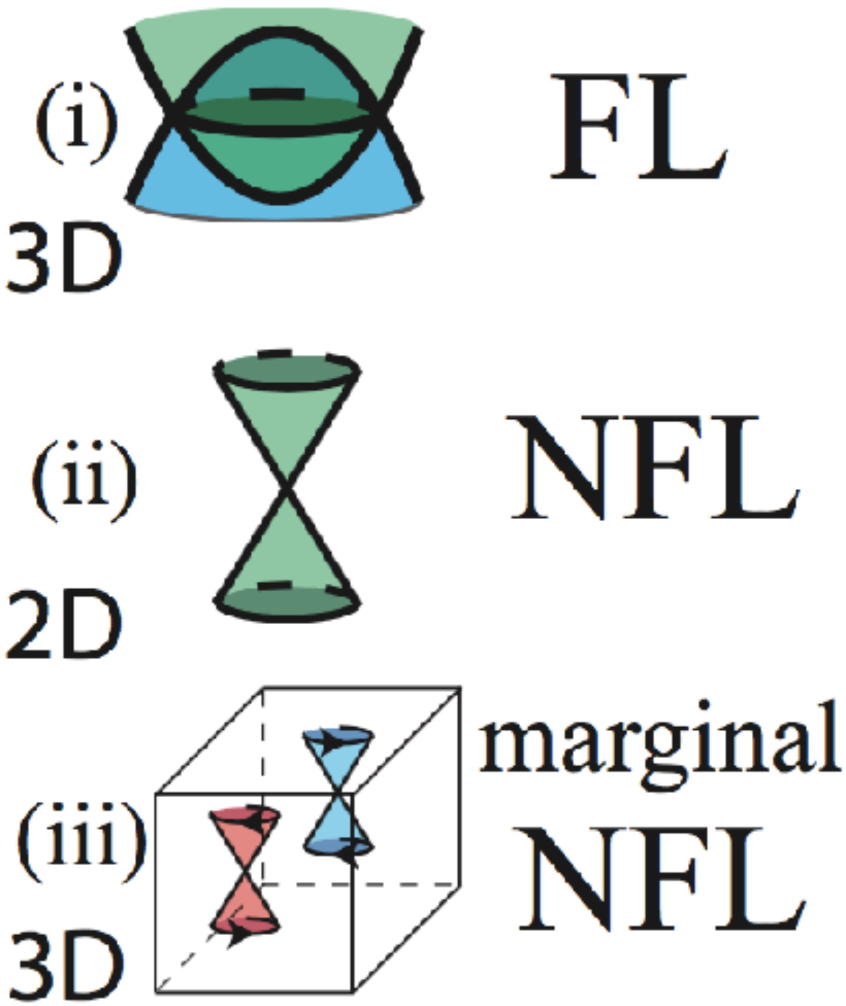
Gapless Particle-Hole Excitations Needed to Drive Novel Metallic Behavior

Band Crossings Close to the Fermi Level !!



Wang et al. PRB 98, 20112 (2018)

Emergent Metallic Behavior in Three Generic Cases



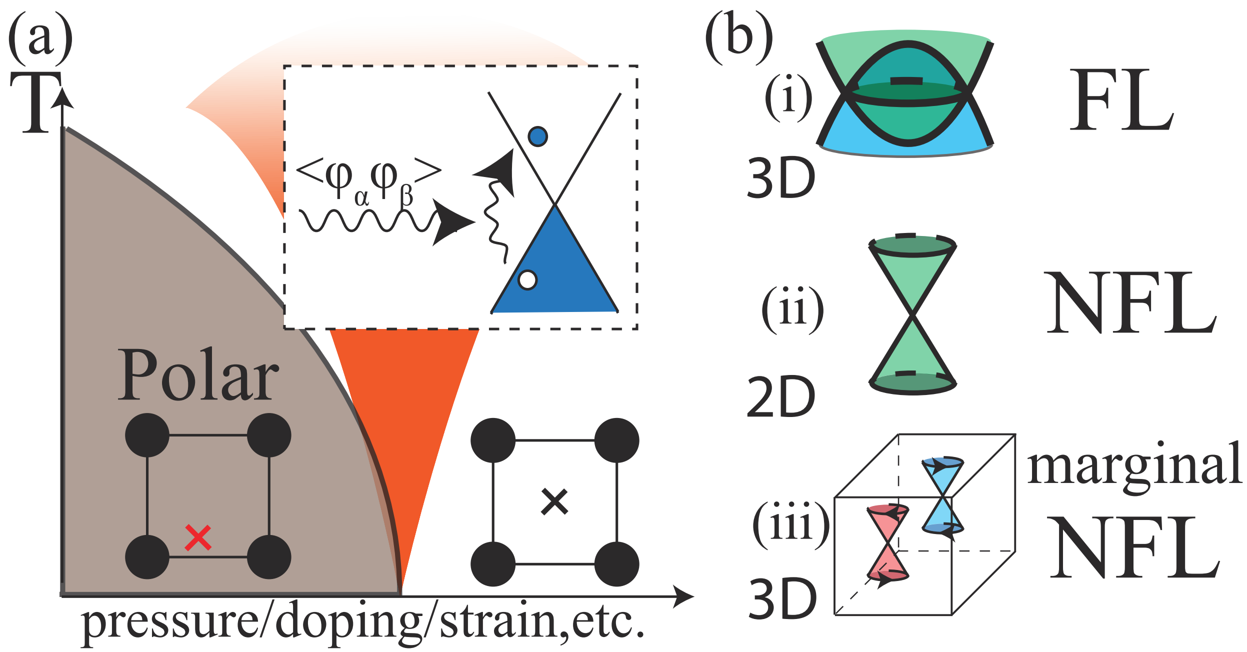
3D Nodal Line

2D Nodal Points

3D Weyl Points
(with Broken Time-Reversal
Symmetry)

Coulomb interactions: anisotropy in (i) and (ii)
gaps the the longitudinal mode (iii)

Multiband Quantum Criticality of Polar Metals



Pavel Volkov (Rutgers)

Novel phases in quantum critical polar metals ??

Nodal multiband metals near polar QCPs promising settings

Experimental Signatures

P.A. Volkov and PC, PRL 124, 237601 (2020)

Summary and Many Open Questions

A Flavor for Two Current Research Projects

Quantum Annealed Criticality

Strongly Correlated Phases in Metals Close to a Polar QCP

T-Dependent Transport ??

Superconductivity Mechanism ??

Multiferroic Quantum Criticality ??

⋮


Thank You
Multumesc
Matondo
Terima Kasih
Obrigado
Dankon
Arigatô
Diolch
Спасибо
ありがとう
Danke
Kiitos
Thank You
감사합니다
Teşekkür ederim
Shukran
Merci
Danke
Thank You
Obrigado
Merci
Matur Nuwun
Maake
Asante
Dank u
Merci
Salamat
Xièxiè
Welalin
Arigatô
Asante
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Shukran
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ありがとう
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Xièxiè