Polar Quantum Criticality





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Polar Materials + Quantum Criticality ??



Quantum Annealed Criticality

Novel Metallicity

Enigmatic Superconductivity



Summary and Outlook

Polar Material ?

Net Dipole Moment/ Volume



No !! (Centrosymmetric)



Example: BaTiO3



Cubic phase



Pup



Polar Materials ? (Simplest Case: Insulators)





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 !

Strong Electromechanical Coupling !

SrTiO₃ - Almost a Ferroelectric



Polar Materials ?



Important for Many Room-Temperature Applications

Can these functional materials "teach" us about some fundamental physics in Nature?



Quantum Fluctuations at Finite Temperature ??

Heisenberg Uncertainty Principle
$$\Delta t \propto \frac{\hbar}{\Delta E}$$

Decoherence Time-Scale (Planck time)
$$t_P \propto \frac{\hbar}{k_B T}$$

Fluctuations purely Quantum up to the Planck time Classical beyond

> T = 0 Quantum Critical Point, Fluctuations are Purely Quantum

Quantum Criticality: Key Concepts

Symmetry-Breaking Phase Transition at T=0

Tuning Parameter is NOT Temperature

Physics determined by Nature of Critical Soft Mode

Importance of Dynamics

Motivation: Exotic Metallicity particularly Unconventional Superconductivity



Polar Materials and Quantum Criticality ?



Classical Polar Transitions Usually First Order !?

Mostly Insulators !? (links to novel metallicity??)





C)

How can Systems that Have Classical First-Order Transitions display Quantum Criticality ??



Quantum Annealed Criticality

PC, P. Coleman, M.A. Continentino, G. G. Lonzarich, Phys. Rev. Res. 2, 043440 (2020)

How can Systems that Have Classical First-Order Transitions display Quantum Criticality ??



Interplay of Classical and Quantum Fluctuations ??

Decrease in T

Quantum fluctuations reduce the amplitudes of thermal fluctuations, weakening the first-order transition

T=0 "Quantum Annealed" Critical Point

Quantum Annealed Criticality

PC, P. Coleman, M.A. Continentino, G. G. Lonzarich, Phys. Rev. Res. 2, 043440 (2020)



(Classical) Larkin-Pikin Mechanism

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

Interaction of strain with squared amplitude of the critical order parameter

Ist Order Transition in the Unclamped System LP Criterion for 1st Order Transition $\kappa < \frac{\Delta C_V}{T_c} \left(\frac{dT_c}{d\ln V}\right)^2$ $\kappa^{-1} = K^{-1} - (K + \frac{4}{3}\mu)^{-1} \qquad \kappa \sim K \frac{c_L^2}{c_T^2}$

Diverging Specific Heat in a Clamped System

Shear Strain Crucial



Coupling of the uniform strain to the energy density

$$\tilde{\kappa} \equiv \kappa - \Delta \kappa$$

$$\downarrow$$
Macroscopic Instability of the Critical Point
$$\downarrow$$

Discontinuous Phase Transition

13

Generalization for the Quantum Case ???

Schematic Flavor of Results



PC, P. Coleman, M.A. Continentino, G. G. Lonzarich, Phys. Rev. Res. 2, 043440 (2020)



Screening of Dipole Moments



Inversion Symmetry-Breaking Transition Remains (Anderson and Blount PRL 12, 217 (1965))

- Intrinsic and "Engineered" Polar Metals Exist
- Search for Weyl semimetals
- **Tuning of the Polar Transition**
 - **Chemical Substitution**
 - Strain/Pressure



Exotic Phases ??

Novel Quantum Critical Polar Metallic Phases ??





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

Can Polar Criticality Drive Dilute Superconductivity ??

Polar Quantum Critical Metals





Usual Frohlich electron-phonon interaction

$$H_{e-ph} = \int d\mathbf{r} \,\nabla \cdot \tilde{\varphi}(\mathbf{r}) \,\, \mathbf{\hat{n}}(\mathbf{r}) \qquad \lim_{q \to 0} \frac{|\nabla \vec{\varphi}|}{|\varphi|} \to 0 \qquad \text{Irrelevant} \quad \text{for the} \\ \text{critical phonon} \quad \text{critical phonon} \quad \text{for the} \\ \text{critical phonon} \quad \text{critical phonon} \quad \text{critical phonon} \quad \text{for the} \\ \text{critical phonon} \quad \text{critical phonon} \quad \text{for the} \\ \text{critical phonon} \quad \text{critical phonon} \quad \text{critical phonon} \quad \text{for the} \\ \text{critical phonon} \quad \text{critical phonon} \quad \text{critical phonon} \quad \text{for the} \quad \text{critical phonon} \quad \text{critical phonon} \quad \text{for the} \quad \text{critical phonon} \quad \text{critical phonon} \quad \text{critical phonon} \quad \text{critical phonon} \quad \text{for the} \quad \text{critical phonon} \quad \text{critical$$

Challenge: Strong Electronic Coupling to the Critical Polar Mode ?

Polar Quantum Critical Metals





Usual Frohlich electron-phonon interaction

$$H_{e-ph} = \int d\mathbf{r} \, \nabla \cdot \tilde{\varphi}(\mathbf{r}) \, \, \mathbf{\hat{n}}(\mathbf{r})$$

$$\lim_{q\to 0} \frac{|\nabla \vec{\varphi}|}{|\varphi|} \to 0$$

Irrelevant for the critical phonon!

Opportunity:

Setting to Study New Collective Electronic Behavior induced by Unconventional Lattice Dynamics ¹⁸

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

Is such a Yukawa-type coupling possible near a 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)

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



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

No ISB without TRSB !!



20

Yukawa Coupling to the Polar Mode

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

$$\begin{split} H^{(a)}_{coupl} &= \lambda \sum_{i,\mathbf{q},\mathbf{k}} f^{i}_{a}(\mathbf{k}) \varphi^{i}_{\mathbf{q}} c^{\dagger}_{\mathbf{k}+\mathbf{q}/2} \sigma_{1} c_{\mathbf{k}-\mathbf{q}/2}, \qquad \mathcal{P} \sim \sigma_{3} \quad \stackrel{\text{(different parity bands)}}{} \\ H^{(b)}_{coupl} &= \lambda \sum_{i,\mathbf{q},\mathbf{k}} f^{i}_{b}(\mathbf{k}) \varphi^{i}_{\mathbf{q}} c^{\dagger}_{\mathbf{k}+\mathbf{q}/2} \sigma_{2} c_{\mathbf{k}-\mathbf{q}/2}, \qquad \mathcal{P} \sim \sigma_{0} \quad \stackrel{\text{(same parity bands)}}{} \end{split}$$



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

Yukawa Coupling to the Polar Mode: Physical Mechanism

(assuming bands arise from two distinct orbitals)

Different Parity Same Parity (a) $\varphi^i = 0$ (d) (c) $\varphi^i \neq 0$

Interorbital Hopping Changes in Both Cases !!

22

Gapless Particle-Hole Excitations Needed to Drive Novel Metallic Behavior

Order Parameter Couples to Interband Particle-Hole Excitations

Best Case Scenario:

Band Crossings close to the Fermi Level



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



What about Superconductivity ??

An Old Tale of Unconventional Superconductivity that Remains a Mystery



25 C. Collignon, X. Lin, C.W. Richau, B. Fauque and K. Behnia, Ann. Rev. Cond. Mat. Phys. 1025 (2019).

Superconductivity in Dilute QC Polar Metals

Challenges:

How to Overcome Coulomb Repulsion ?? No retardation Isotropic (s-wave)

Tc Increases with Proximity to Polar QCP !!



Enderlein et al. Nat. Comm. (2020)

Critical Mode = Transverse Optical Phonon

Negligible Direct Coupling between Electrons and Soft Mode (unless there is spin-orbit coupling)

Can Polar Criticality Drive Dilute Superconductivity ?26

Superconductivity in Dilute QC Polar Metals: Context



Multivalley

Plasmons

Two-Phonon Processes

$$\mathcal{S}^{2ph} = \sum_{\mathbf{kq}} g_{2ph} \ c^{\dagger}_{s,\mathbf{k+q}} c_{s,\mathbf{k}} \ \mathbf{u}^{2}_{\mathbf{q}}$$



Koonce et al., PR (1967)

Quantum criticality important Multiband Effects Spin-Orbit Coupling $S^{2ph} = \sum_{\mathbf{kq}} g_{SOC} \left[c^{\dagger}_{s,\mathbf{k}+\frac{\mathbf{q}}{2}} (\mathbf{k} \times \sigma_{ss'}) c_{s',\mathbf{k}-\frac{\mathbf{q}}{2}} \right] \cdot \mathbf{u_q}$

M.N. Gastiasoro, J. Ruhman and R. M Fernandes, Annals of Physics 417, 168107 (2020)

Guiding Observations





Electrons do not directly interact with zero-point fluctuations

²⁸

Electrons Interact with the Energy Density of the Critical TO Phonons

Model for this Coupling





Suppression of the zero-point fluctuations of the critical phonons near the electrons

Reduction of chemical potential of nearby electrons

Fluctuations of the critical phonon energy density near the electrons result in an attractive potential

Weak vs. Strong Coupling ?

Coulomb/Kinetic Energy

$$r_s = 1/(k_F a_B)$$
$$k_F \sim n^{\frac{1}{3}}$$

Dilute Quantum Critical Polar Metals $4\pi\varepsilon\hbar^2$

$$a_B = \frac{1}{m^* e^2}$$
$$\varepsilon \sim \varepsilon(\vec{q}, \omega)|_{q=2k_F, \omega=E_F} \approx \frac{\Omega_0^2}{(2c_s k_F)^2} \gg 1$$

 $r_s << 1$ Weakly Interacting !!



Dilute Quantum Critical Polar Metals ??

Coupling to Energy Fluctuations (g finite)



Coupling to Energy Fluctuations (g finite)

Finite Electron Density

$$n = \langle \rho_e(x) \rangle \quad \longrightarrow \quad$$

$$\omega_T^2(n) = \omega_{T0}^2 + gn\varepsilon_0\Omega_0^2$$

Suppression of Polar State by Charge Doping

Shift of the Quantum Critical Point

Energy Fluctuation Coupling Cannot be Integrated Out Exactly



Perturbative Effects (Weak Coupling)

Effective Electron-Electron Interaction

$$V_{En}^{Pair}(x) \sim -g^2 [D_T(x)]^2 \sim -\frac{g^2}{x^4}$$

Quantum Critical Point (QCP) $(\omega_T(n) = 0)$

$$x^2 = \vec{x}^2 + c^2 \tau^2$$

Effective Electron-Electron Interaction





(b)
$$\frac{1}{k_F} << \xi << \frac{1}{E_F}$$

$$(c) \quad \xi << \frac{1}{k_F}, \frac{1}{E_F}$$

Quantum Critical in Space and Time (High Density)

Quantum Critical in Space Local in Time (Low Density)

Local in Space and Time (Ultralow Density)







 $-E_F^{-1}$



 k_F^{-1}

Effective Electron-Electron Interaction

$$V_{En}^{Pair}(x) \sim -g^2 [D_T(x)]^2 \sim -\frac{g^2}{x^4}$$

Quantum Critical Point (Q.C.P.)

$$(\omega_T(n)=0)$$

$$x^2 = \vec{x}^2 + c^2 \tau^2$$

Interaction relevant for electron pairing

$$\langle V(k-k') \rangle = \langle V(k_F,\theta) \rangle_{\theta} \sim -\frac{g^2}{c_s^3} \log \left[\frac{\Omega_T}{\max(\omega_T, c_s k_F, E_F)} \right]$$
$$\Omega_T = \max_{\vec{q}} \omega_T(\vec{q}) \text{ cutoff} \qquad \text{large momenta contribute}$$

Density-Dependence of the Effective Attraction



Superconductivity

For low carrier density close to the polar QCP, the attractive electron-electron interaction will overcome Coulomb repulsion leading to superconductivity.



Attractive part of the effective electron coupling

Superconductivity

For low carrier density close to the polar QCP, the attractive electron-electron interaction will overcome Coulomb repulsion leading to superconductivity.



$$T_c \propto E_F \ e^{-rac{1}{\lambda}}$$
 $\left(rac{2\Delta}{T_c}
ight) = 3.5$ Gorkov and Melik-Barkhudarov (1961) Gorkov (2016)

T_c has dome-behavior as a function of the carrier density n

Superconductivity in Doped SrTiO₃

$$g/a_0^3 = .68$$



Superconductivity in Doped SrTiO₃



Superconductivity in Doped 2D SrTiO3



Distinguishing Features of the Energy Fluctuation Mechanism

$$\label{eq:phi} \begin{split} \rho \propto T^2 & \text{Dominant Coupling to Energy Fluctuations} \\ \omega_T^2(n_e) - \omega_{TO}^2 \propto g n_e & \text{Suppression of Polar State} \\ \omega_T^2(n_e) - \omega_{TO}^2 \propto g n_e & \text{Suppression of Polar State} \\ 0.5 < g/a_0^3 < 0.7 & (\text{n-doped STO}) & \checkmark \\ \end{split}$$

Scaling of T_c with phonon frequency and sensitivity to carrier density at low doping concentrations

Normal State near the Polar QCP = Fermi liquid

Distinguishing Features of the Energy Fluctuation Mechanism

$$\label{eq:starsest} \begin{split} \rho \propto T^2 & \text{Dominant Coupling to Energy Fluctuations} \\ \omega_T^2(n_e) - \omega_{TO}^2 \propto g n_e & \text{Suppression of Polar State} \\ \omega_T^2(n_e) - \omega_{TO}^2 \propto g n_e & \text{Suppression of Polar State} \\ 0.5 < g/a_0^3 < 0.7 & (\text{n-doped STO}) & \checkmark \\ \end{split}$$

Take-Home Message: Unconventional Superconductivity can be Driven by Multiple Critical Transverse Phonons

New Channel for Superconductivity in Materials with Large Anharmonicity Setting to Study Nontraditional Electron-Phonon Interactions Novel Metallic Phases

Enigmatic Superconductivity Driven by Multiple Transverse Phonons

Future Directions

Mixed parity polar superconducting states?

Polarization Textures ?

Light-Induced Dynamical Quantum Criticality ?

Please come and join in the good fun !!



A Technical Flavor for the 2D Dirac Point Results

Example: CDW in graphene

No Coulomb Interactions: Gross-Neveu-Yukawa Model

NFL



$$H_{Dir} = v_F (k_x \sigma_x + k_y \sigma_y)$$
$$H_{coupl} = \lambda \sum_{\mathbf{q},\mathbf{k}} \varphi_{\mathbf{q}} c_{\mathbf{k}+\mathbf{q}/2}^{\dagger} \sigma_3 c_{\mathbf{k}-\mathbf{q}/2}$$

Emergent Lorentz invariance z = 1

Renormalization of critical phonon velocity $c_s \rightarrow v_F$

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 !!



A Technical Flavor for the 2D Dirac Point Results

Example: CDW in graphene

Include Coulomb Interactions:

$$[q_x] = [\omega, q_y]^{3/2}$$

$$H_{Dir} = v_F (k_x \sigma_x + k_y \sigma_y)$$
$$H_{coupl} = \lambda \sum_{\mathbf{q},\mathbf{k}} \varphi_{\mathbf{q}} c_{\mathbf{k}+\mathbf{q}/2}^{\dagger} \sigma_3 c_{\mathbf{k}-\mathbf{q}/2}$$

One-Loop RG





Mihaila et al. PRB 96, 165133 (2017); Lang and Lauchli PRL 123, 137602 (2019)

Can the strength of the spin-orbit mediated coupling to soft polar modes be probed experimentally ??





Abhishek Kumar (Rutgers)



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Accessible with Current Experimental Techniques with Reasonable Fields

A. Kumar, PC and P.A. Volkov, PRB 105, 125142 (2022).

DFT Studies with Rutgers colleagues also in Progress...

Novel phases in quantum critical polar metals ?? V



Yukawa coupling to critical (TO) phonon

Possible in multiband systems without SOC Strong correlations near Band Crossings

3D Nodal Line (LiOsO₃)

Fermi Liquid Unconventional Phonon Spectrum

2D Nodal Point

Non-Fermi Liquid (NFL) Anisotropy induced by Coulomb interactions

3D Weyl Point

Logarithmic NFL corrections



54

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





In all three cases the critical polar mode is strongly affected by interactions close to the polar QCP (dispersion renormalization and smearing of the spectral weight)