Quantum Criticality in Polar Materials I :

New Perspectives on Quantum Criticality from Polar Materials (pedagogical)

P. Chandra
(Rutgers)

I. Title Unpacked

II. Why ??

III. Historical Perspectives and Current Challenges

PC, G.G. Lonzarich, S.E. Rowley and J.F. Scott, Reports on the Progress of Physics 80, 112502 (2017)

What does quantum critical mean?

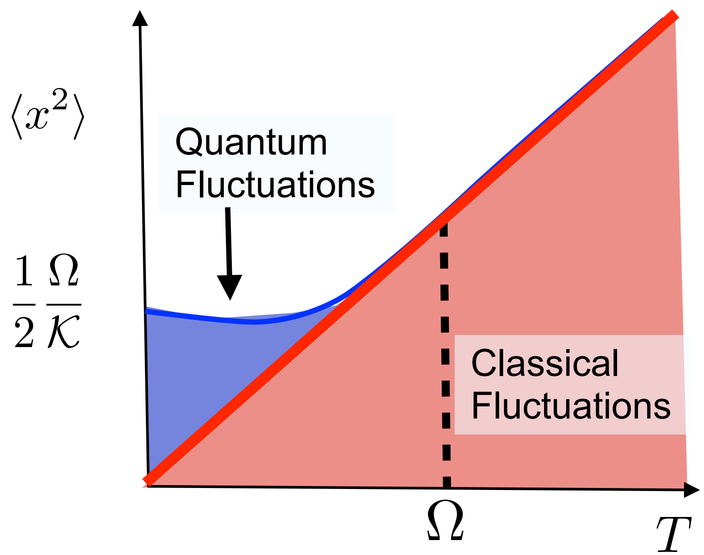
Aren’t quantum fluctuations only important at T = 0 ?

“The career of a young theoretical physicist consists of treating the harmonic oscillator in ever-increasing levels of abstraction.”

Sidney Coleman

Simple Harmonic Oscillator (1d)

Variance $$\langle x^2 \rangle = \frac{\Omega}{\mathcal{K}} \left\{ \frac{1}{e^{\frac{\Omega}{T}} - 1} + \frac{1}{2} \right\}$$ $(\hbar = 1, \; k_B = 1)$



$\Omega < T$ Thermal (classical) Fluctuations $\langle x^2 \rangle \sim \frac{T}{\mathcal{K}}$

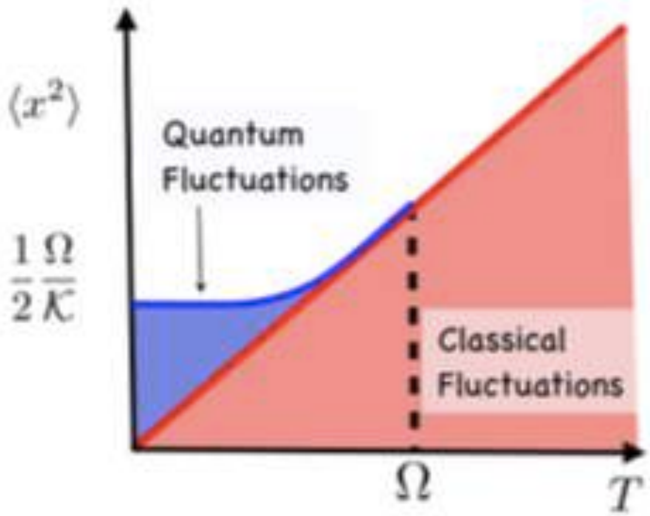
$0 < T < \Omega$ Thermal-Quantum Fluctuations

$T = 0$ Pure Quantum Fluctuations $\langle x^2 \rangle = \frac{\Omega}{2\mathcal{K}3}$

What does the behavior of a SHO have to do with phase transitions and criticality ?

Order Parameter Fluctuations

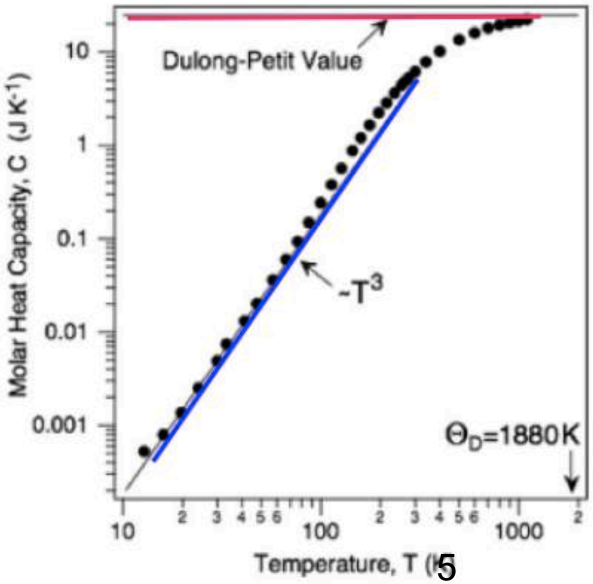
Variance of each of their Fourier Components, a mode of wavevector q whose behavior can be mapped onto a SHO



At a continuous phase transition $\mathcal{K} \to 0 \quad \Rightarrow \quad \langle x^2 \rangle \to \infty$

What about the specific heat ?

In diamond effects of quantum
fluctuations present at room temperatures !



How to think about temperature near a quantum critical point?

- Temperature is NOT a tuning parameter
- Temperature is a boundary effect!

$$\Delta t \propto \frac{\hbar}{\Delta E} \rightarrow t_{dec} \propto \frac{\hbar}{k_B T}$$

Fluctuations are Purely Quantum
up to this Time-scale

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Back to the SHO ......

$$\langle x^2 \rangle = \left\{ n_\Omega + \frac{1}{2} \right\} \Omega \chi \qquad \chi = \frac{1}{\mathcal{K}} (= \mathrm{Re}\ \chi_{\omega=0})$$

$$\mathrm{Im}\ \chi_\omega = \frac{\pi}{2} \omega\ \chi\ \delta(\omega - \Omega) \qquad (\omega > 0)$$

$$\langle x^2 \rangle = \frac{2}{\pi} \int_0^\infty d\omega \left\{ n_\omega + \frac{1}{2} \right\} \mathrm{Im}\ \chi_\omega$$

Nyquist Theorem

Generalization to all modes in the Brillouin Zone

$$\langle \delta\phi^2 \rangle = \frac{2}{\pi} \sum_q \int_0^\infty d\omega \left\{ n_\omega + \frac{1}{2} \right\} \mathrm{Im}\ \chi_{q\omega}$$

Scalar Order Parameter

$$\phi = \bar{\phi} + \delta\phi$$

Average $\langle \delta\phi \rangle = 0$

$$\mathrm{Im}\ \chi_{q\omega} = \frac{\pi}{2}\ \omega\ \chi_q\ \delta(\omega - \omega_q) \qquad (\omega > 0)$$

(propagating limit, simplest case)

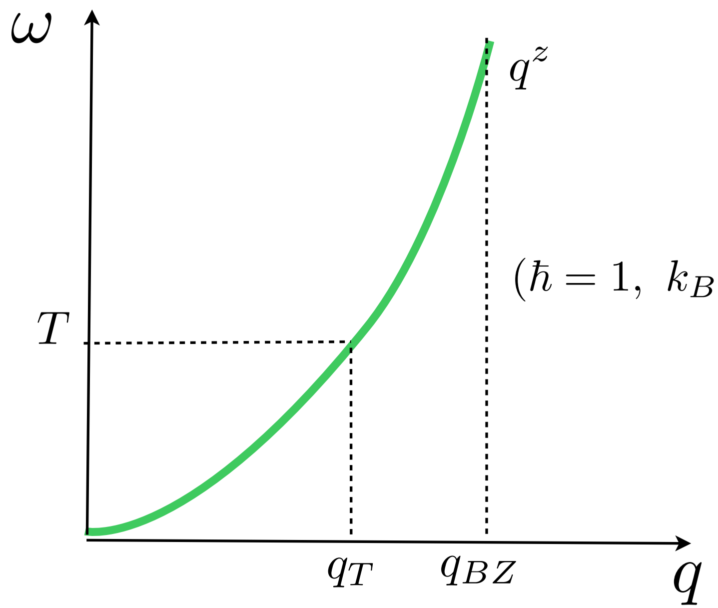
Generalization to all modes in the Brillouin Zone

$$\langle \delta\phi^2 \rangle = \frac{2}{\pi} \sum_q \int_0^\infty d\omega \left\{ n_\omega + \frac{1}{2} \right\} \mathrm{Im}\ \chi_{q\omega}$$

Our Focus: $\langle \delta\phi_T^2 \rangle$

Strongly Temperature-Dependent Contribution
Dominant in Determining Temperature-Dependence
of Observable Properties

Dispersion and Important Wavevectors



$(\hbar = 1,\ k_B = 1)$

$$q_T \propto T^{\frac{1}{z}}$$

$q_{BZ} < q_T$ Purely Classical Fluctuations

$q_{BZ} > q_T$ Quantum Fluctuations Present

Generalization to all modes in the Brillouin Zone

$$\langle \delta\phi^2 \rangle = \frac{2}{\pi} \sum_q \int_0^\infty d\omega \left\{ n_\omega + \frac{1}{2} \right\} \text{Im } \chi_{q\omega}$$

Focus: $\langle \delta\phi_T^2 \rangle$

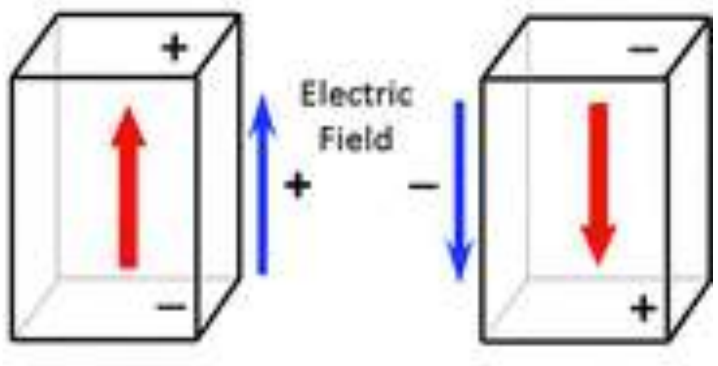
$$\langle \delta\phi_T^2 \rangle \approx T \sum_{q<q_{BZ}} \chi_q \qquad (T \gg \omega_q \quad \text{for} \quad q < q_{BZ})$$

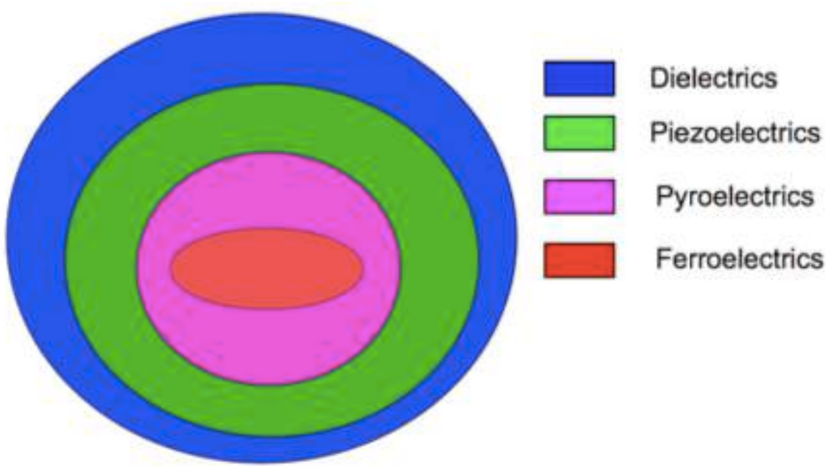
$$\langle \delta\phi_T^2 \rangle \approx T \sum_{q<q_T} \chi_q \qquad (T \ll \omega_q \quad \text{for} \quad q < q_T)$$

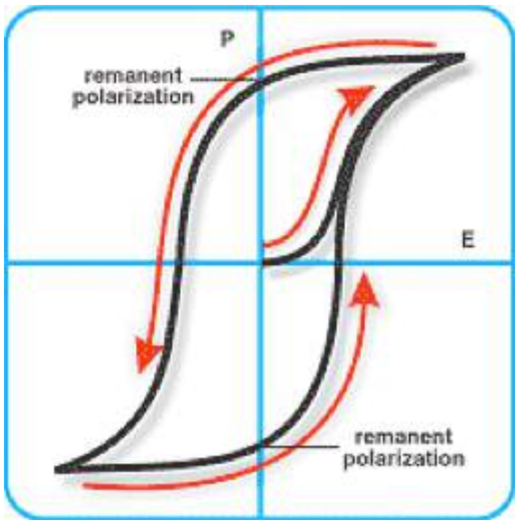
$$(\chi_q^{-1} \propto \kappa^2 + q^2) \qquad (\chi^{-1} \propto \kappa^2)$$

Ferroelectrics: The Simplest Polar Materials

A FE is a material that has a spontaneous polarization that is switchable by an electric field of practical magnitude

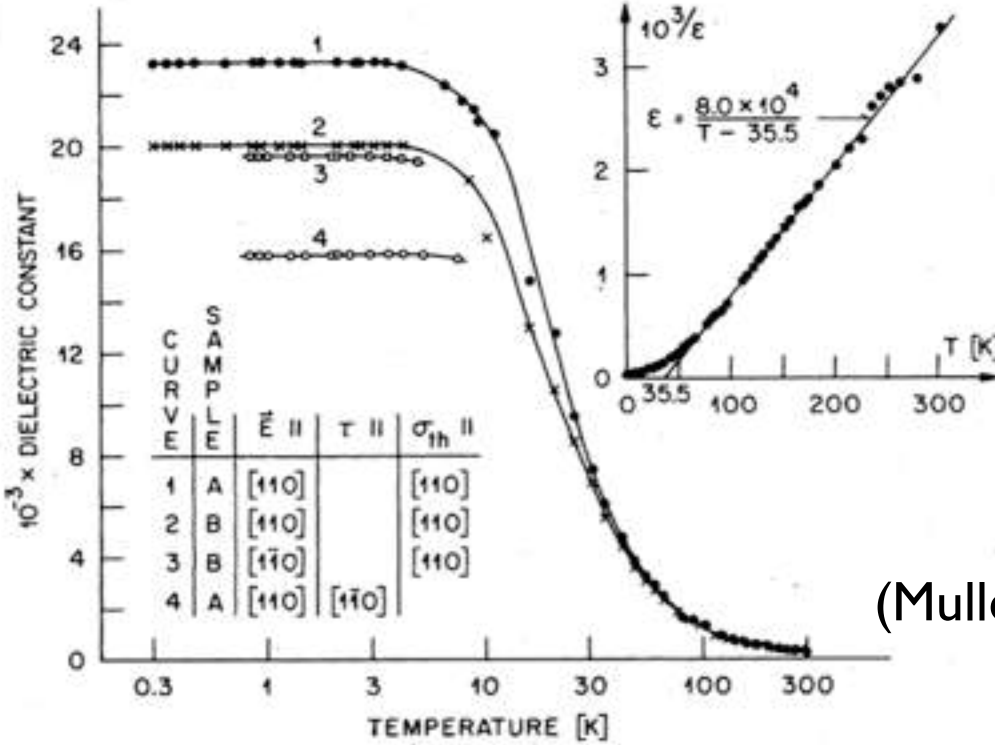


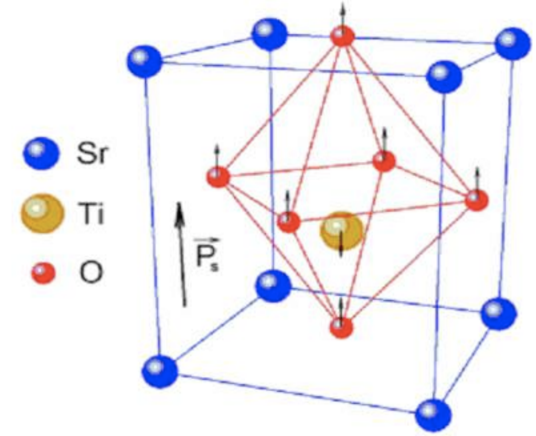





Actuator
Piezoelectricity
Piezoelectric
Pyroelectric
Ferroelectric
Thermal infrared switch
Electro-optical activity
DRAM storage capacitor
High permittivity
Pyroelectricity
Polarizability
Infrared sensors
NVFRAM memory cell

$SrTiO_3$ - Almost a Ferroelectric

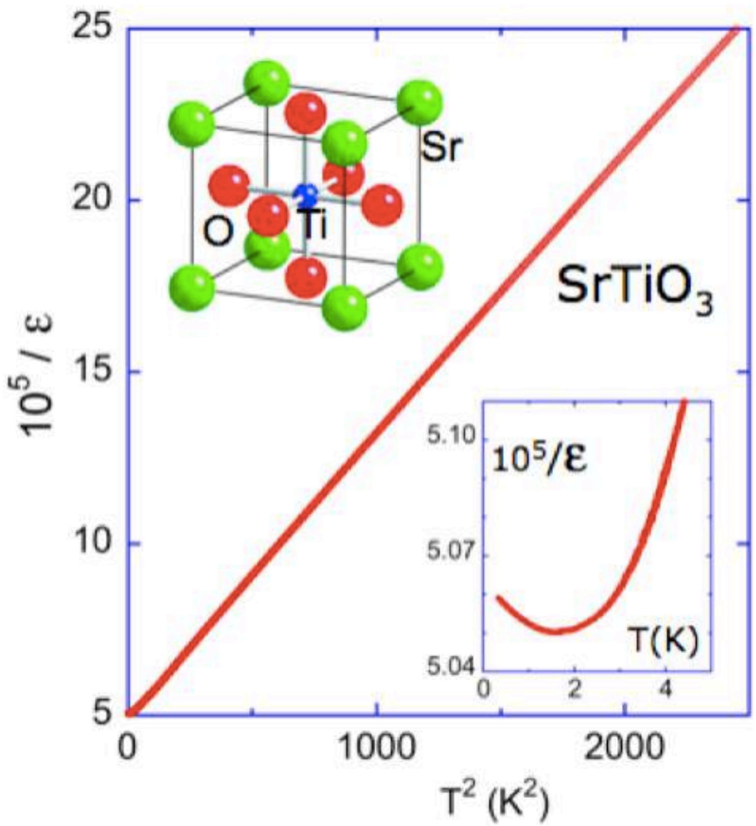


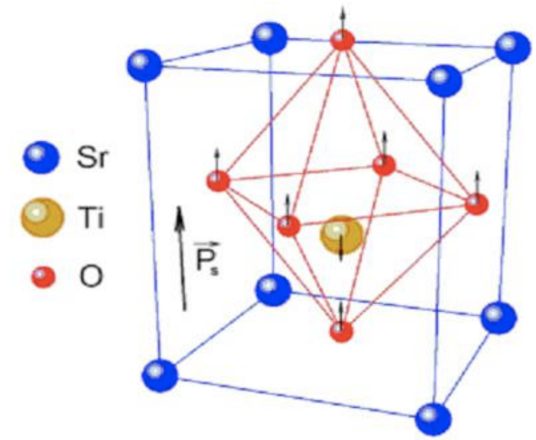


(Muller and Burkhard 79)

Ferroelectricity <u>induced</u> by
Uniaxial Stress, Ca and O-18 Substitution

$SrTiO_3$ - Almost a Ferroelectric





(Rowley et al. 14)

Ferroelectricity induced by
Uniaxial Stress, Ca and O-18 Substitution

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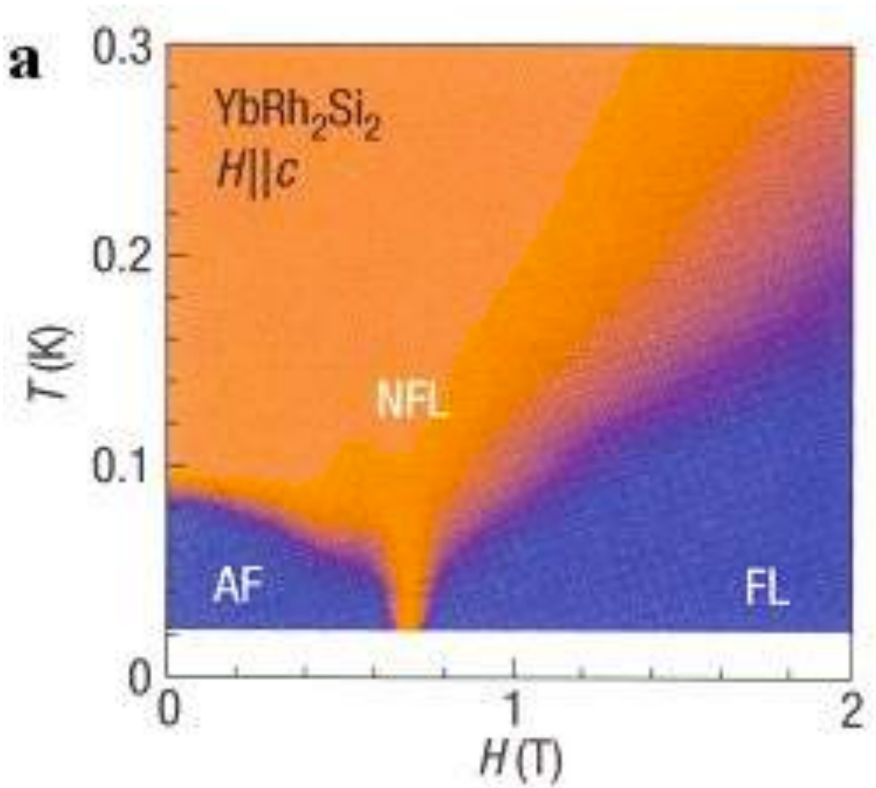
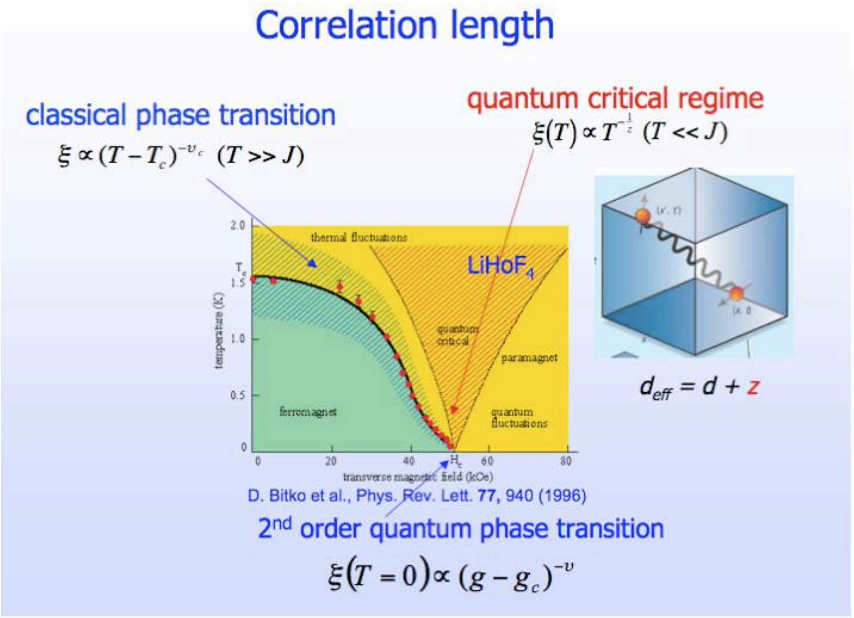
What do FEs have to do with Quantum Criticality ?

Insulators (link to novel metals and superconductivity?) !?

Classical FE transitions usually 1st order !?

Many, many (magnetic) settings to study quantum criticality....
why do we need more ??





Important Role in (Classical) Critical Phenomena

SOVIET PHYSICS JETP VOLUME 29, NUMBER 6 DECEMBER, 1969

PHASE TRANSITION IN UNIAXIAL FERROELECTRICS

A. I. LARKIN and D. E. KHMEL'NITSKIĬ

Institute of Theoretical Physics, U.S.S.R. Academy of Sciences

Submitted January 16, 1969

Zh. Eksp. Teor. Fiz. 56, 2087–2098 (June, 1969)

The form of the singularity of thermodynamic quantities at the phase transition point in a uniaxial ferroelectric substance is determined. The results differ from the predictions of the phenomenological theory by logarithmic factors. Similar results have been obtained for four-dimensional models discussed in Appendix 2.


First Calculation of Logarithmic Corrections to Mean-Field Theory in d=d* !!

Uniaxial Ferroelectric

$$d_{eff}^{space} = d + 1$$

All dipoles in z direction

$$W(q) \propto \frac{q_z^2}{q^2}$$

TO phonon dispersion

$$\omega^2(q) = c^2 q^2 + \Delta^2 + \beta \frac{q_z^2}{q^2} \quad (1)$$

Application of Simple Scaling

$$q^2 \approx q_x^2 + q_y^2$$

$$\tilde{q}_{x(y)} = \frac{q_{x(y)}}{b}, \qquad \tilde{q}_z = \frac{q_z}{b^k}, \qquad b, k > 1 \quad (2)$$

Simultaneous Satisfaction of (1) and (2) ⟶ k=2

q_z "counts" for effectively two dimensions

Why Study FE Quantum Criticality ?

Quest for Universality

Simplicity

Controlled Additional Degrees of Freedom
(and maybe novel metals and exotic superconductors)

(Possible Applications)

SOVIET PHYSICS JETP VOLUME 33, NUMBER 2 AUGUST, 1971

CONTRIBUTION TO THE THEORY OF SECOND-ORDER PHASE TRANSITIONS AT LOW TEMPERATURES

A. B. RECHESTER

L. D. Landau Institute of Theoretical Physics, USSR Academy of Sciences

Submitted August 21, 1970

Zh. Eksp. Teor. Fiz. 60, 782–796 (February, 1971)

Quantum effects are investigated in second-order phase transitions at low temperatures. The temperature dependence of the gap in the spectrum of the critical optical phonons is calculated in first approximation of perturbation theory and in the "parquet" approximation. The results are compared with the experimental data for SnTe and $KTaO_3$. The transition at T = 0 is also investigated.

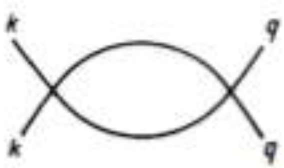


FIG. 8

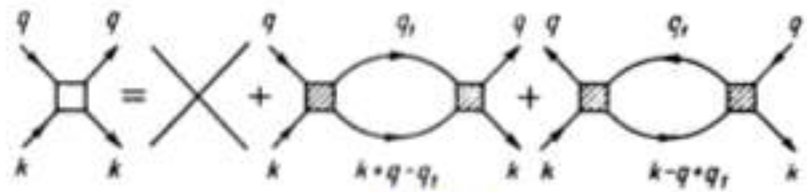
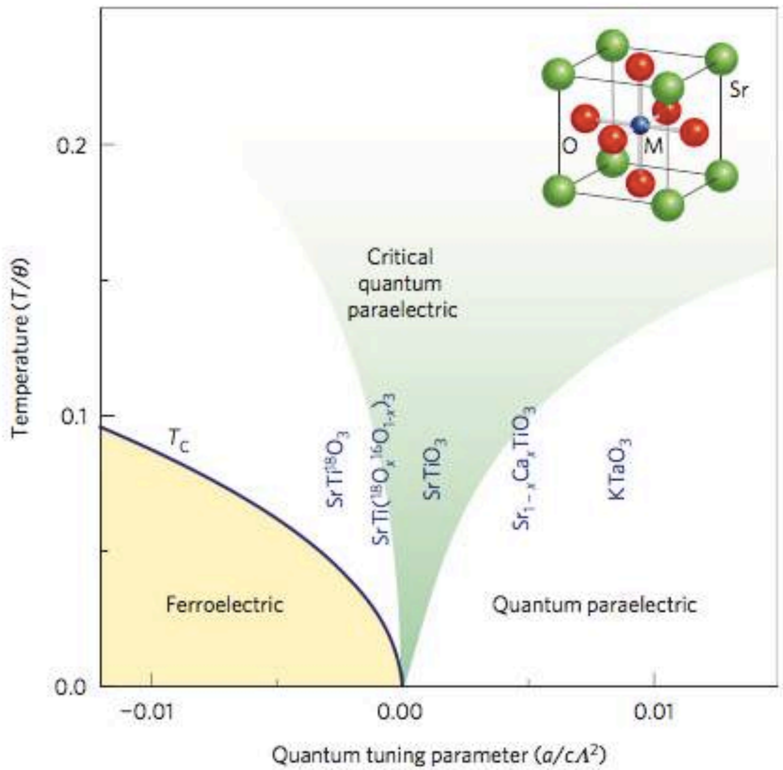
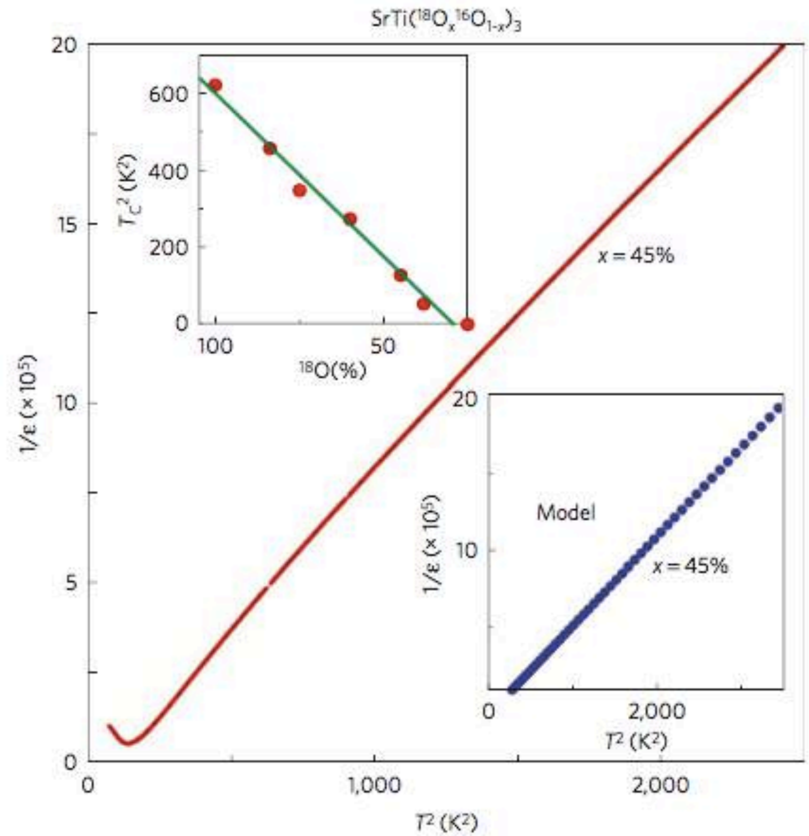


FIG. 9

$$\chi^{-1} \propto T^2$$

Simpler way to get this result ??





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)

Self-consistent Landau Approach

$$f = \frac{1}{2}\alpha\phi^2 + \frac{1}{4}\beta\phi^4 + \frac{1}{2}\gamma|\nabla\phi|^2 - \mathcal{E}\phi$$

Minimization

$$\mathcal{E} = \alpha\phi + \beta\phi^3 - \gamma\nabla^2\phi$$

Observed moment requires fluctuation-averaging
(due to coarse-graining over q_T)

$$\phi \rightarrow \overline{\phi} + \delta\phi$$

$$\mathcal{E} = (\alpha + 3\beta\langle\delta\phi^2\rangle)\overline{\phi} + \gamma\nabla^2\overline{\phi}$$

We can Fourier transform in the limit $\phi,\ \mathcal{E} \to 0$ to obtain

$$\chi_q^{-1} = (\alpha + 3\beta\langle\delta\phi^2\rangle) + q^2$$

Most probable vs. average values...coarse-graining over q_T!

$$\lim_{T\to 0} \kappa^2 \propto \langle\delta\phi_T^2\rangle$$

$$\kappa^2 \propto \sum_{q<q_T} \frac{T}{\kappa^2 + q^2} \approx T \int_{\kappa}^{q_T} \frac{q^{d-1}}{q^2} \approx T\ q_T^{d-2} \left\{1 - \left(\frac{\kappa}{q_T}\right)^{d-2}\right\}$$

Temptation…

$$\chi^{-1} \propto \kappa^2 \propto T^{\frac{(d+z-2)}{z}}$$

When is this approach valid ?

$$\left(\frac{\kappa}{q_T}\right)^2 \propto T^{\frac{(d+z-4)}{z}} \left\{1 - \left(\frac{\kappa}{q_T}\right)^{d-2}\right\}$$

$$\lim_{T\to 0}\left(\frac{\kappa}{q_T}\right) \to 0 \qquad \text{if} \qquad d_{eff} \equiv d + z > 4$$

Ferroelectrics d = 3, z = 1

$$\chi^{-1} \propto \kappa^2 \propto T^{\frac{(d+z-2)}{z}} = T^2$$ (log terms)

Agrees with previous calculation by different methods

Finite-Size Scaling in Space and T

- Space (near CCP) $\xi \sim t^{-\nu}$

$$\chi \sim t^{-\gamma} \Phi \left(\frac{L}{\xi} \right) \sim t^{-\gamma} \Phi \left(\frac{L}{t^{-\nu}} \right)$$

For $L << \xi$ $\quad \chi = \chi(L)$

$$\chi \sim t^{-\gamma} \left(\frac{L}{\xi} \right)^{p} \sim t^{-\gamma} \Phi \left(\frac{L}{t^{-\nu}} \right)^{\frac{\gamma}{\nu}} \sim L^{\frac{\gamma}{\nu}}$$

- Time

  (near QCP)

$$\xi \sim g^{-\nu} \longrightarrow \xi_\tau \sim g^{-z\nu}$$

$$L_\tau = \frac{\hbar}{k_B T}$$

$(\omega \propto q^z \rightarrow [\xi_\tau] = [\xi^z])$

$$\chi \sim g^{-\gamma}\Phi\left(\frac{L_\tau}{\xi_\tau}\right) \sim g^{-\gamma}\Phi\left(\frac{L_\tau}{g^{-z\nu}}\right)$$

For $L_\tau << \xi_\tau$ $\quad \chi = \chi(L_\tau)$

$$\chi \sim g^{-\gamma}\left(\frac{L_\tau}{\xi_\tau}\right)^p \sim g^{-\gamma}\Phi\left(\frac{L_\tau}{g^{-z\nu}}\right)^{\frac{\gamma}{z\nu}} \sim L_\tau^{\frac{\gamma}{z\nu}} \sim T^{-\frac{\gamma}{z\nu}}$$

(near FE-QCP)

$(\text{here } z = 1, \nu = 1/2, \gamma = 1 \rightarrow \frac{\gamma}{z\nu} = 2)$

$$\chi^{-1} \propto T^2$$

Gruneisen Ratio $$\Gamma = \frac{1}{V}\frac{\partial V}{\partial U} = \frac{\alpha_{Th}}{c_P}$$

Zhu et al (13)

$$F(\delta\phi, \delta V) = \frac{\alpha}{2}\phi^2 + \frac{a}{2}\delta V^2 - \eta(\delta V)(\delta\phi^2)$$

Minimization + Fluctuation-Averaging

$$\Gamma_{FE} = \frac{1}{V}\frac{\partial V}{\partial U} \propto \frac{\langle \delta\phi^2 \rangle}{\delta U}$$

Near Classical Phase Transition

$$\Gamma_{CFE}(T \to T_c) \propto (T - T_c)^0$$

(supported by experiment)

Gruneisen Ratio $\Gamma = \frac{1}{V}\frac{\partial V}{\partial U} = \frac{\alpha_{Th}}{c_P}$

Zhu et al (13)

$$F(\delta\phi, \delta V) = \frac{\alpha}{2}\phi^2 + \frac{a}{2}\delta V^2 - \eta(\delta V)(\delta\phi^2)$$

Minimization + Fluctuation-Averaging

$$\Gamma_{FE} = \frac{1}{V}\frac{\partial V}{\partial U} \propto \frac{\langle \delta\phi^2 \rangle}{\delta U}$$

In the vicinity of a (d=3) FE-QCP

$$\Gamma_{QFE} \propto \left(\frac{\langle \delta\phi_T^2 \rangle}{\delta U} \right) \propto \frac{\chi^{-1}}{T q_T^d} = \frac{T^2}{T^4} = \frac{1}{T^2}$$

Zhu et al (13)

Scaling Approach to the Gruneisen Ratio

$$\Gamma = \frac{\alpha}{c_P} = -\frac{1}{V_m T}\frac{\partial S/\partial V}{\partial S/\partial T}$$

Dimensionally

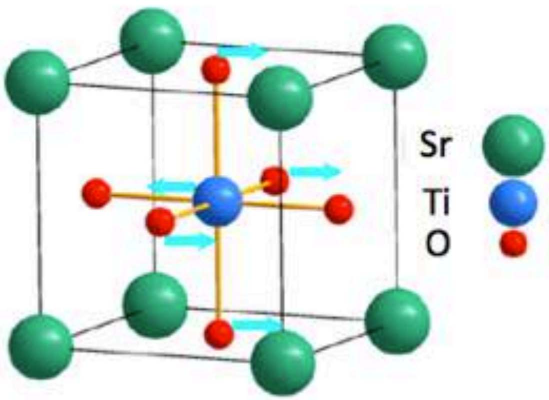
$$[\Gamma] = \left[\frac{1}{g}\right]$$

Near a (FE)-QCP

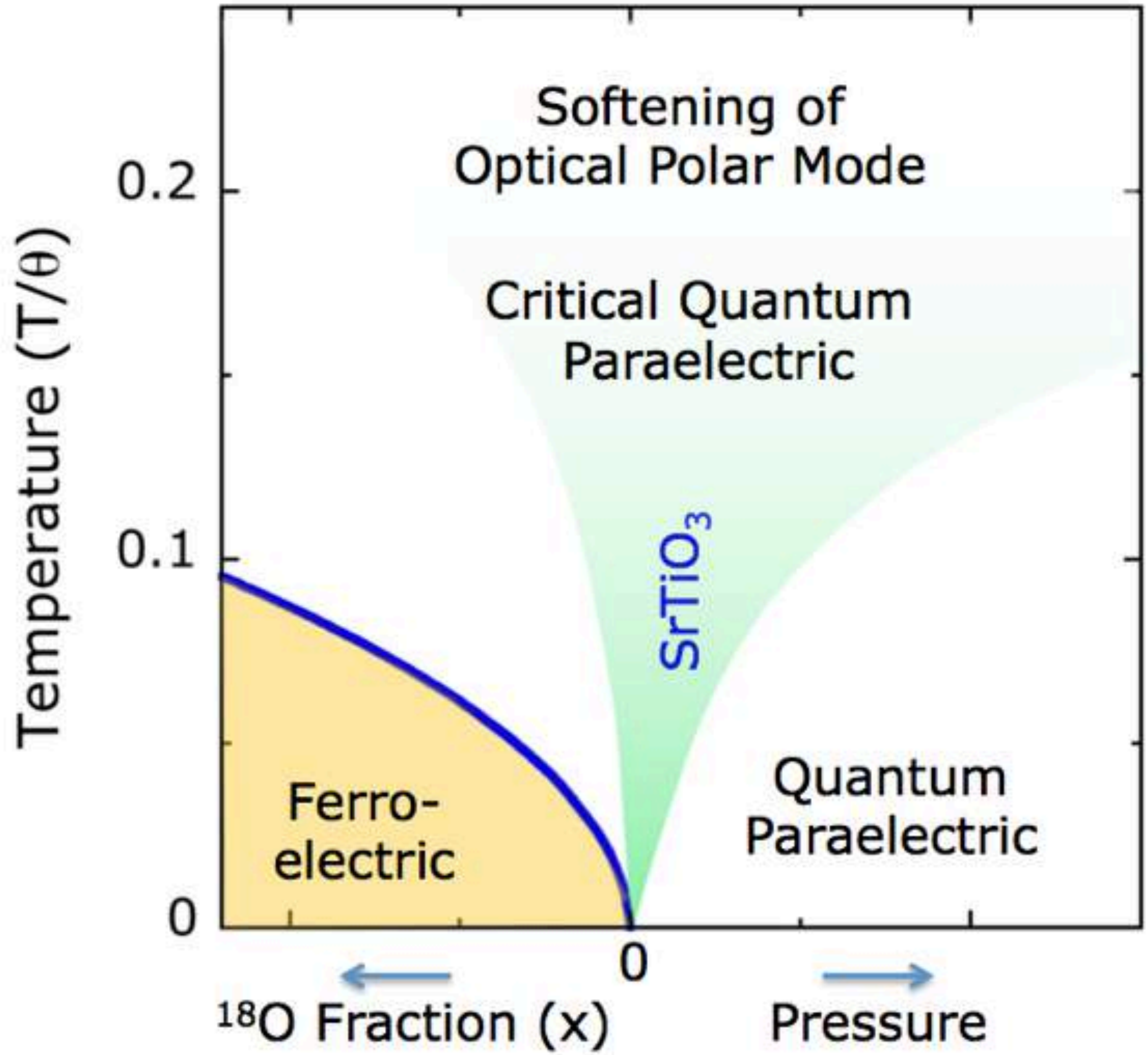
$$\Gamma = \frac{1}{g}\Phi\left(\frac{L_\tau}{\xi_\tau}\right) = \frac{1}{g}\Phi\left(\frac{L_\tau}{g^{-z\nu}}\right) = \tilde{\Gamma}_0 L_\tau^{\frac{1}{z\nu}} = \Gamma_0 T^{-\frac{1}{z\nu}}$$

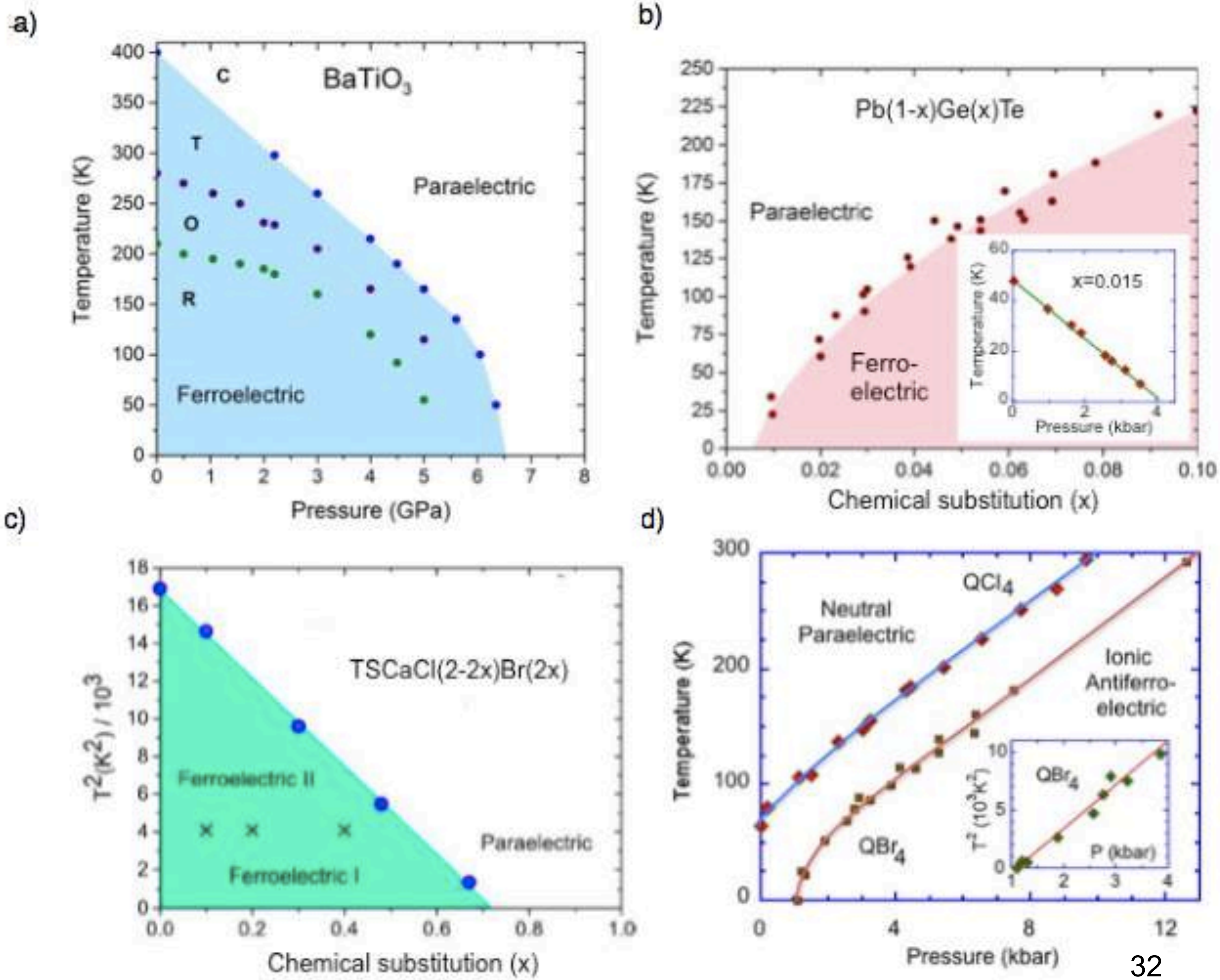
$$\Gamma^{-1} \propto T^2$$

$(z = 1, \nu = \frac{1}{2})$



Optical Polar Mode





a)
BaTiO3
C
T
O
R
Paraelectric
Ferroelectric
Temperature (K)
Pressure (GPa)
b)
Pb(1-x)Ge(x)Te
Paraelectric
Ferro-
electric
x=0.015
Temperature (K)
Pressure (kbar)
Chemical substitution (x)
c)
TSCaCl(2-2x)Br(2x)
Ferroelectric II
Ferroelectric I
Paraelectric
T2(K2) / 103
Chemical substitution (x)
d)
QCl4
Neutral
Paraelectric
Ionic
Antiferro-
electric
QBr4
T2 (103K2)
P (kbar)
Temperature (K)
Pressure (kbar)

Why Study Ferroelectric Quantum Criticality?

Quest for Universality in Quantum Criticality

Simple Examples: Few Degrees of Freedom and Non-Dissipative Dynamics

Reside in marginal dimension allowing for detailed interplay between experiment and theory

Additional Degrees of Freedom (e.g. Spin and Charge) can be added Systematically

Open Questions for Future Research

Specific FE/PE materials for Study at low T

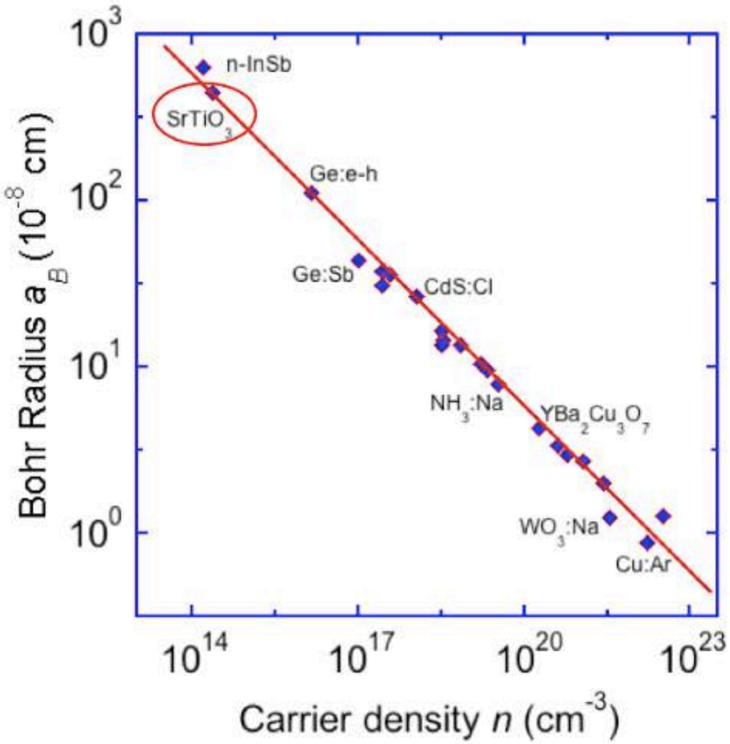
Add Spin: A Multiferroic QCP

Add Charge: An Exotic Metal and an Unexpected Superconductor!

Thoughts on n-doped STO

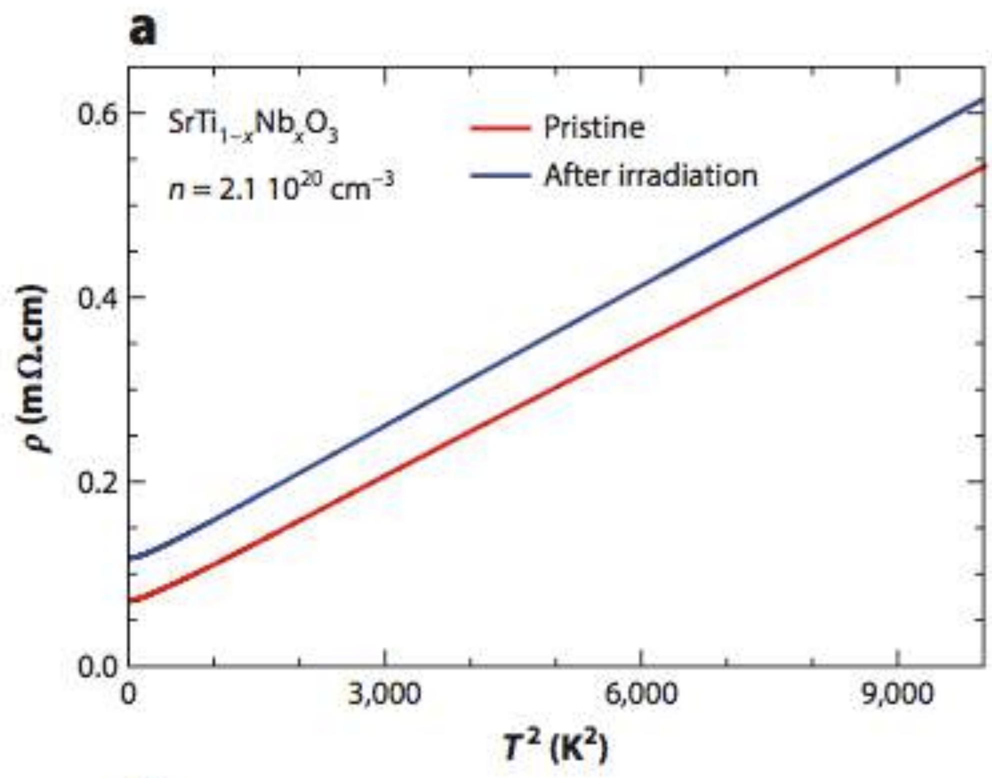
Mott criterion for doped semiconductors

$$n_c^{\frac{1}{3}} a_B^* \approx 0.26 \qquad \left(a_B^* = \frac{\epsilon \hbar^2}{m^* e^2} \right)$$



Transport in n-doped STO

$$\rho = \rho_0 + AT^2 \qquad A = f(n)$$



Origin of this Robust T-Dependence ??

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

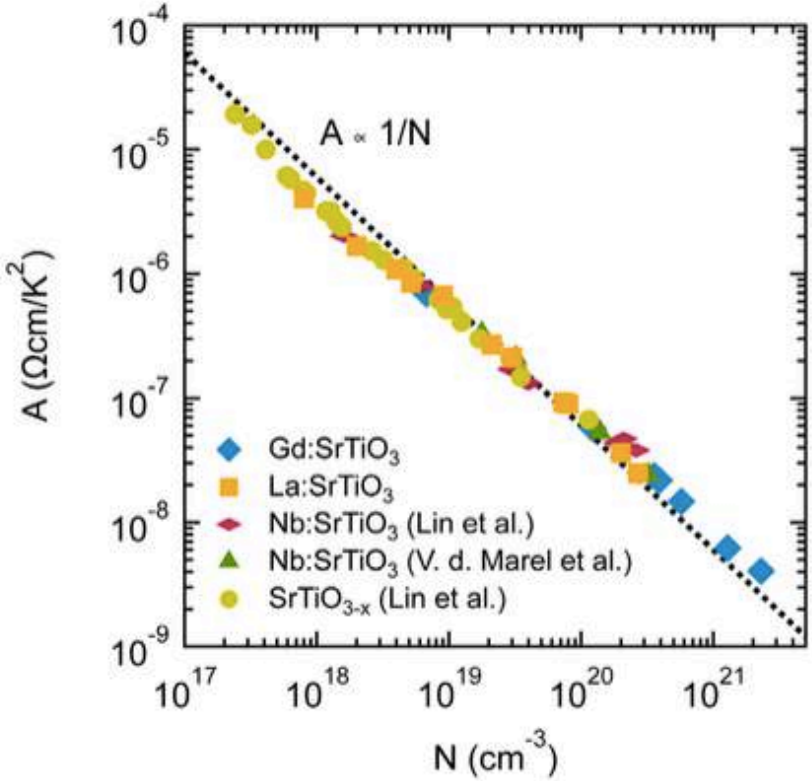


Figure 3. Carrier density dependence of the *A*-coefficient of the T^2 resistivity term for 3D electron gases in $SrTiO_3$ doped with different dopants (see legend). Data is from thin films (La:$SrTiO_3$ and Gd:$SrTiO_3$) grown by MBE and bulk single crystal data from [44, 45]. The *A*-coefficient approximately follows a 1/*N* dependence on the carrier density *N* over orders of magnitude in *N*, as can be seen by comparison with the black dotted line. Slight deviations from the 1/*N* behavior are expected even if the scattering rate is independent of the carrier density, because the carrier mass also changes as higher lying bands are filled. Reprinted from [56]. CC BY 4.0.

$$\rho = \rho_0 + AT^2$$

Drude Model

$$AT^2 = \frac{m^*}{Ne^2}\frac{1}{\tau}$$

S. Stemmer and J. Allen ROPP 81, 062502 (2018)

Energy Scales

$$T \propto k_F^2 \propto n^{\frac{2}{3}}$$

$$V \propto \frac{1}{r} \propto n^{\frac{1}{3}}$$

$$r_s \propto \frac{V}{T} \propto \frac{1}{n^{\frac{1}{3}} a_B^*} \approx 10^{-2}$$

weak elector-electron interactions

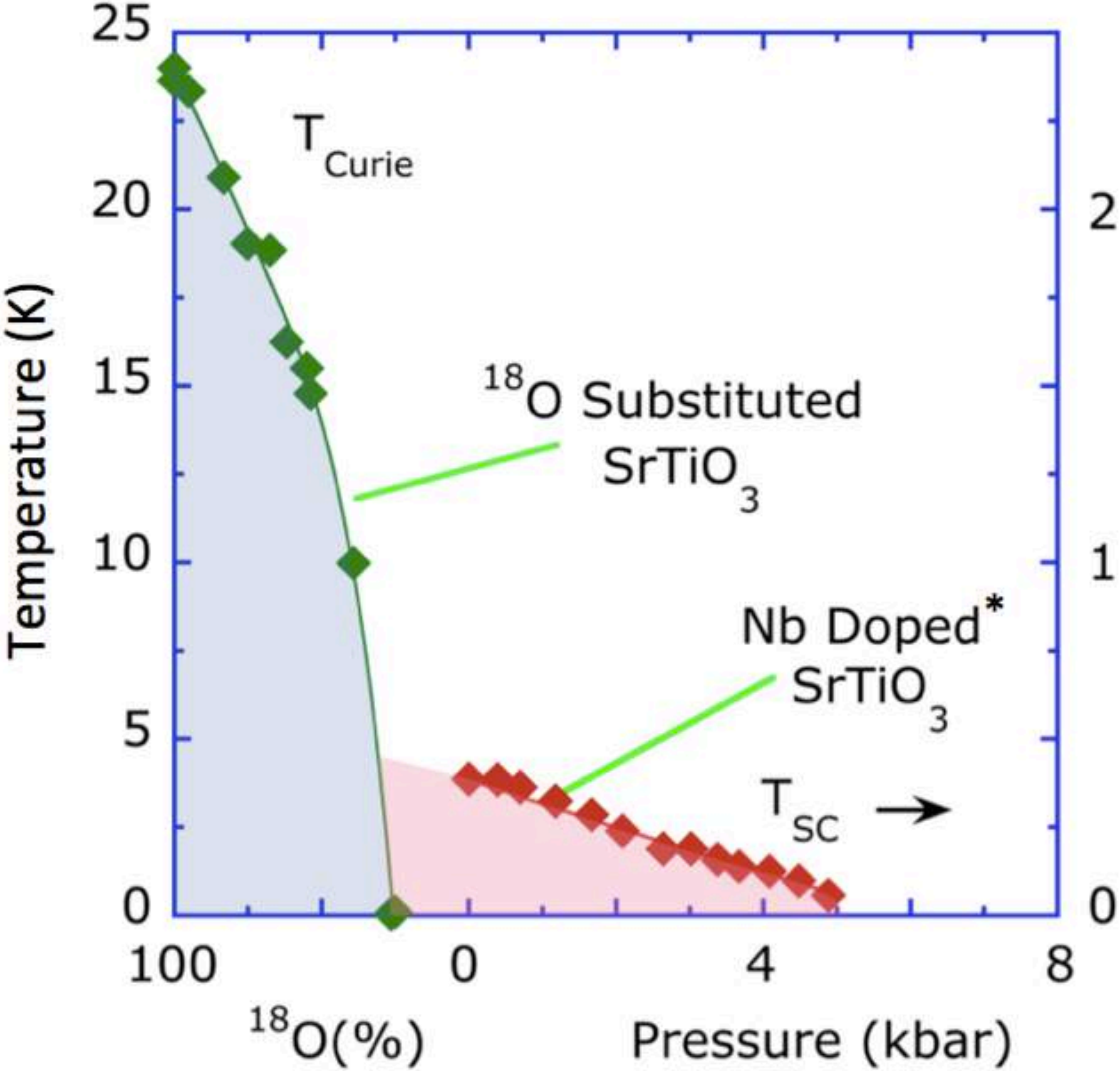
$$T_F \sim 13K$$

$$n = 5.5 \times 10^{17} cm^{-3}$$

$$T_D \sim 400K$$

$$T_F \ll T_D$$

Slow Electrons and Fast Phonons !



(S. Rowley et al., arXiv:1801:08121)

Isotope effect in superconducting n-doped $SrTiO_3$

A. Stucky, G. W. Scheerer, Z. Ren, D. Jaccard, J.-M. Poumirol, C. Barreteau, E. Giannini & D. van der Marel

Sc. Reports 2016

$$\alpha = -\frac{d(\ln T_C)}{d\ln M} = -10 \qquad (\alpha = 0.5 \quad \text{BCS})$$

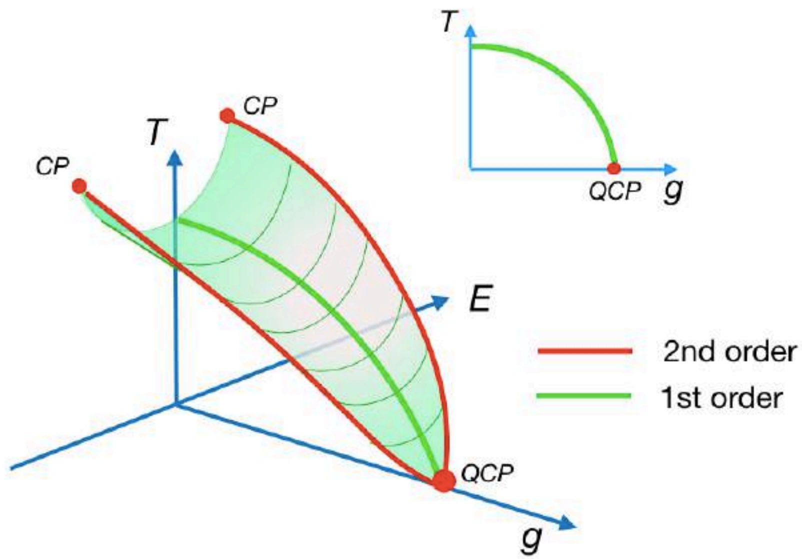
Quantum critical fluctuations enhance superconductivity ??!

Soft TO phonons (very weak coupling to charge density)

Plasmons (much fine-tuning required)

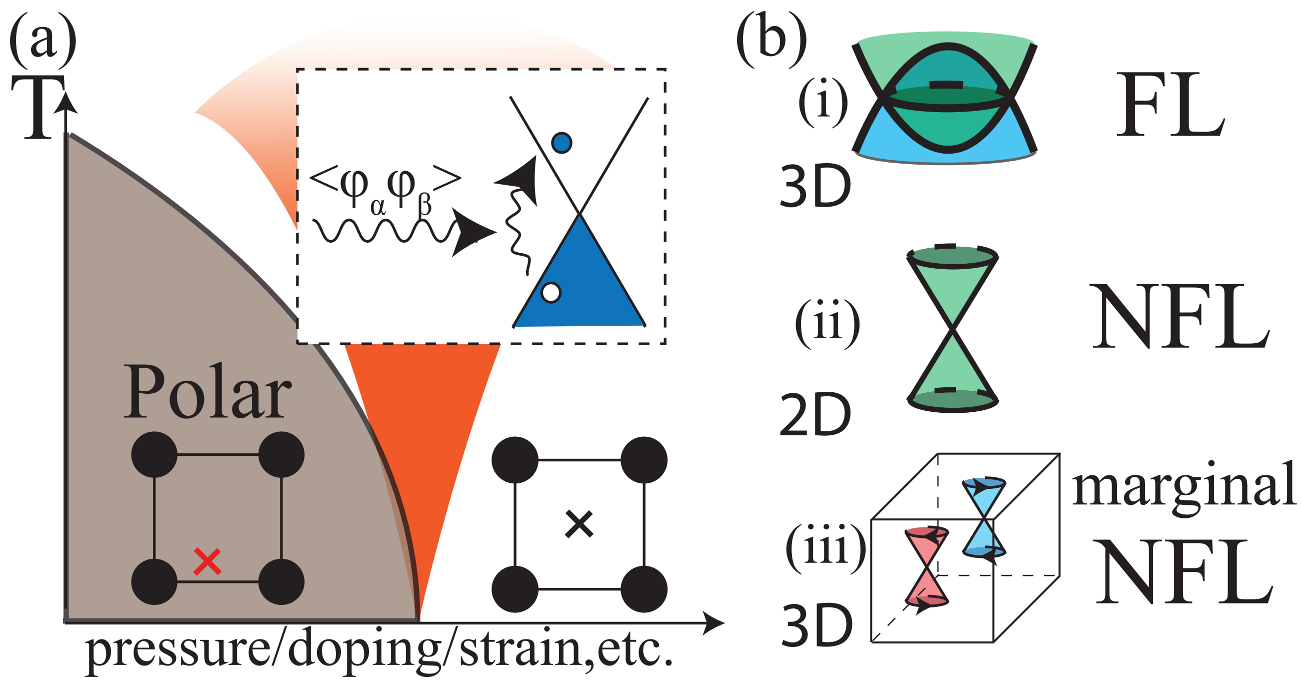
Wanted: How to get (s-wave) Cooper pairing without retardation!!

Next Time: A Flavor for Two Current Research Projects



Can quantum fluctuations “toughen” a system against macroscopic instabilities resulting in a line of classical first-order transitions ending in a quantum critical point ?

Next Time: A Flavor for Two Current Research Projects



When do metals close to polar quantum critical points develop strongly interacting novel phases ??


thank you
danke
謝謝
teşekkür ederim
gracias
спасибо
Баярлалаа
рахмат
dank je
tapadh leat
bedankt
hvala
mauruuru
dziękuję
obrigado
sagolun
sukriya
kop khun krap
grazie
taiku
go raibh maith agat
mochchakkeram
arigatō
takk
dakujem
мерси
terima kasih
ありがとう
감사합니다
ευχαριστώ
merci