Mott metal-insulator transition on compressible lattices

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Universität zu Köln

in collaboration with :

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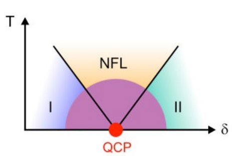
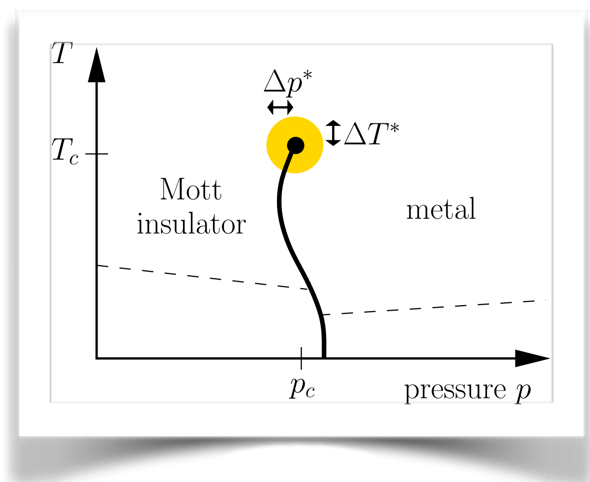
Lorenz Bartosch (Frankfurt)





Outline

- Introduction: Mott transition
- Universality of the Mott endpoint
- Experiments
- Theory: Mott endpoint on compressible lattices
- Summary

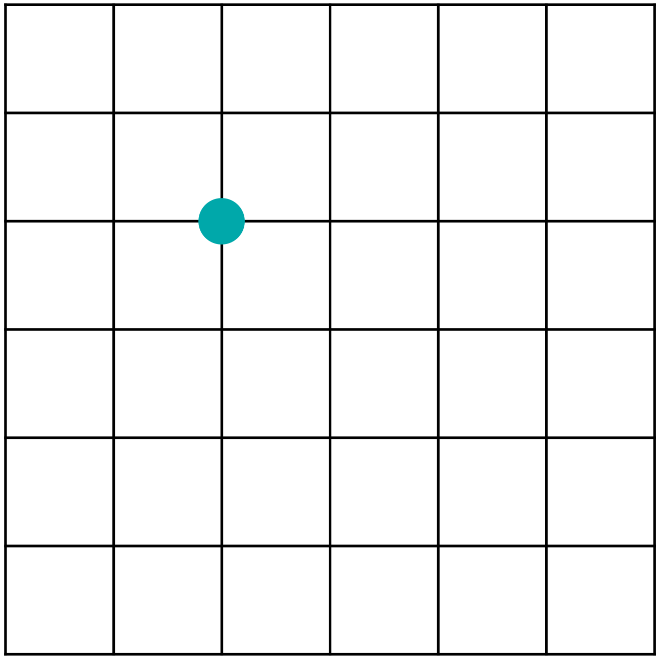
Introduction: Mott transition

Mott metal-insulator transition

Hubbard model: $$\mathcal{H} = -t \sum_{\sigma\langle ij\rangle} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

hopping on a lattice

simplification: on-site repulsion
(screened Coulomb interaction)



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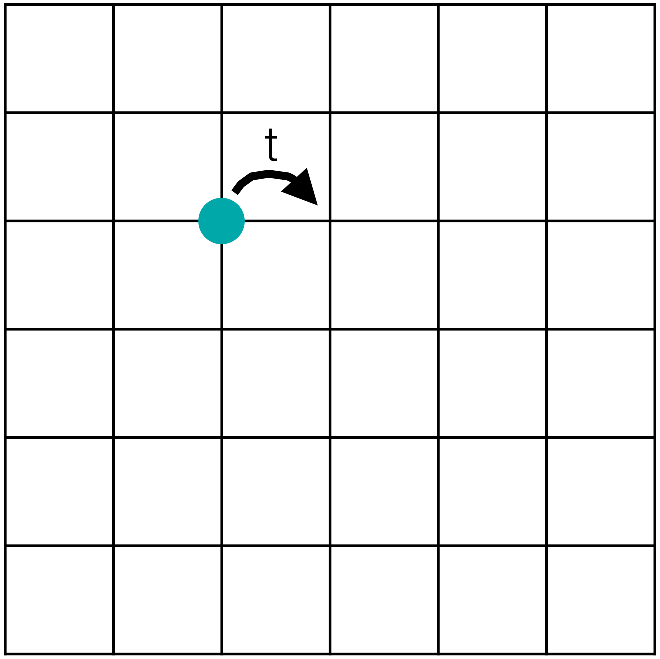

hopping:
gain of kinetic energy t

Mott metal-insulator transition

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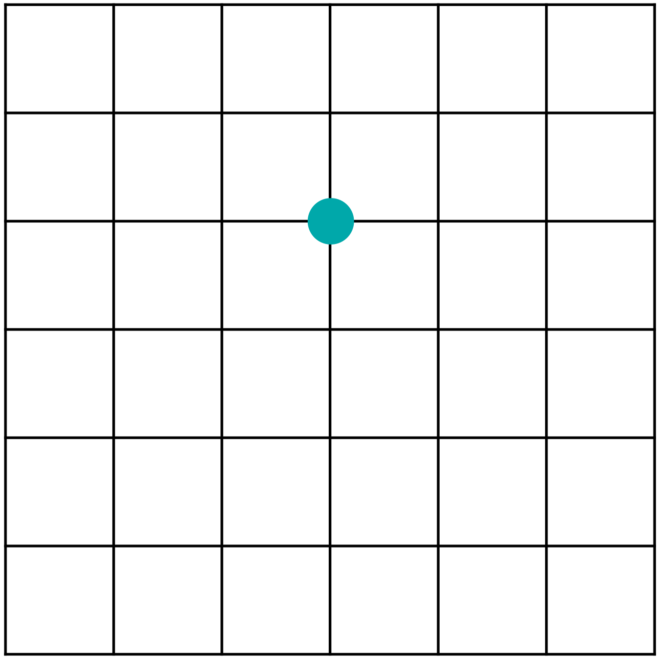

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Mott metal-insulator transition

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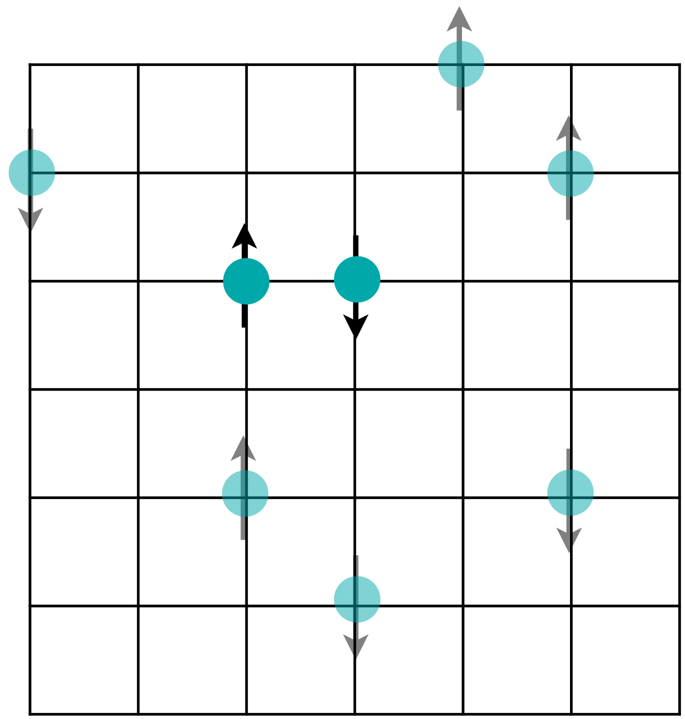

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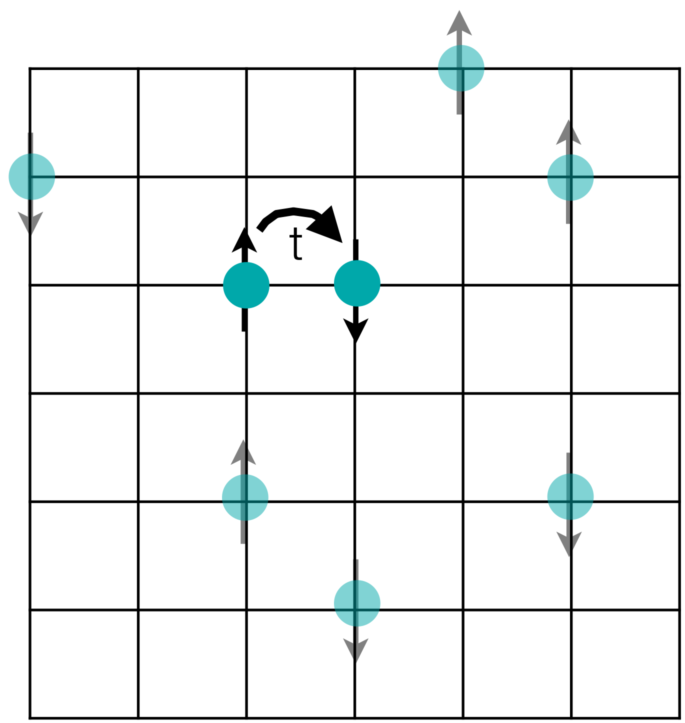

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hopping on a lattice

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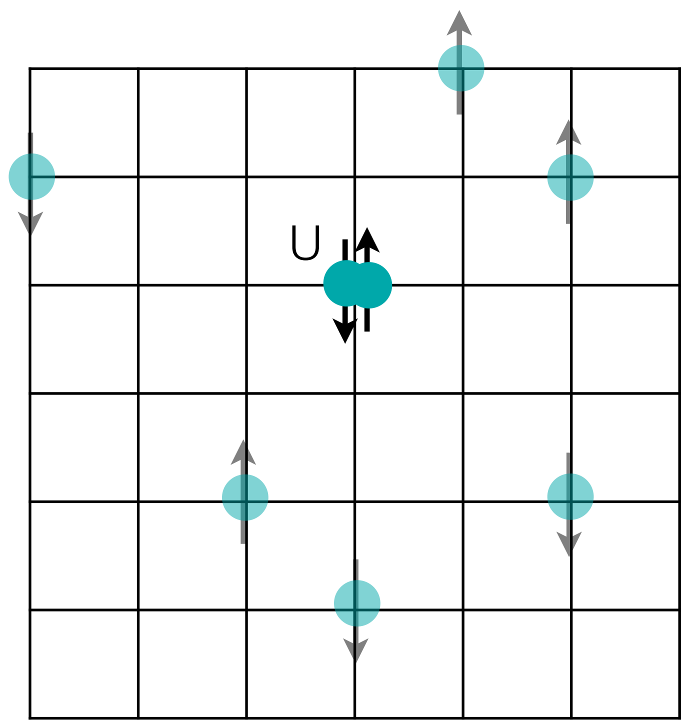


hopping:
gain of kinetic energy t

doubly occupied site:
cost of energy U

Mott metal-insulator transition

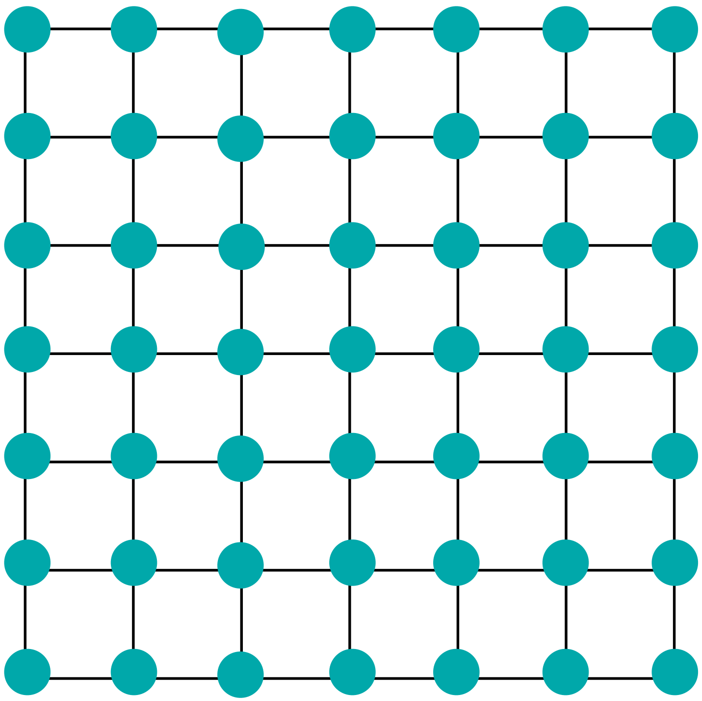
Hubbard model: $$\mathcal{H} = -t \sum_{\sigma\langle ij\rangle} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$$

hopping on a lattice

simplification: on-site repulsion
(screened Coulomb interaction)

at half-filling:

strong competition between kinetic energy and on-site repulsion

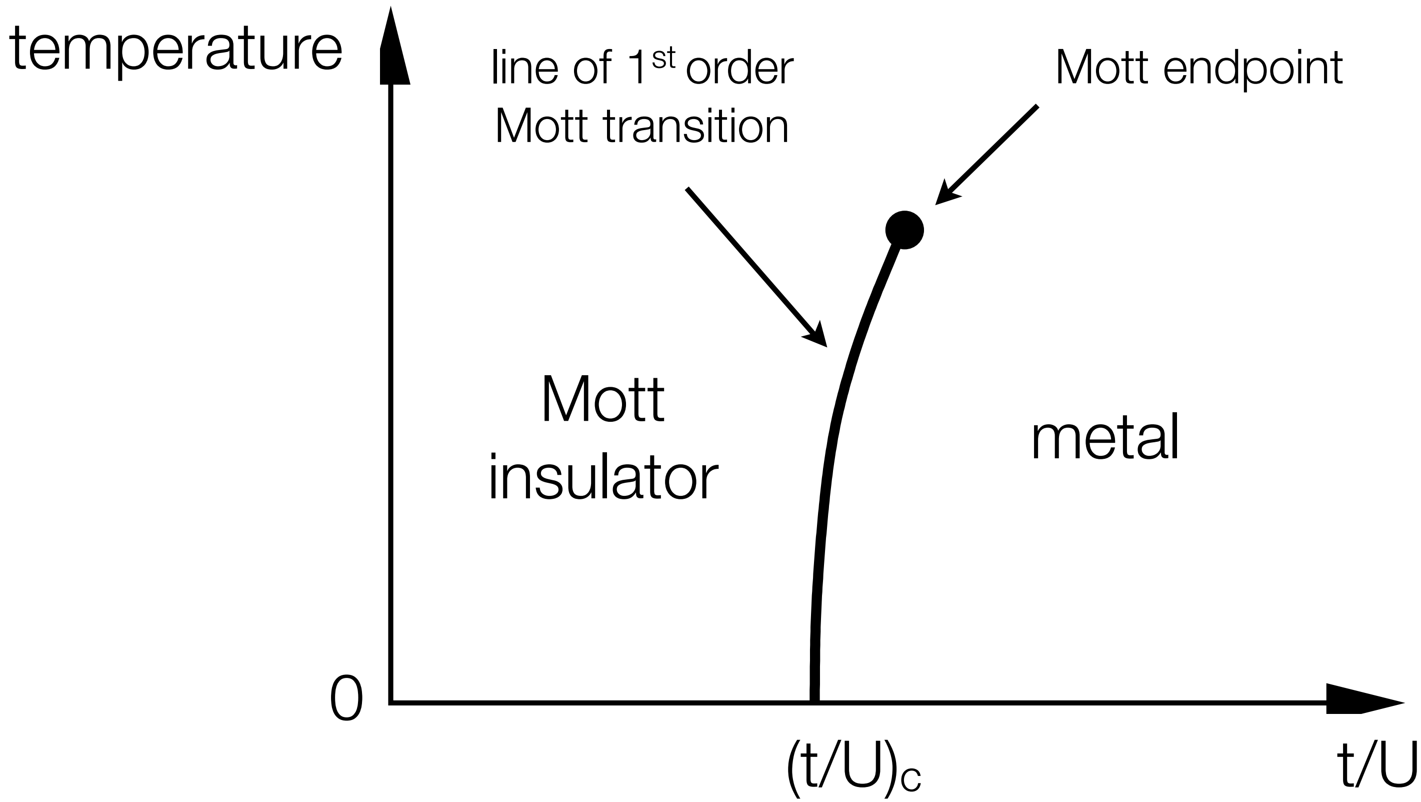


metallic for t >> U
(without nesting)

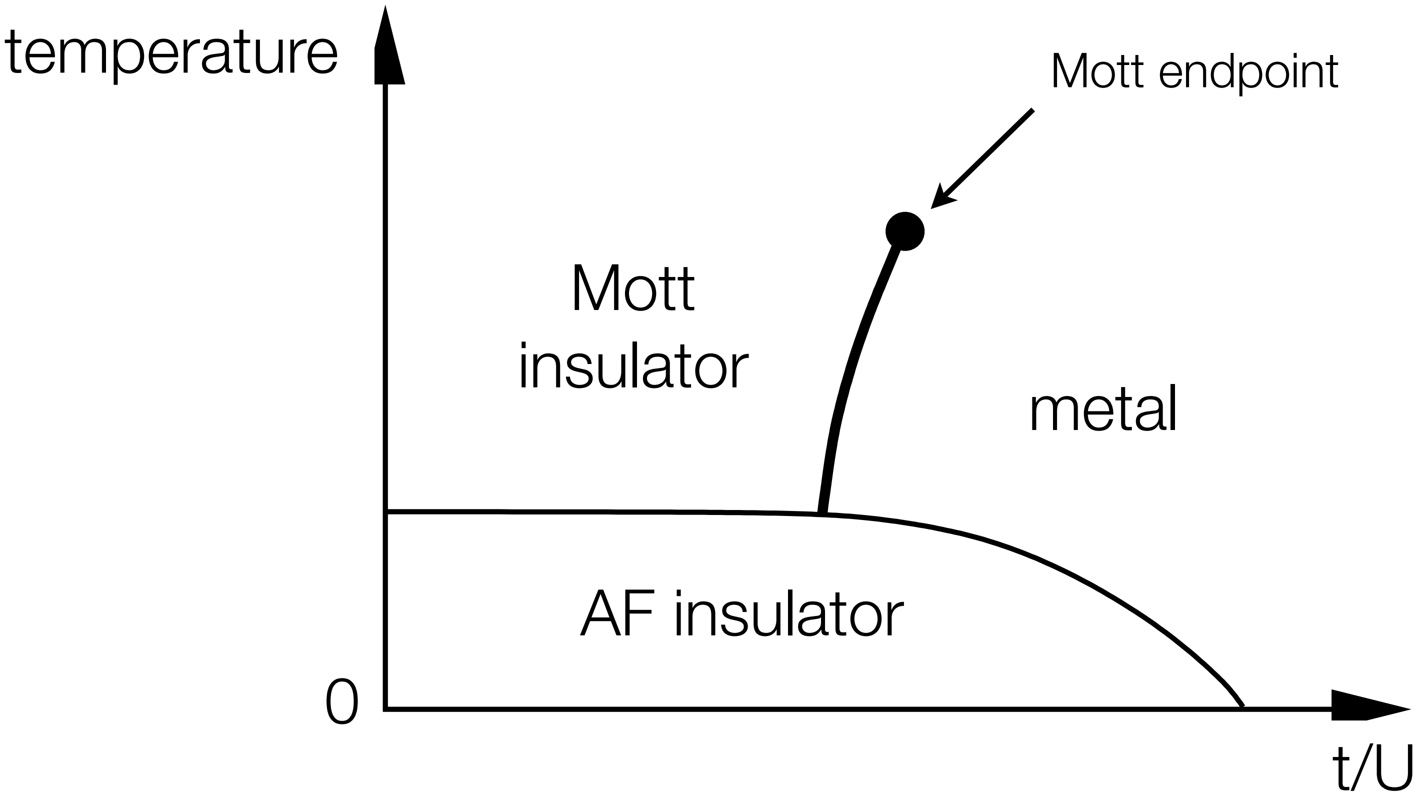
insulating for t << U

metal-insulator transition at a critical ratio t/U

Phase diagram

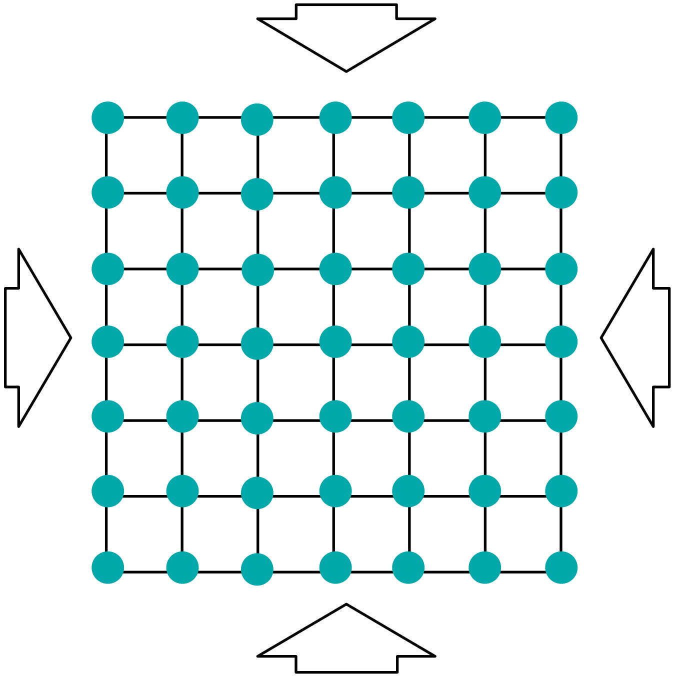


Phase diagram



to release spin entropy: magnetic ordering at low T

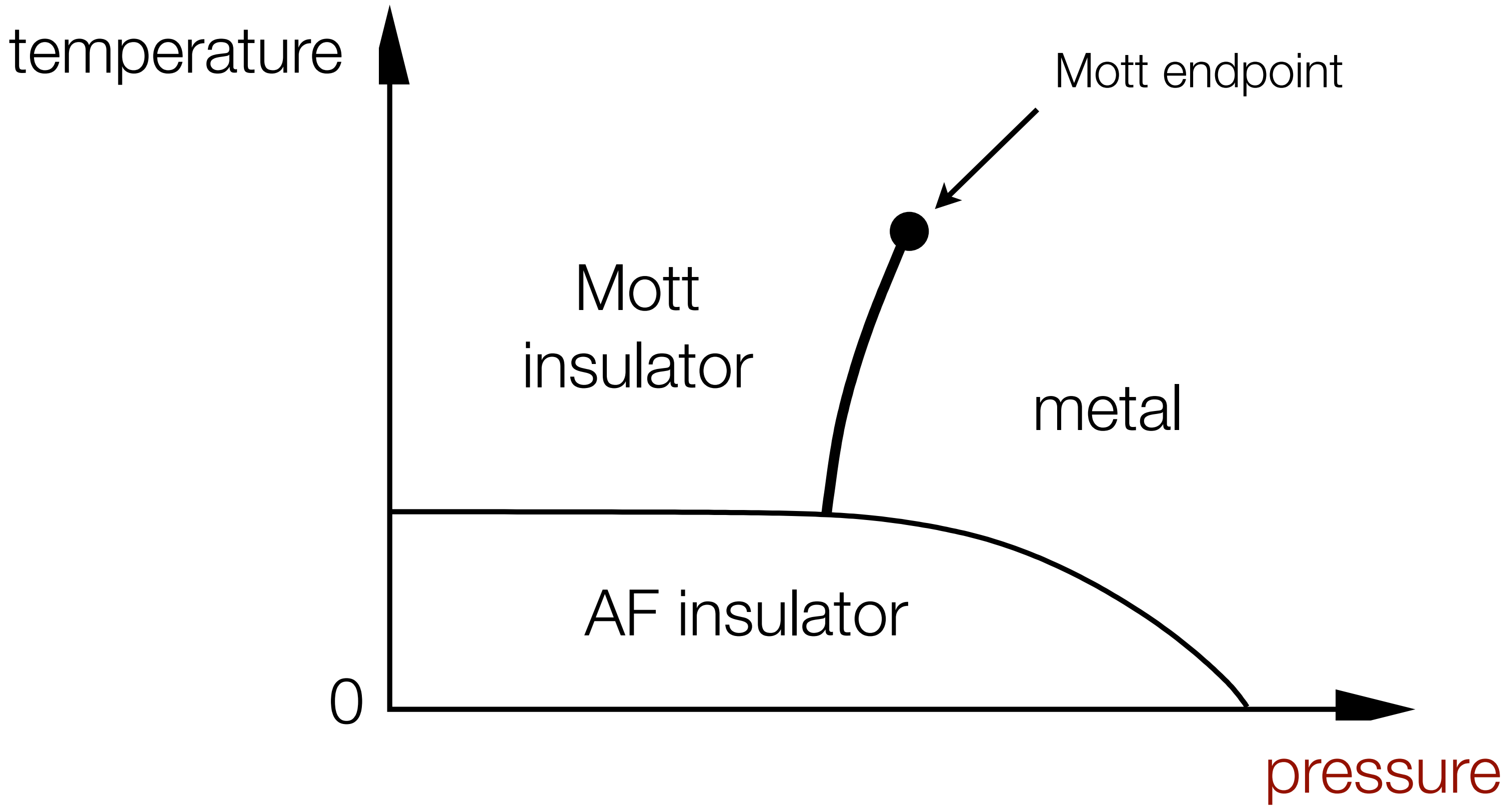
Tuning by pressure



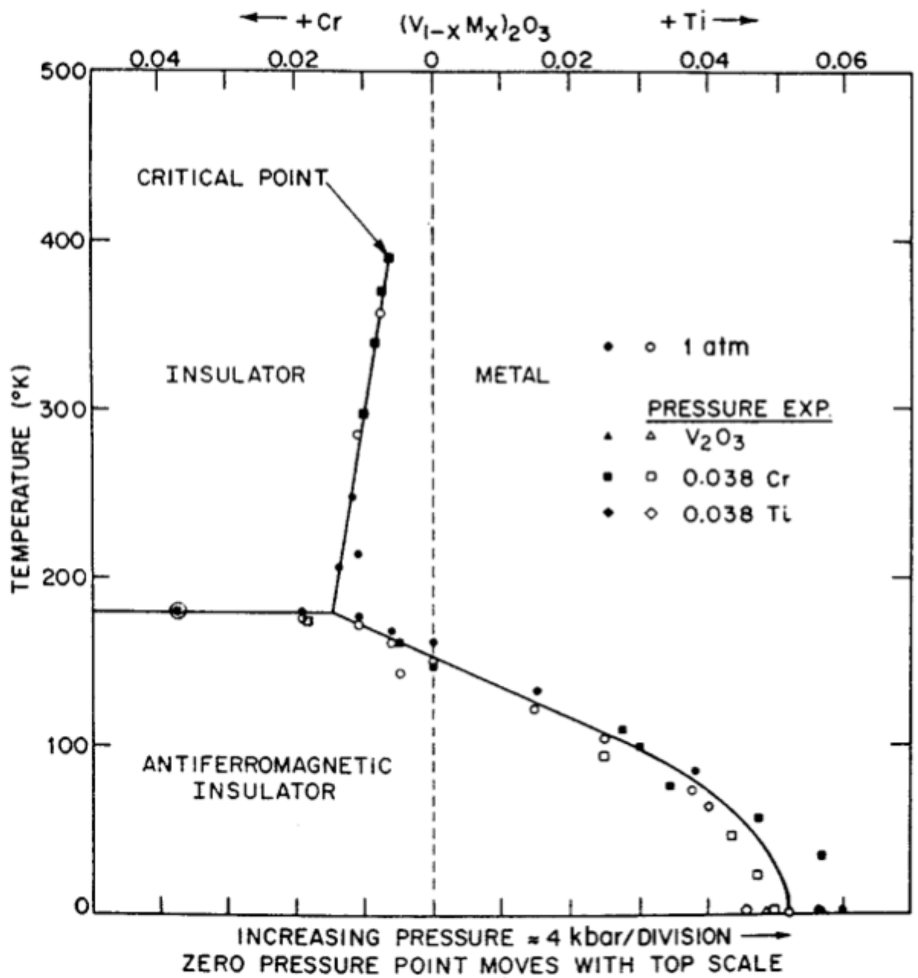
applying pressure reduces lattice constant

⇨ increases overlap of electron wavefunctions,
enhancement of hopping amplitude t

Phase diagram with pressure tuning



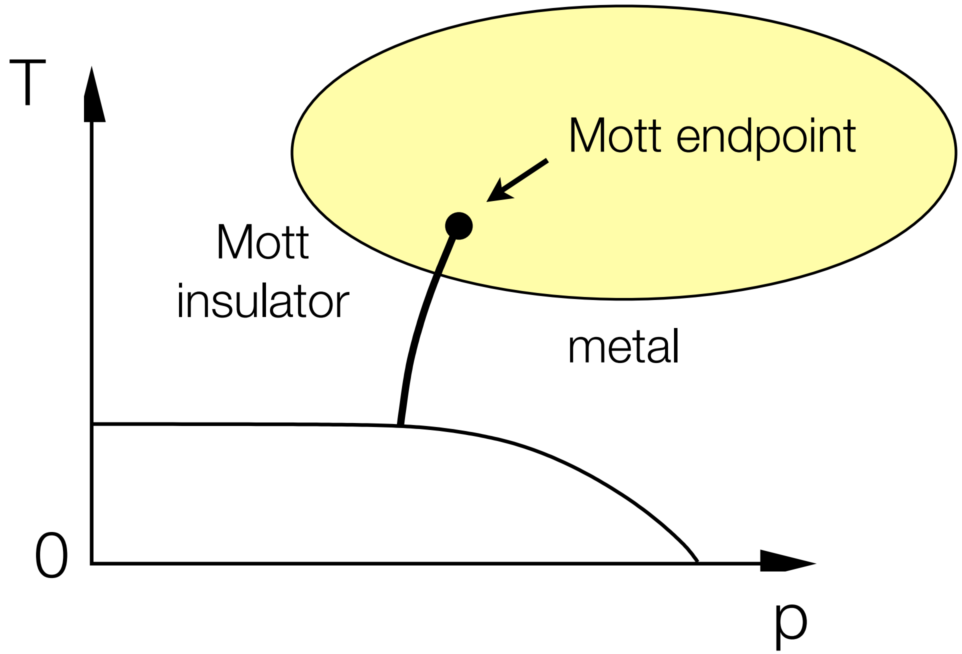
Phase diagram of V_2O_3



McWhan et al PRB (1973)

Universality of the Mott end point

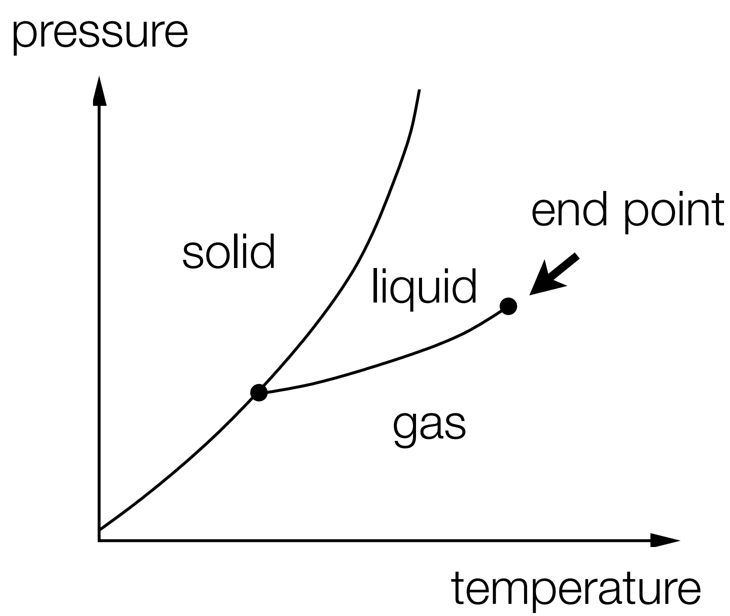
Mott critical endpoint



What are the critical properties of the Mott endpoint?

Liquid-gas end point

line of first-order liquid-gas transitions terminates at second-order end point



line defines an emergent mirror symmetry ⇨ Ising symmetry

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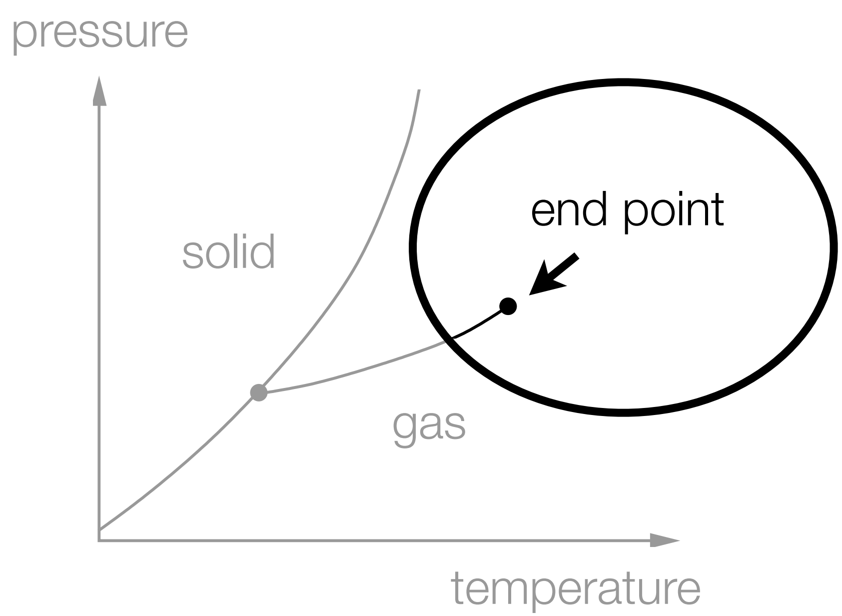
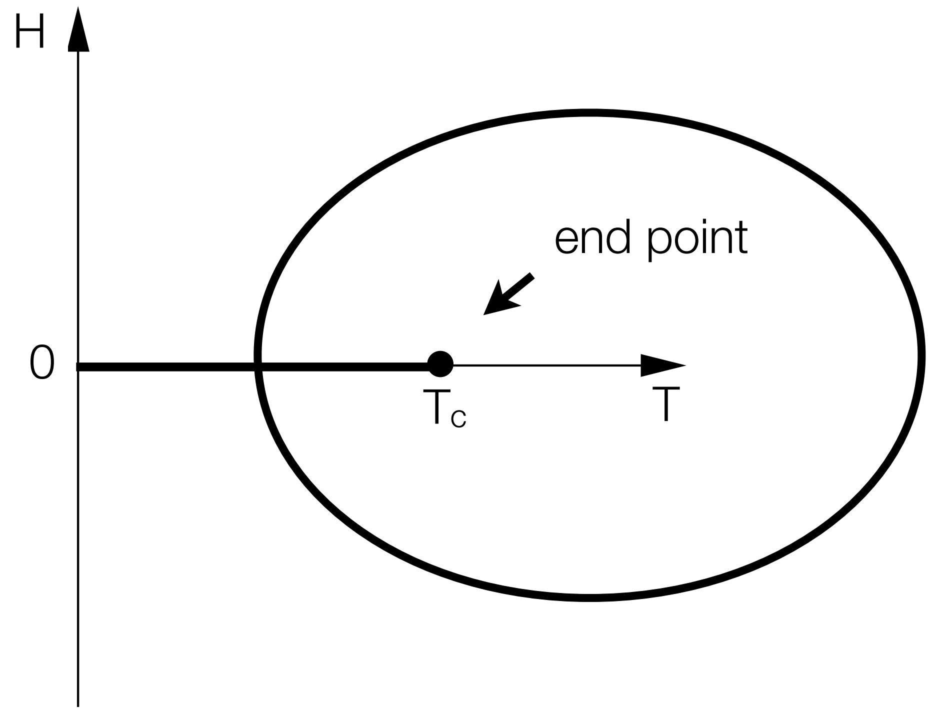


line defines an emergent mirror symmetry ⇨ Ising symmetry

Ising criticality

Ising magnet in a field: $\mathcal{L} = \frac{T - T_c}{2T_c} M^2 + (\nabla M)^2 + \frac{u}{4!} M^4 - HM$



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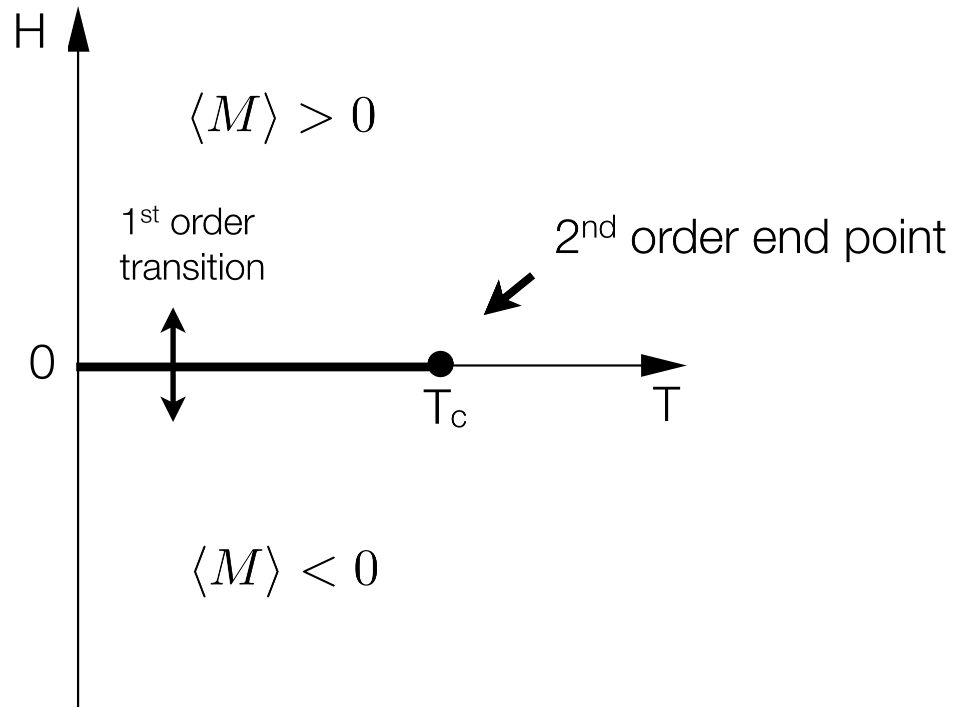

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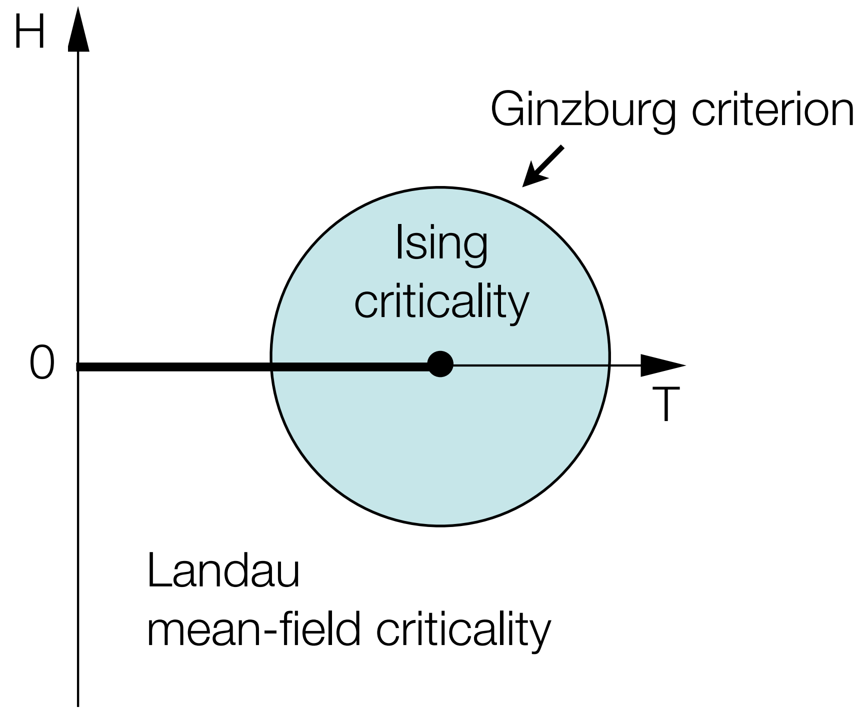
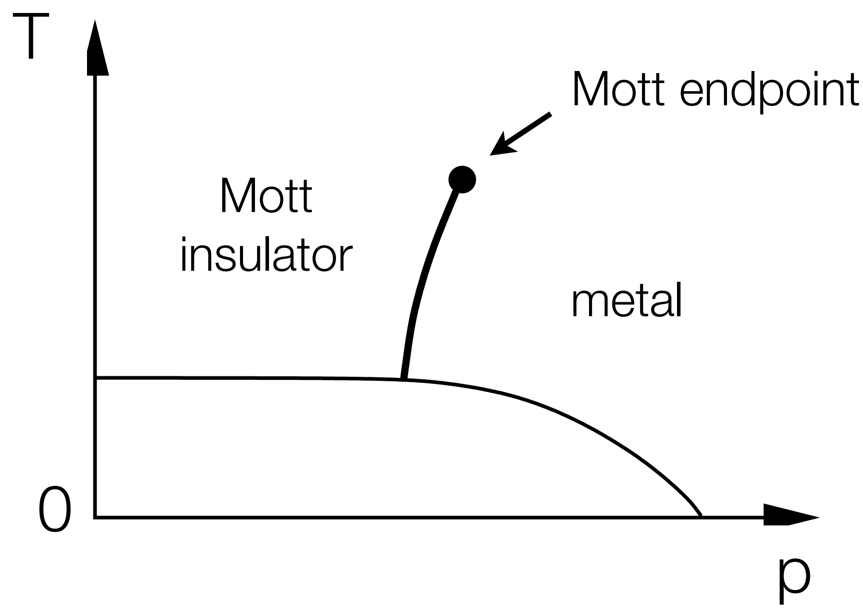
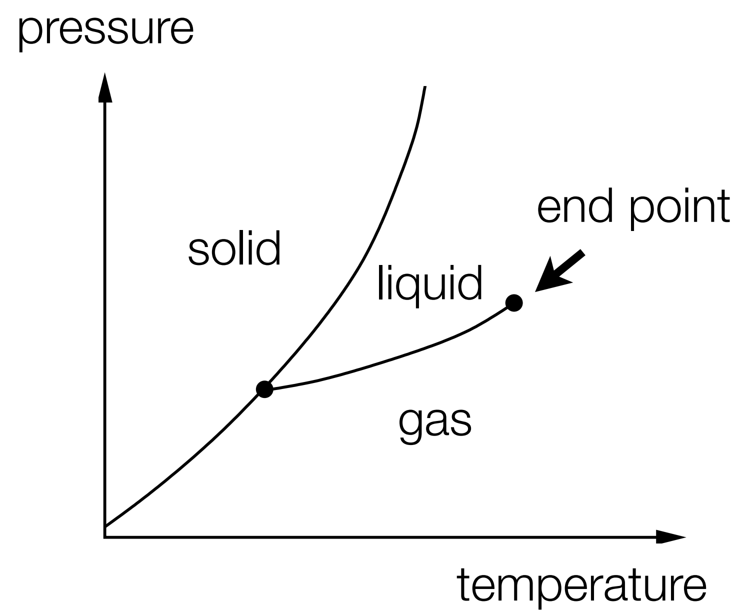


critical behavior: non-trivial Ising exponents close to endpoint

Universality of the Mott end point: Experiments

Mott critical endpoint



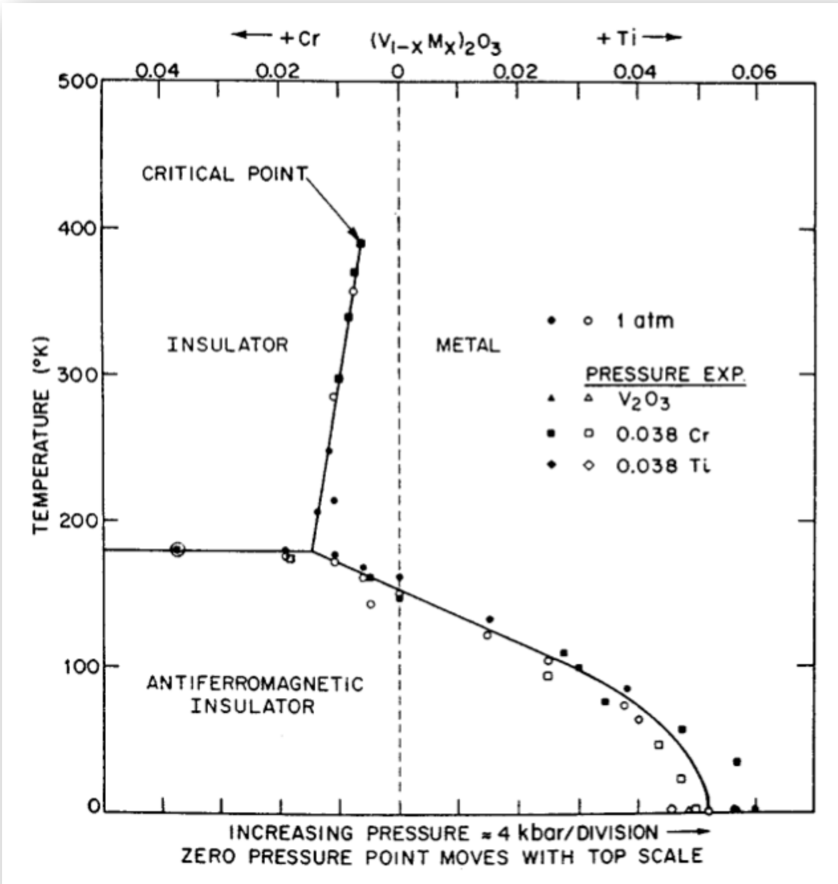


Is the Mott endpoint analogous to the liquid-gas endpoint?

Is it in the Ising universality class?

Mott end point of Cr-doped V_2O_3

Science **302**, 89 (2003)



Universality and Critical Behavior at the Mott Transition

P. Limelette,[1*] A. Georges,[1,2] D. Jérome,[1] P. Wzietek,[1] P. Metcalf,[3] J. M. Honig[3]

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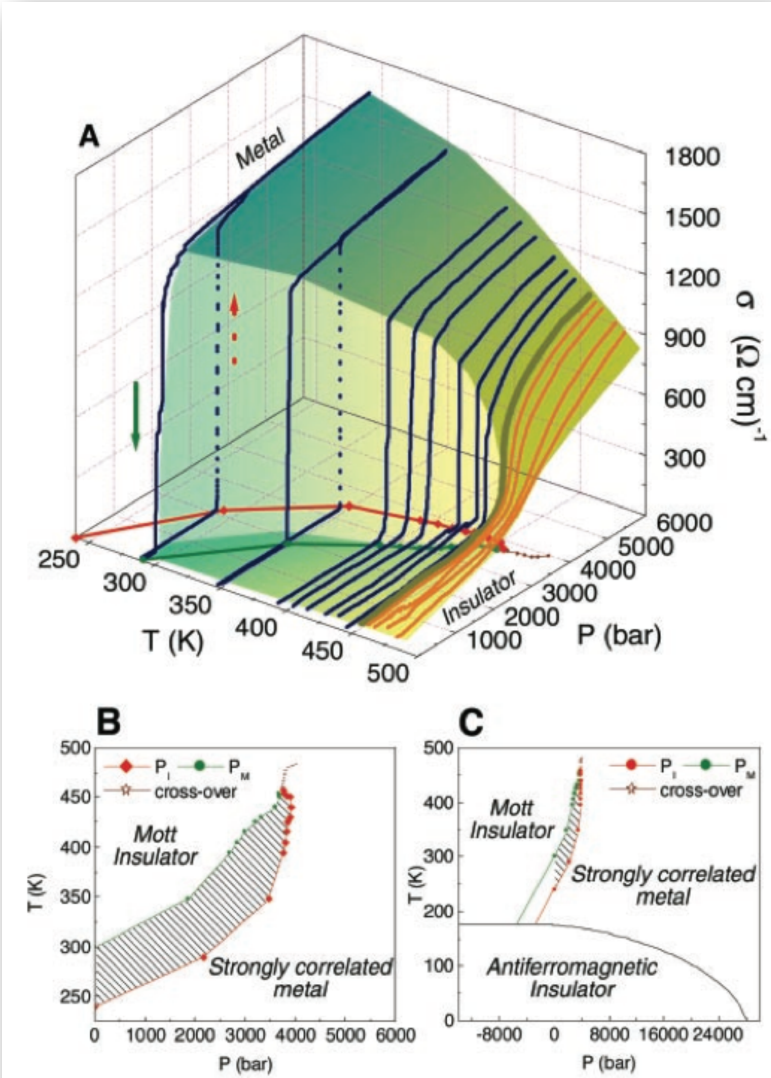

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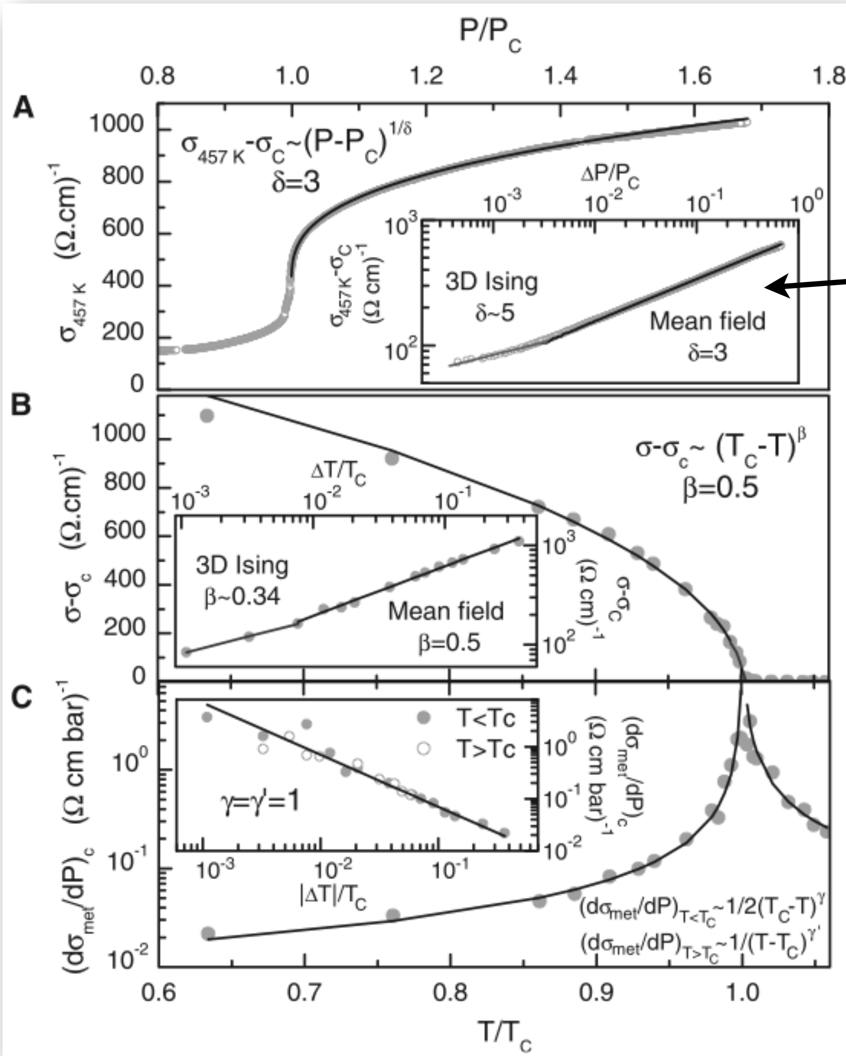

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Landau mean-field exponents

indications for Ising exponents close to the endpoint?

non-trivial assumption of the scaling analysis:

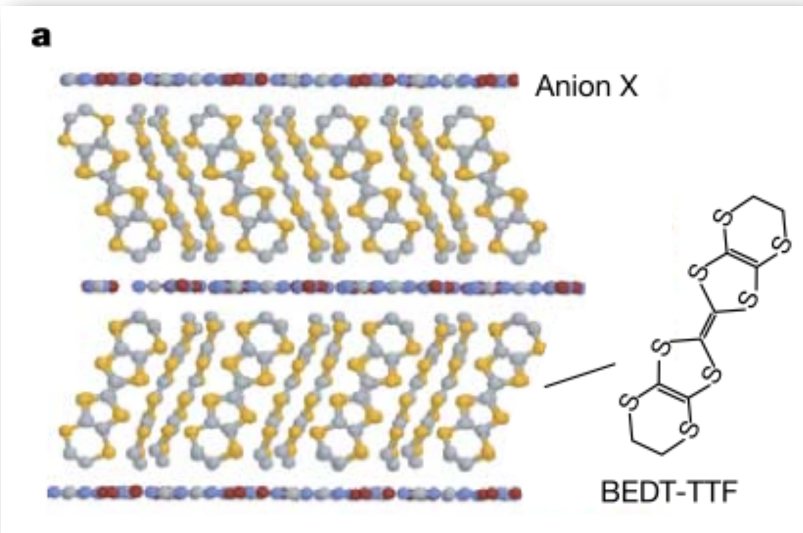
conductivity is the Ising order parameter!

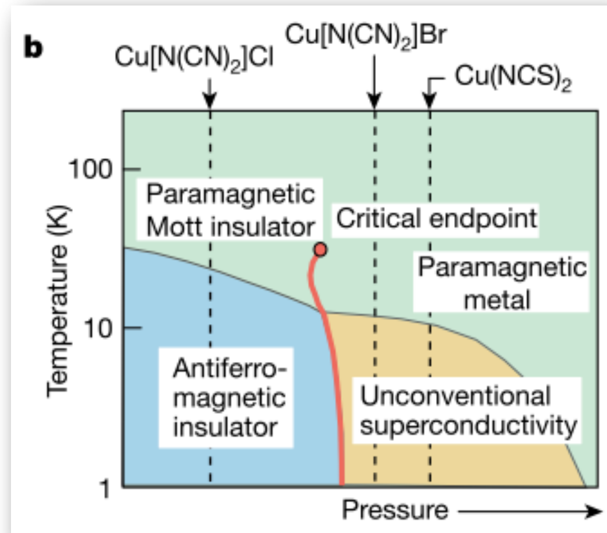
Mott end point of κ-(BEDT-TTF)$_2$X

Unconventional critical behaviour in a quasi-two-dimensional organic conductor

F. Kagawa[1], K. Miyagawa[1,2] & K. Kanoda[1,2]

nature Vol 436|28 July 2005|**doi:10.1038/nature03806**





conducting 2D layers of BEDT-TTF

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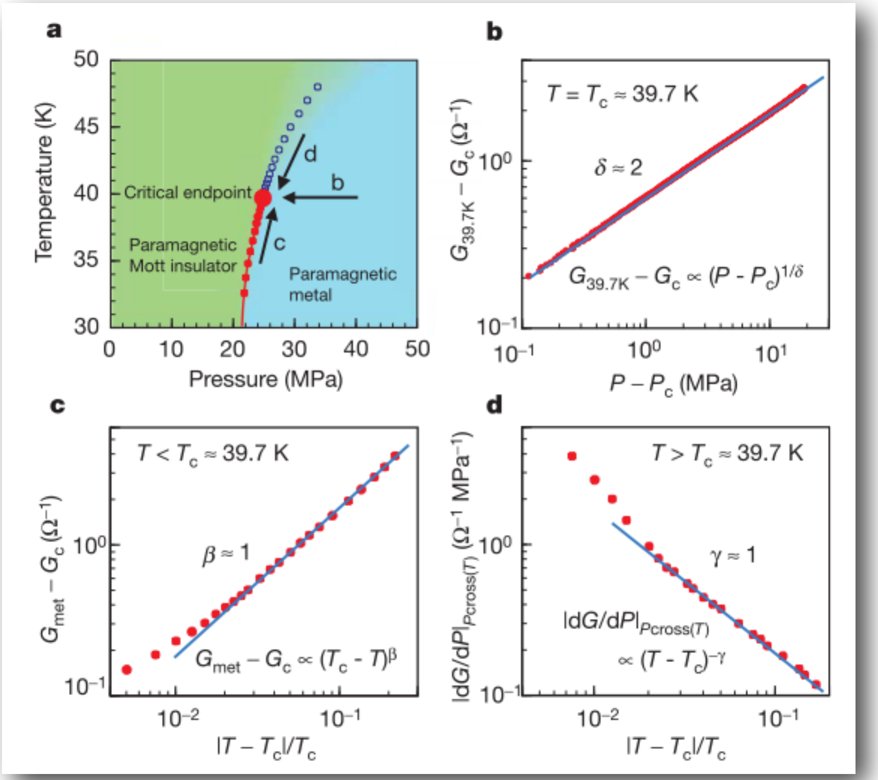

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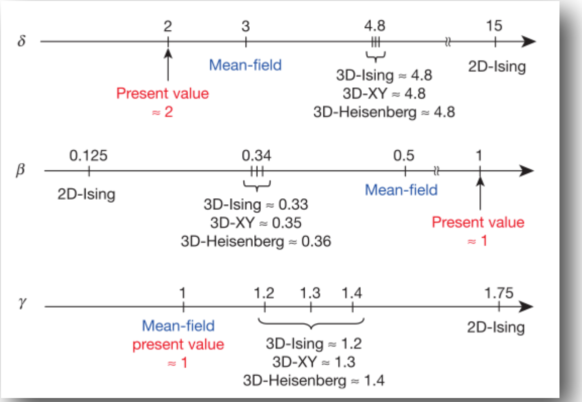

exponents neither Landau nor Ising?

unconventional universality class?

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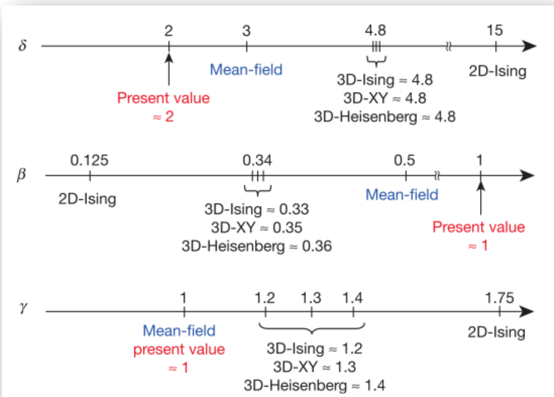


exponents neither Landau nor Ising?

unconventional universality class?

S. Papanikolaou et al. PRL (2008): NO!

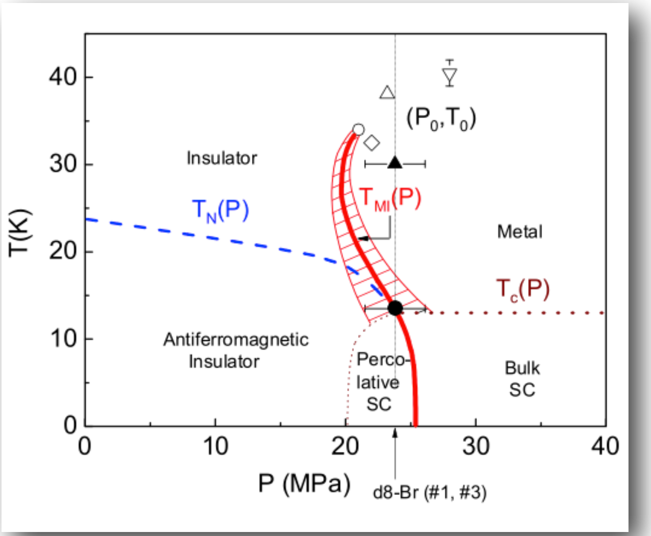
conductivity NOT necessarily the Ising order parameter!

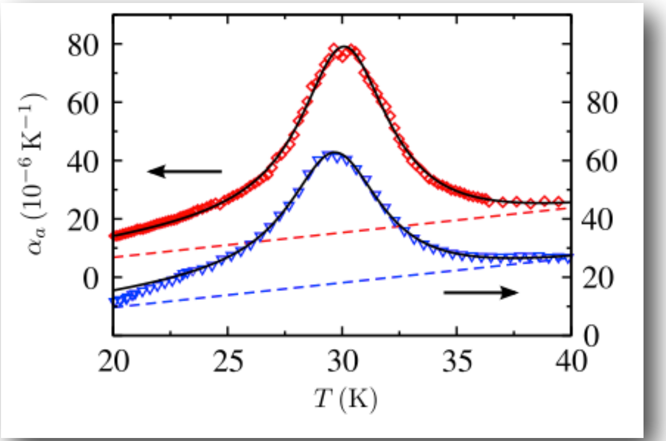
instead: conductivity ~ energy density (cf. Fisher-Langer scaling)

⇨ consistency with Ising criticality!

Mott end point of κ-(BEDT-TTF)$_2$X

Thermodynamics easier to interpret than transport:



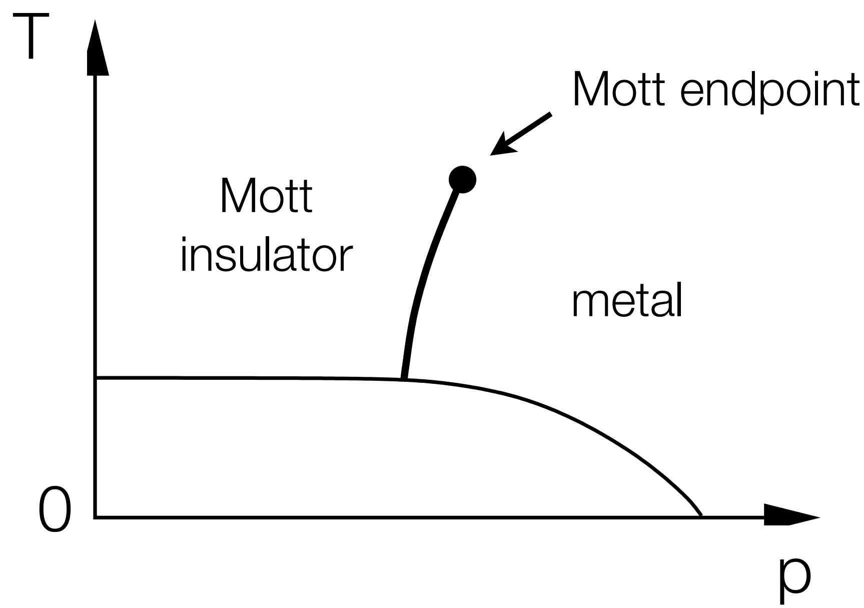


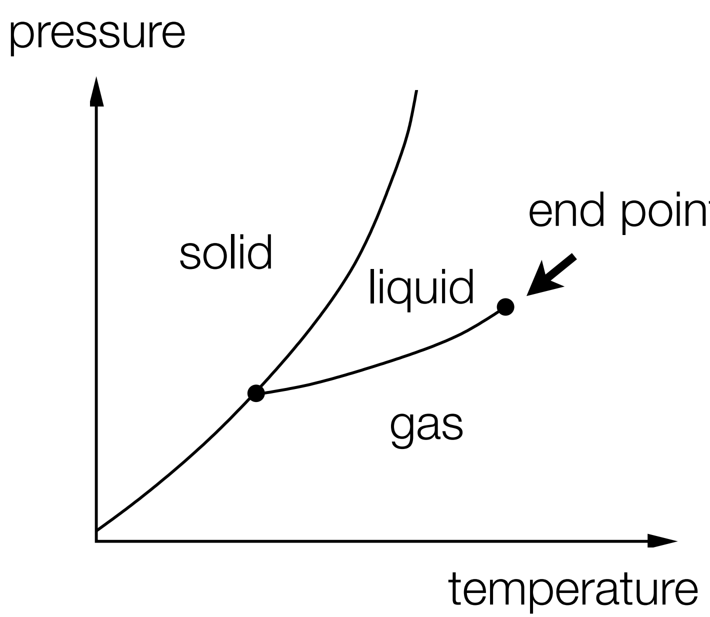
thermal expansion as a function of T:
consistent with 2d Ising critical behavior

M. de Souza, A. Brühl, Ch. Strack, B. Wolf, D. Schweitzer, and M. Lang, PRL (2007)
L. Bartosch, M. de Souza, and M. Lang, PRL (2010)

Universality of the Mott end point:
Theory

Mott critical endpoint





Is the Mott endpoint analogous to the liquid-gas endpoint?

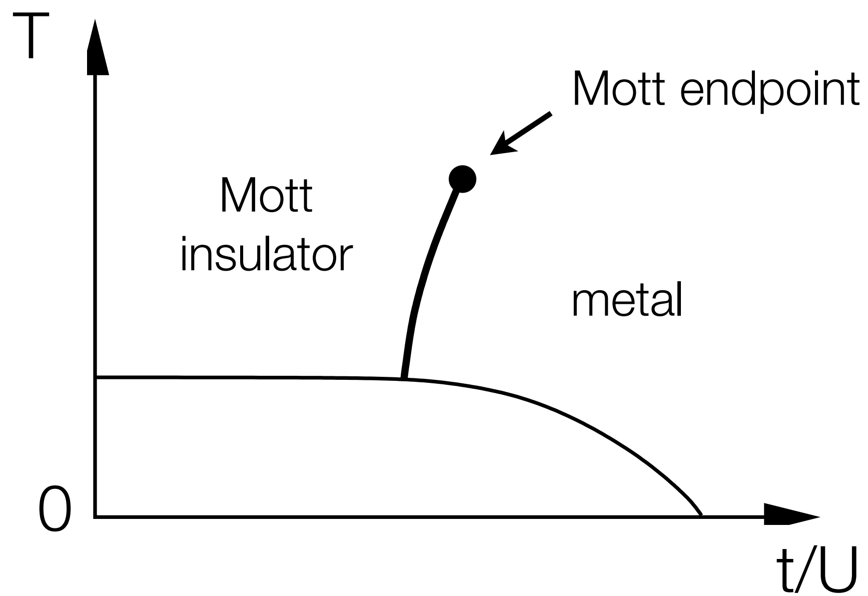
Is it really in the Ising universality class?

Mott transition on incompressible lattices

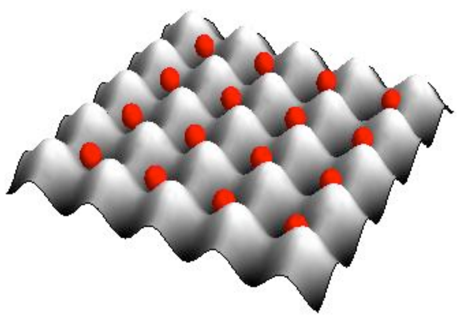
Mott transition on incompressible lattices

YES! Mott endpoint ≙ liquid-gas endpoint

at least for the Hubbard model. Subtler: long-range Coulomb



eg. optical lattice



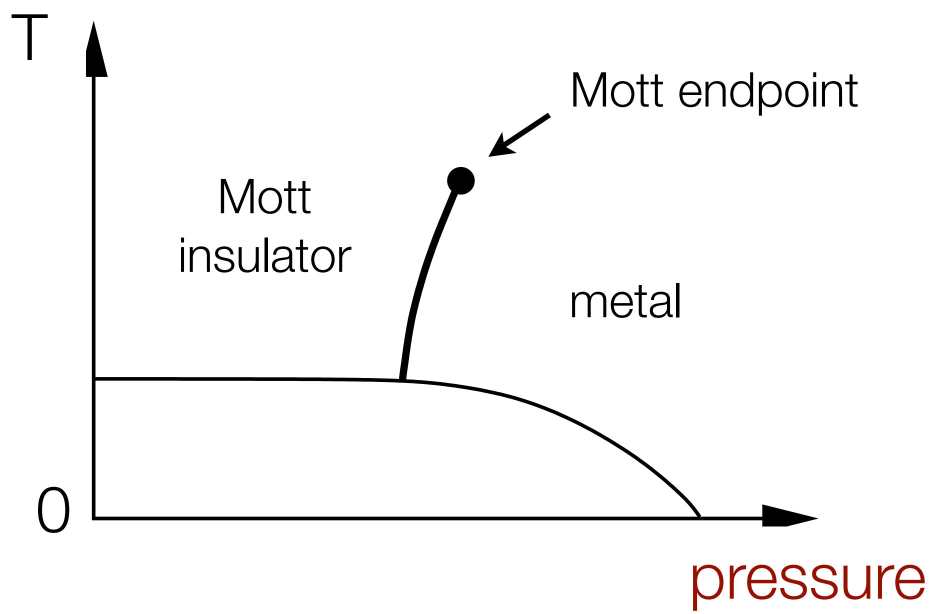
Castellani et al. PRL (1979); Kotliar et al. PRL (2000); Papanikolaoou et al. PRL (2008)

Mott transition on compressible lattices

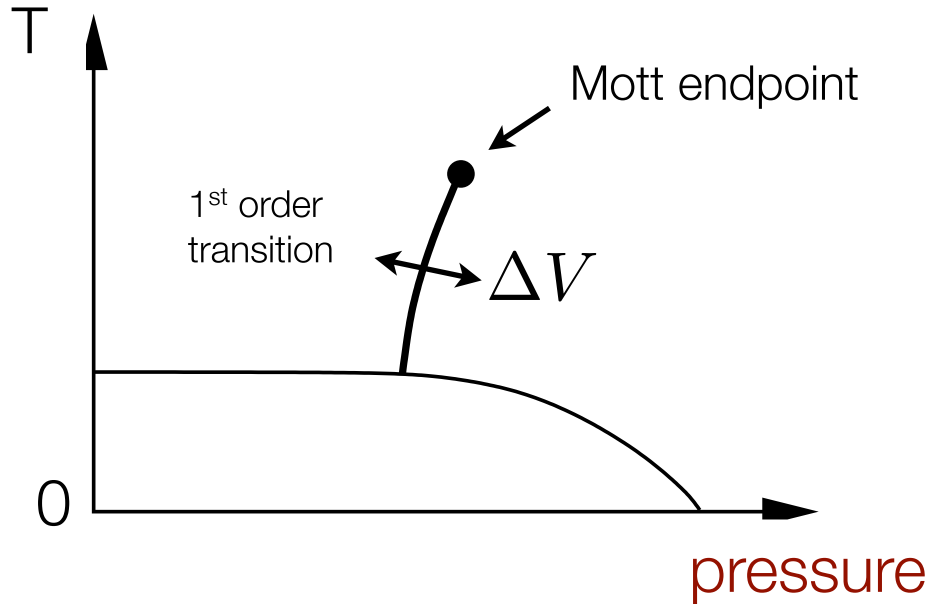
Mott transition on compressible lattices

NO! Mott endpoint $\neq$ liquid-gas endpoint

i.e. for basically all solid state realizations!



Mott transition on compressible lattices



at the first order transition: jump of conjugate quantity, i.e. volume ΔV

⇨ solid-to-solid isostructural transition

Mott endpoint ≙ solid-solid endpoint

PHYSICAL REVIEW B VOLUME 2, NUMBER 9 1 NOVEMBER 1970

Critical Behavior of the Mott Transition in Cr-Doped V_2O_3

A. Jayaraman, D. B. McWhan, J. P. Remeika, and P. D. Dernier
Bell Telephone Laboratories, Murray Hill, New Jersey 07974
(Received 24 April 1970)

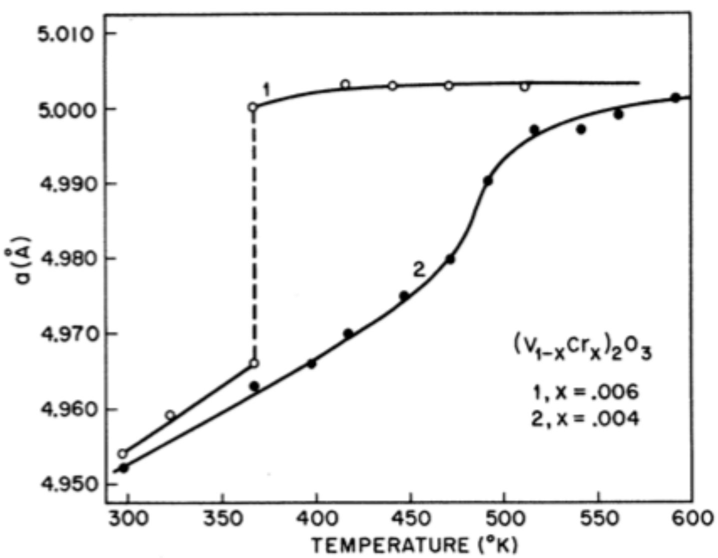


FIG. 7. Change in the lattice constant (a) for two Cr-doped V_2O_3 samples as a function of temperature. The sample with $x = 0.006$ exhibits a discontinuous jump. Sample with $x = 0.004$ shows a continuous and smooth but somewhat anomalous variation. The former is charac-terist of suberitical and the latter of supercritical behavior.

15 of Ref. 2). Based on an extrapolation of the M-I transition boundary to pure V_2O_3 and from the nature of the resistance anomaly observed in pure V_2O_3 in the 500–600 °K region,[3] it has been suggested[1] that the M-I phase boundary terminates at a critical point. In this paper we present results of resistance-versus-pressure studies on several Cr-doped V_2O_3 samples and show that the M-I phase boundary does terminate at a critical point in the pressure-temperature plane, in accordance with the earlier prediction.[1] Results of x-ray diffraction studies on several of these samples at different temperatures are presented which are consistent with the termination of the Mott transition at a solid-solid critical point.

I. EXPERIMENTAL RESULTS

Single crystals of Cr-doped V_2O_3 were grown by a new flux technique.[2] For resistivity measurements, samples were contacted with four leads placed approximately at the corners of a square.

Mott transition on compressible lattices

Mott endpoint $\triangleq$ solid-solid endpoint $\neq$ liquid-gas endpoint

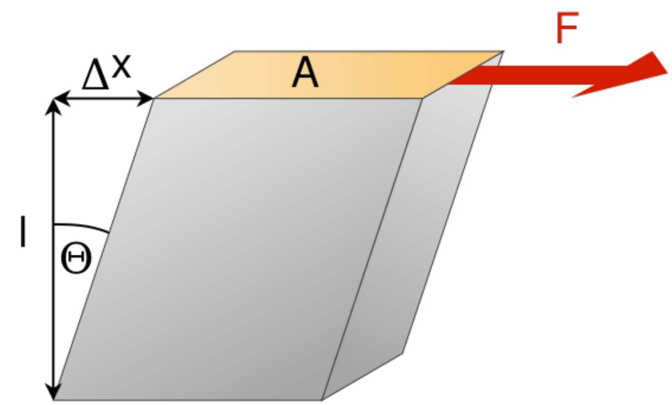
Difference between a solid and a liquid:

Mott transition on compressible lattices

Mott endpoint ≙ solid-solid endpoint ≠ liquid-gas endpoint

Difference between a solid and a liquid:

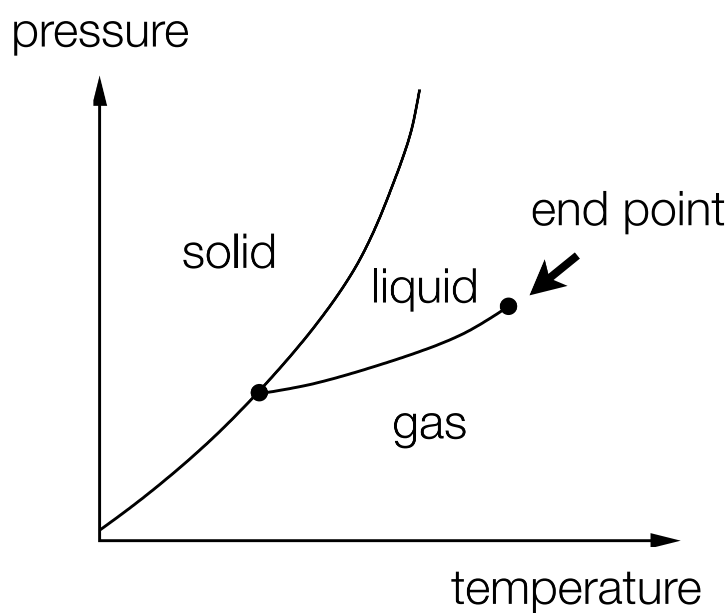
finite shear modulus



$$G = \frac{Fl}{A\Delta x}$$

wikipedia

Liquid-gas critical point



order parameter: change in density $\delta\rho$

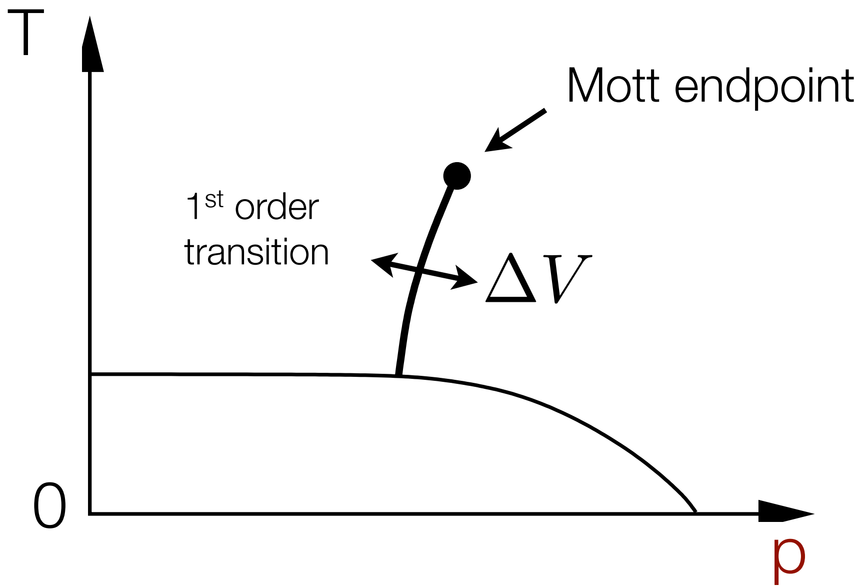
compressibility $\kappa = -\frac{1}{V}\frac{\partial V}{\partial p} = \frac{1}{\rho}\frac{\partial \rho}{\partial p}$

diverges at the endpoint

speed of sound vanishes $c^2_{\mathrm{sound}} = \frac{\partial p}{\partial \rho} = \frac{1}{\rho\kappa}$

vanishing sound velocity at the liquid-gas endpoint

Solid-solid critical point



order parameter: change in volume ΔV

compressibility $\kappa = -\frac{1}{V}\frac{\partial V}{\partial p} = \frac{1}{K}$

diverges at the endpoint

Isotropic solid: longitudinal sound waves $c_l^2 = \frac{K + \frac{4}{3}G}{\rho}$

shear sound waves $c_s^2 = \frac{G}{\rho}$

remain finite for K→ 0
due to shear modulus G!

finite sound velocity at the solid-solid endpoint

Macroscopic instability of a solid

elasticity theory: $$\mathcal{L} = \frac{1}{2}\epsilon_{ij}\, C_{ijkl}\, \epsilon_{kl}$$

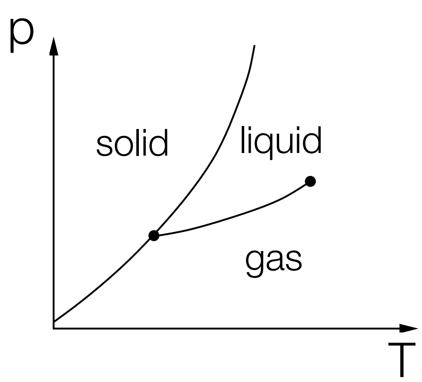
solid becomes unstable if a eigenvalue of C_{ijkl} vanishes: $$\det C_{ijkl} = 0$$

phonon velocities are determined by a different matrix: $$D_{ij} = C_{ijkl}\hat{q}_k\hat{q}_l$$

BUT: $$\boxed{\det C_{ijkl} = 0 \quad \not\Rightarrow \quad \det D_{ij} = 0}$$

⇨ phonon velocities generally stay finite!

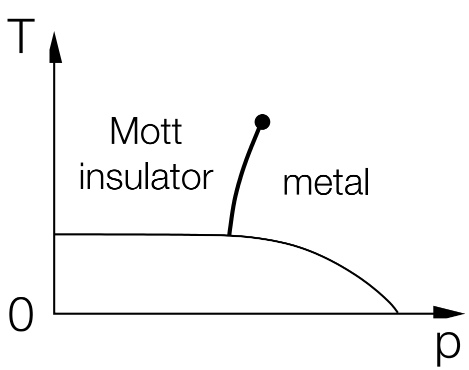
Universality classes



Liquid-gas critical point:

vanishing sound velocity ➔ critical microscopic fluctuations

⇨ Ising criticality



Solid-solid critical point:

isostructural transition, no change in crystal symmetry

finite sound velocity ➔ absence of critical fluctuations

⇨ Landau (mean-field) criticality

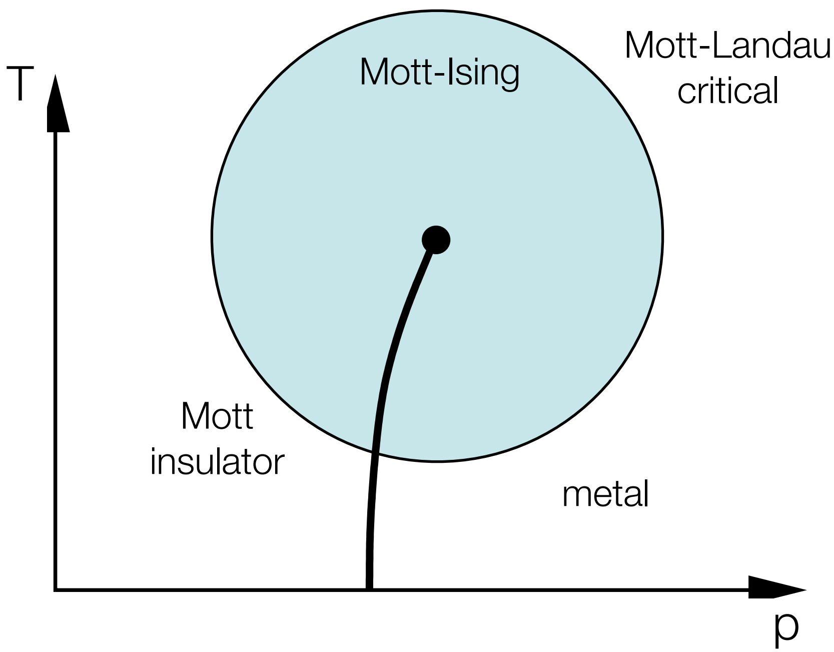
applies to all crystal symmetries:

Cowley, PRB (1976), Folk, Iro, Schwabl, Z Physik B (1976)

Mott critical endpoint ⇨ Landau criticality

Two scenarios:

weak Mott-elastic coupling:



crossover from Mott-Landau to
Mott-Ising to elastic Landau criticality

Mott critical endpoint ⇨ Landau criticality

Two scenarios:

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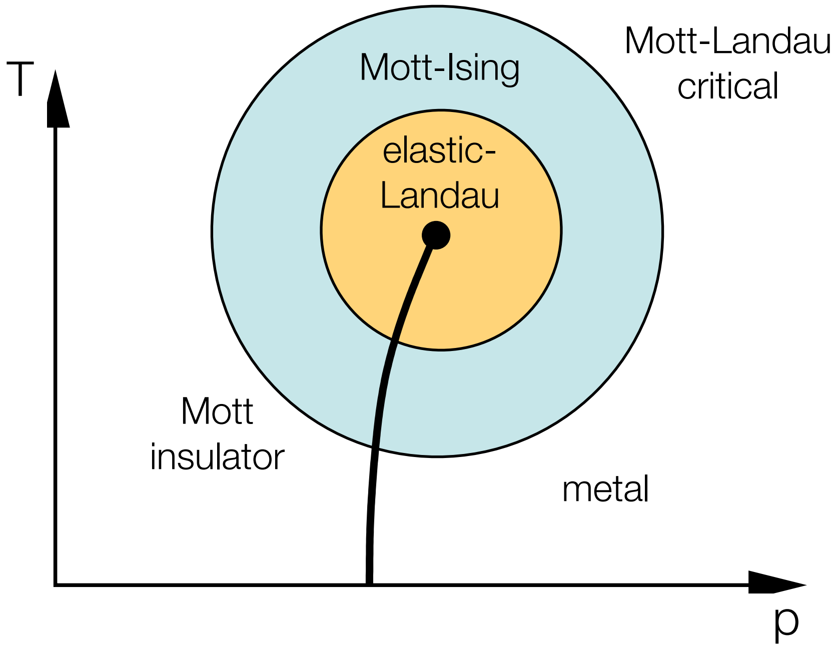

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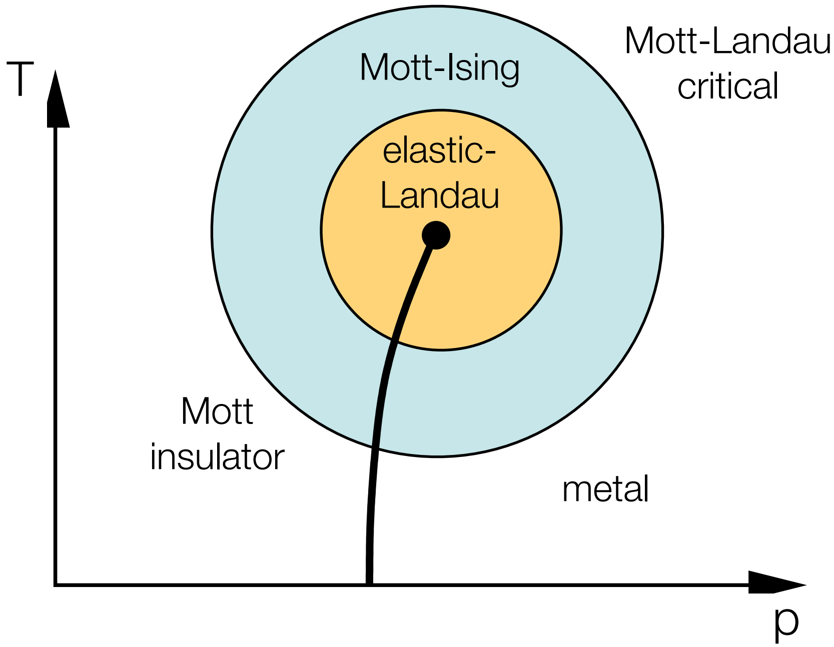

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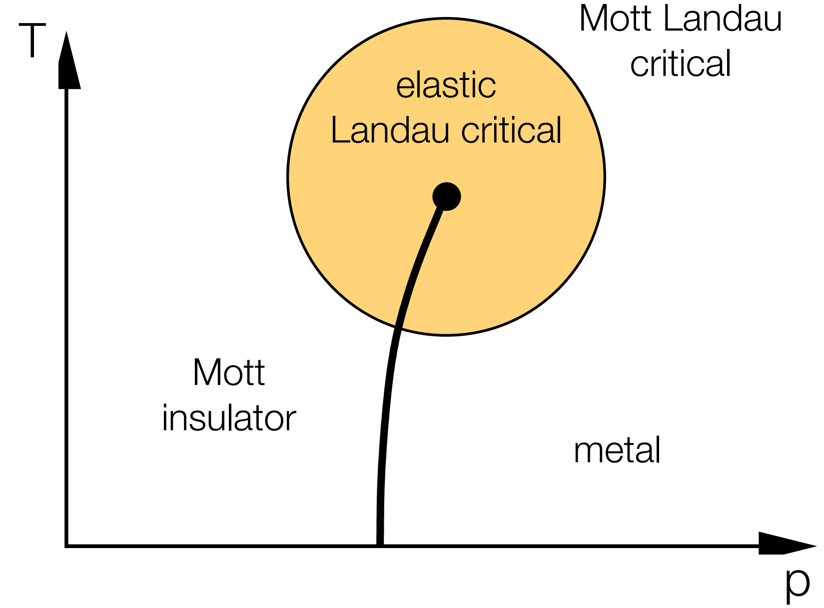


single crossover from Mott- to elastic Landau criticality

Theory and relation to experiments

Theory for the Mott endpoint

Assumption:

Mott endpoint without coupling to the lattice = Ising critical

How does the Ising order parameter ϕ couple to strain?

$$\mathcal{L}_{\rm int} = -\gamma_1 \varepsilon \phi + \frac{1}{2}\gamma_2 \varepsilon \phi^2$$

ε: singlet irred. representation of crystal group

linear coupling allowed as Ising symmetry is emergent!

Linear coupling only to singlet ε $\rightarrow$ no crystal symmetry breaking isostructural instability!

similar to critical piezoelectric ferroelectrics

Levanyuk and Sobyanin JETP Lett. (1970), Villain, SSC (1970)

Theory for the Mott endpoint

How does the Ising order parameter ϕ couple to strain?

$$\mathcal{L}_{\text{int}} = -\gamma_1 \varepsilon \phi + \frac{1}{2}\gamma_2 \varepsilon \phi^2$$

Effective theory: neglect non-critical phonons

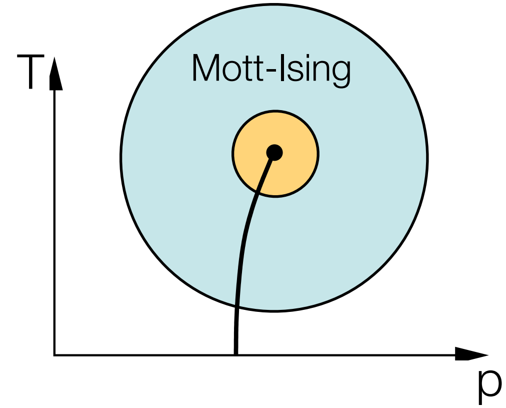
→ effective potential for macroscopic strain singlet

$$\mathcal{V}(\varepsilon) = \frac{K_0}{2}\varepsilon^2 - \varepsilon p + f_{\text{sing}}(t_0 + \gamma_2 \varepsilon, h_0 + \gamma_1 \varepsilon)$$

bare modulus

pressure

free energy density
of the Ising model



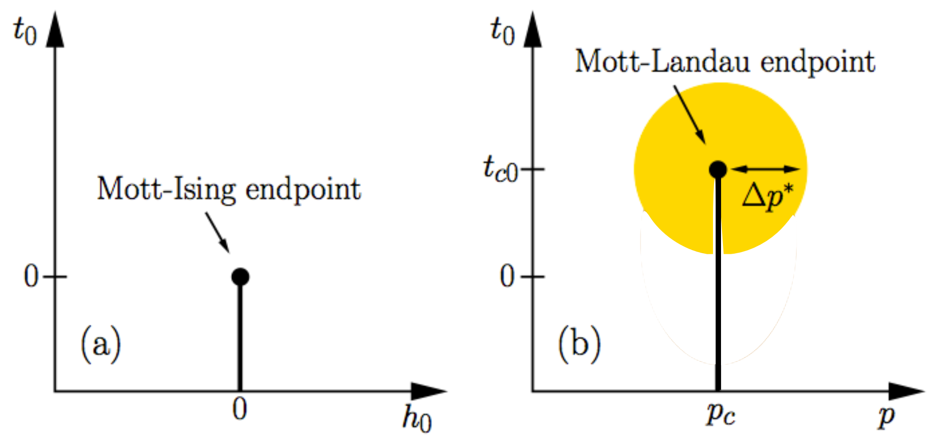
weak Mott-elastic coupling

Theory for the Mott endpoint

effective potential: $$\mathcal{V}(\varepsilon) = \frac{K_0}{2}\varepsilon^2 - \varepsilon p + f_{\mathrm{sing}}(t_0 + \gamma_2\varepsilon, h_0 + \gamma_1\varepsilon)$$

without coupling to crystal elasticity: $\gamma_1 = \gamma_2 = 0$

with coupling to crystal elasticity: $\gamma_1 \neq 0; \gamma_2 = 0$

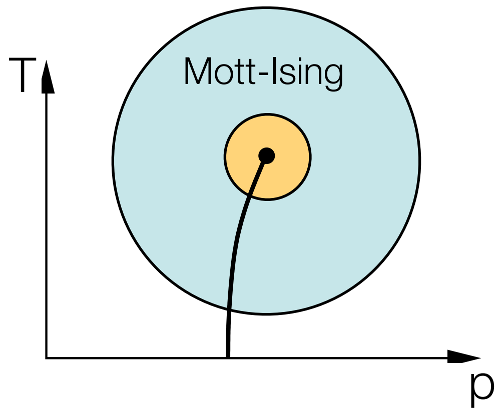


Mott-Ising endpoint preempted by isostructural instability

mean-field exponents!

Theory for the Mott endpoint

effective potential: $$\mathcal{V}(\varepsilon) = \frac{K_0}{2}\varepsilon^2 - \varepsilon p + f_{\rm sing}(t_0 + \gamma_2 \varepsilon, h_0 + \gamma_1 \varepsilon)$$



away from the critical point (blue regime):

perturbative minimization: $\varepsilon \approx p/K_0$

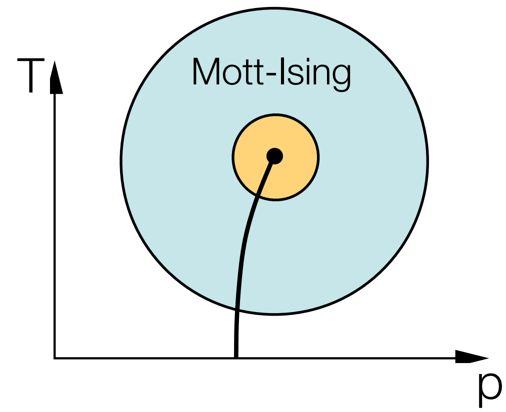
$$\Rightarrow \quad \mathcal{F}_{\rm pert} = -\frac{p^2}{2K_0} + f_{\rm sing}(t_0 + \gamma_2 p/K_0, h_0 + \gamma_1 p/K_0)$$

pressure dependence of tuning parameters

used by Bartosch et al. PRL (2010)

Theory for the Mott endpoint

yellow non-perturbative regime: elastic Landau-critical



expansion in $\delta\varepsilon = \varepsilon - \bar{\varepsilon}$

$$\mathcal{V}(\varepsilon) \approx \frac{K}{2}\delta\varepsilon^2 - \delta\varepsilon\,(p - \bar{p}) + \frac{u}{4!}\delta\varepsilon^4 + f_{\rm sing}(\bar{t}, \bar{h})$$

with $\bar{\varepsilon}$ chosen such that cubic term vanishes

and $\bar{h} = h_0 + \gamma_1 \bar{\varepsilon}$ and $\bar{t} = t_0 + \gamma_2 \bar{\varepsilon}$

renormalized modulus:

$$K = K_0 - \gamma_1^2 \chi_{\bar{h}\bar{h}} - 2\gamma_1\gamma_2 \chi_{\bar{h}\bar{t}} - \gamma_2^2 \chi_{\bar{t}\bar{t}}$$

most singular correction due to linear coupling: $\chi_{\bar{h}\bar{h}} = -\partial_{\bar{h}}^2 f_{\rm sing}(\bar{t}, \bar{h})$

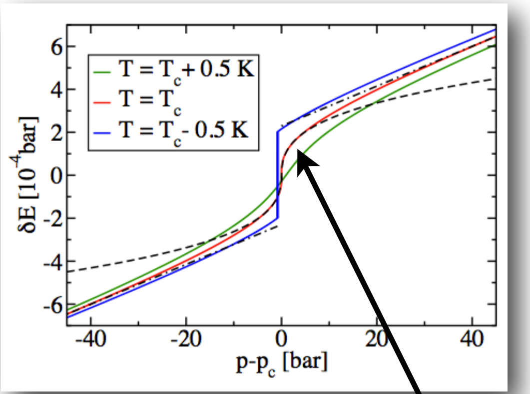
diverges and drives bulk modulus to zero!

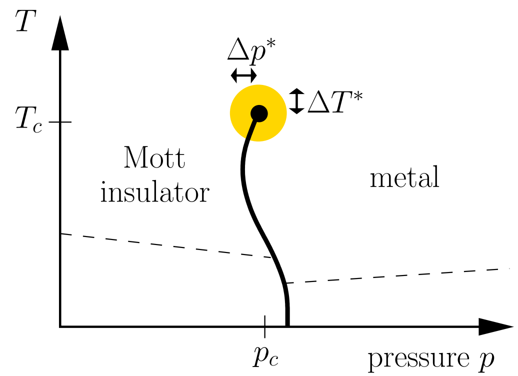
For $K \approx 0$ minimization yields:

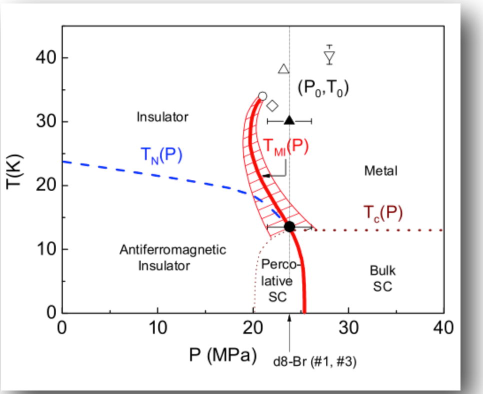
$\delta\varepsilon = (6(p - \bar{p})/u)^{1/3}$ breakdown of Hooke's law! with mean-field exponent

Application to κ-(BEDT-TTF)$_2$X

breakdown of Hooke's law: smoking-gun criterion for elastic Landau critical regime with non-perturbative Mott-elastic coupling







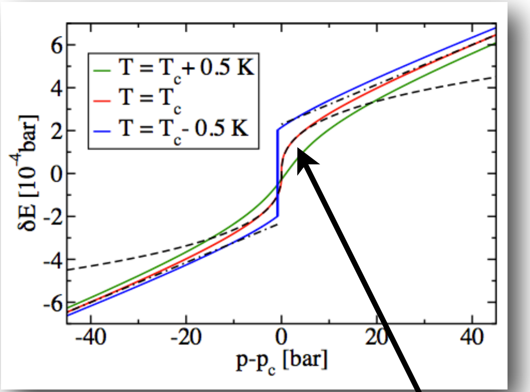
non-linear strain-stress relation

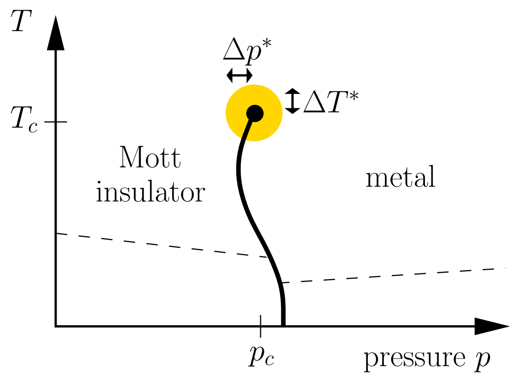
width of the elastic Landau regime:

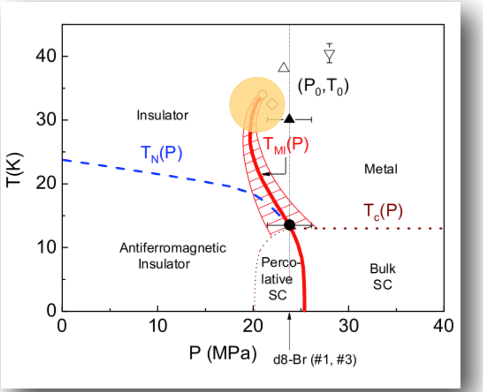
$$\Delta p^* \approx 45\,\mathrm{bar} = 4.5\,\mathrm{MPa}$$
$$\Delta T^* \approx 2.5\,\mathrm{K}$$

Application to κ-(BEDT-TTF)$_2$X

breakdown of Hooke's law: smoking-gun criterion for elastic Landau critical regime with non-perturbative Mott-elastic coupling







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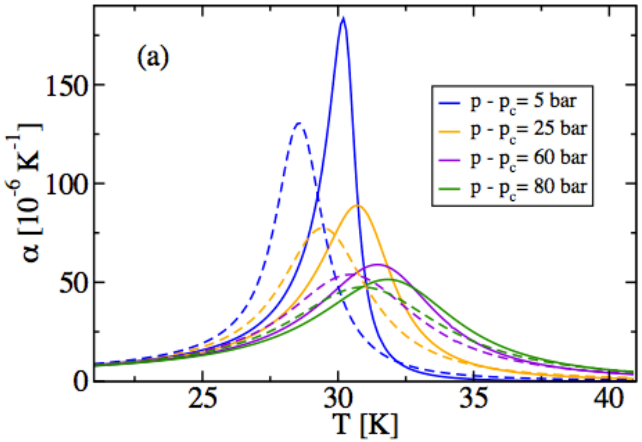
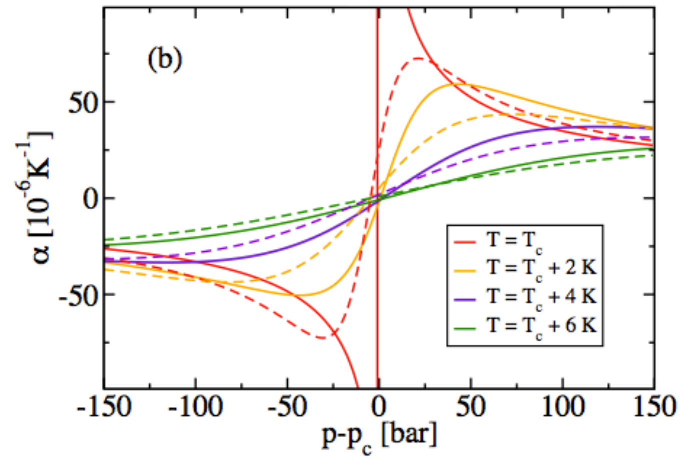
Application to κ-(BEDT-TTF)$_2$X

using fitting parameters of Bartosch et al. PRL (2010):





dotted line: perturbative; solid line: full solution

width of the elastic Landau regime:

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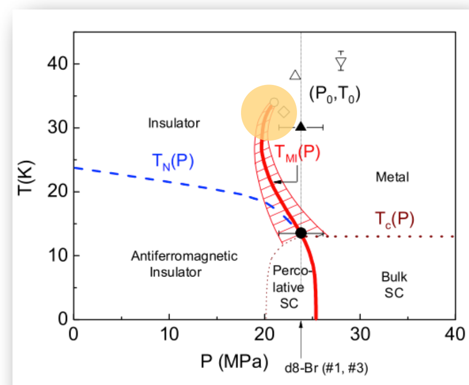

Mott end point of Cr-doped V_2O_3

What is the critical singlet irred. representation of strain for V_2O_3?

PHYSICAL REVIEW B VOLUME 24, NUMBER 6 15 SEPTEMBER 1981

Elastic constants of V_2O_3 between 300 and 640 K: Anomalies near the high-temperature electrical transition

D. N. Nichols, R. J. Sladek, and H. R. Harrison
Department of Physics, Purdue University, West Lafayette, Indiana 47907
(Received 12 May 1981)

determined elastic constant matrix
by measureing various sound velocities

trigonal crystal symmetry

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & 0 & 0 \\ C_{12} & C_{11} & C_{13} & -C_{14} & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ C_{14} & -C_{14} & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & C_{14} \\ 0 & 0 & 0 & 0 & C_{14} & \frac{C_{11}-C_{12}}{2} \end{pmatrix}$$

TABLE I. Sample length at room temperature, wave propagation, and polarization directions, and elastic stiffness ρv^2, where ρ is the sample density and v the wave velocity.

Sample length (cm)	Propagation $\vec{q}$ and polarization $\hat{e}$	ρv^2 [a]
0.5465	$\vec{q}_L \parallel [001] \parallel \hat{e}$	C_{33}
0.5465	$\vec{q}_s \parallel [001] \parallel \hat{e}_s$	C_{44}
0.4925	$\vec{q}_L \parallel [100] \parallel \hat{e}$	C_{11}
0.4925	$\vec{q}_s \parallel [100]$ $\hat{e}_s$: $-37°$ from basal plane	$C_{FT} = \frac{1}{4}(C_{11} - C_{12} + 2C_{44}) + \frac{1}{4}[(C_{11} - C_{12} - 2C_{44})^2 + 16C_{14}^2]^{1/2}$
0.4925	$\vec{q}_s \parallel [100]$ $\hat{e}_s$: $53°$ from basal plane	$C_{ST} = \frac{1}{4}(C_{11} - C_{12} + 2C_{44}) - \frac{1}{4}[(C_{11} - C_{12} - 2C_{44})^2 + 16C_{14}^2]^{1/2}$
0.3683	$\vec{q}_s$: $45°$ from c axis in the mirror plane $\hat{e}_s \parallel [100]$	$C_T = \frac{1}{4}(4C_{14} + 2C_{44} + C_{11} - C_{12})$
0.4563	$\vec{q}_L \parallel \hat{e}$: $45°$ from c axis in the mirror plane	$C_{QL} = \frac{1}{4}(C_{11} + C_{33} + 2C_{44} - 2C_{14}) + \frac{1}{2}[\frac{1}{4}(C_{11} - C_{33} - 2C_{14})^2 + (C_{13} + C_{44} - C_{14})^2]^{1/2}$

[a] Equations are from Ref. 16.

phonon velocities related to eigenvalues of $D_{ij} = C_{ijkl}\hat{q}_k\hat{q}_l$

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TABLE II. Expressions relating the eigenvalues (λ_i) of the elastic constant matrix to the independent elastic constants (C_{ij}) and the strain associated with each eigenvalue for trigonal crystals with point group $\bar{3}m$, and eigenvalues for V_2O_3 at 300 K.

Eigenvalue relations	Strain	V_2O_3 at 300 K λ_i (10^{11} dyn/cm^2)	λ_{i+1}
$\lambda_{1,2} = \frac{1}{2}(C_{11}-C_{12}+C_{44}) \pm \frac{1}{2}[(C_{11}-C_{12}-C_{44})^2+8C_{14}^2]^{1/2}$	$(e_1-e_2) - \frac{2C_{14}}{\lambda_{1,2}-C_{44}}e_4$	19.3,	7.8
$\lambda_{3,4} = \frac{1}{2}(C_{11}+C_{12}+C_{33}) \pm \frac{1}{2}[(C_{11}+C_{12}-C_{33})^2+8C_{13}^2]^{1/2}$	$(e_1+e_2) - \frac{2C_{13}}{\lambda_{3,4}-C_{33}}e_3$	56.7,	13.7
$\lambda_{5,6} = \frac{1}{4}(C_{11}-C_{12}+2C_{44}) \pm \frac{1}{4}[(C_{11}-C_{12}-2C_{44})^2+16C_{14}^2]^{1/2} = C_{FT}, C_{ST}$	$e_5 + \frac{\lambda_{5,6}-C_{44}}{C_{14}}e_6$	11.0,	6.8

crystal stability: eigenvalues must be positive

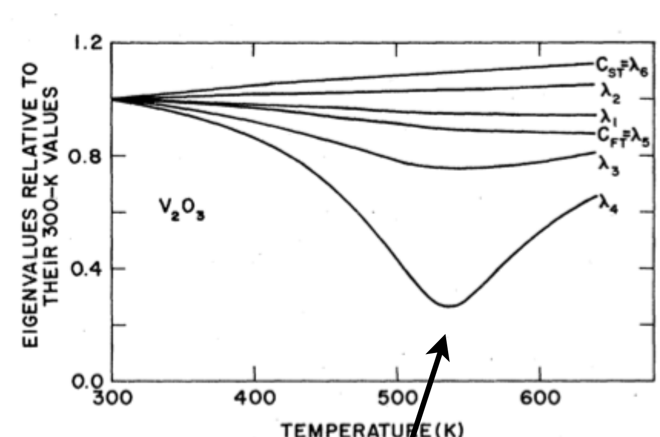


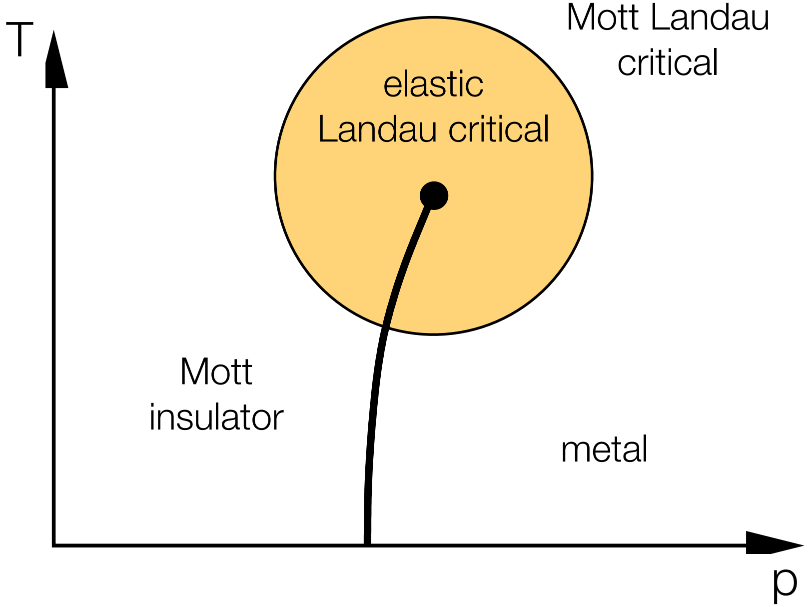
FIG. 5. Eigenvalues of the elastic constant matrix for V_2O_3 relative to their 300-K values as a function of temperature.

strong softening!
Singlet!

Mott end point of Cr-doped V_2O_3

strong softening close to critical temperature already in undoped V_2O_3!

probably no regime with non-trivial Ising criticality!



strong Mott-elastic coupling

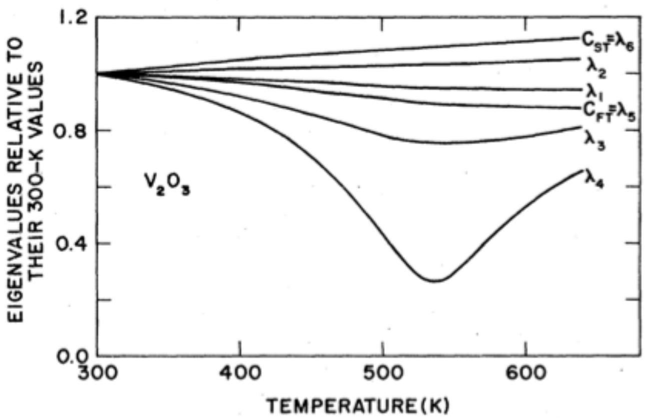
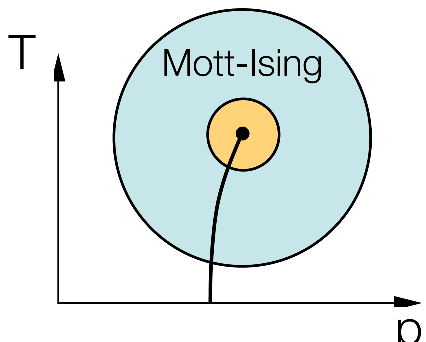


FIG. 5. Eigenvalues of the elastic constant matrix for V_2O_3 relative to their 300-K values as a function of temperature.

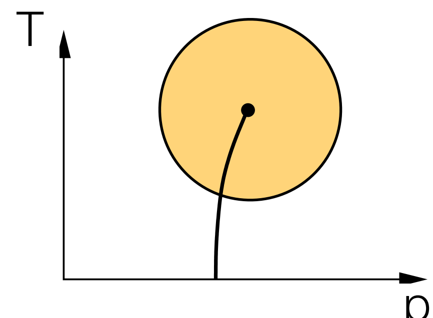
Summary

Phys. Rev. Lett. 109, 176401 (2012)

- Mott endpoint ≠ liquid-gas endpoint
- Mott endpoint = solid-solid endpoint
- Mott endpoint criticality: Landau (mean-field) not Ising
- critical elasticity regime: breakdown of Hooke's law
- two scenarios:



κ-(BEDT-TTF)$_2$X



V_2O_3

- estimate for κ-(BEDT-TTF)$_2$X:

$$\Delta p^* \approx 45\,\mathrm{bar} = 4.5\,\mathrm{MPa}$$

$$\Delta T^* \approx 2.5\,\mathrm{K}$$