# Nematic quantum criticality in a metal: A Quantum Monte Carlo study

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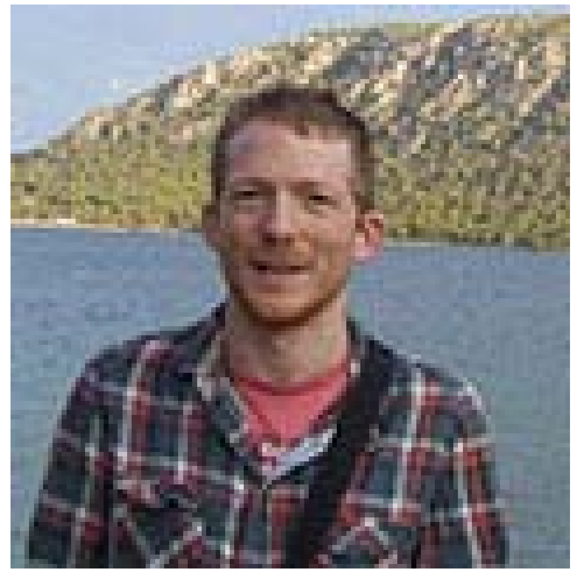
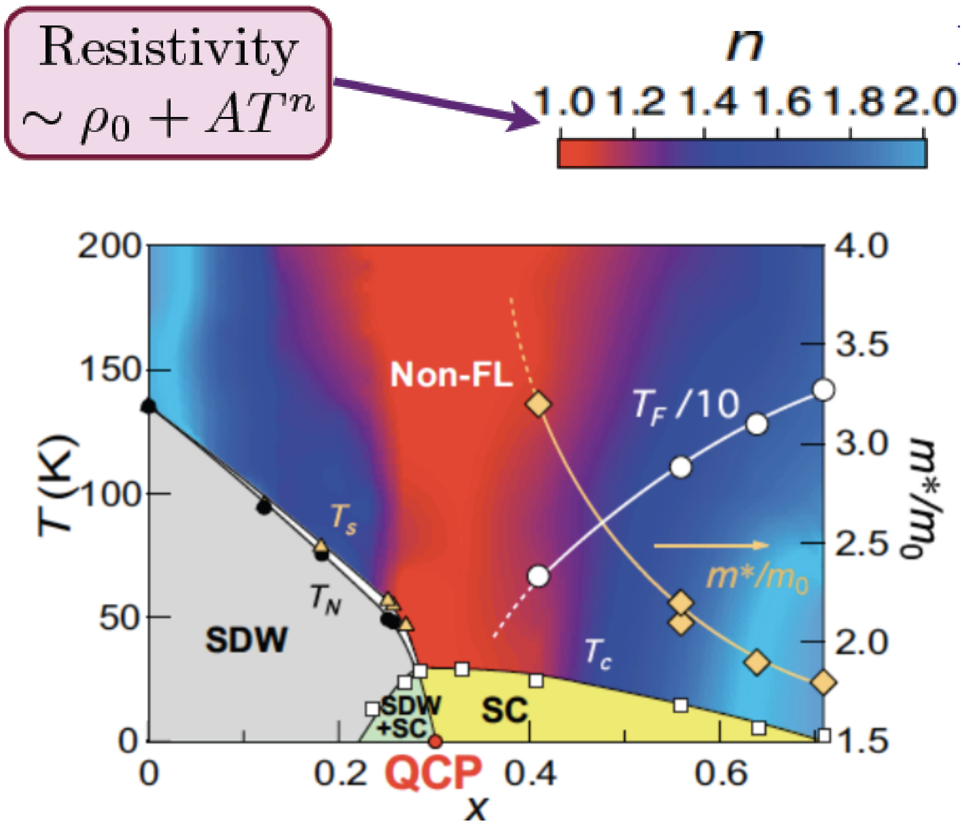
**Sam Lederer**
**(Stanford → MIT)**

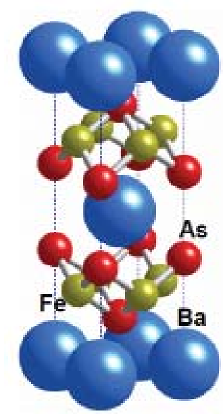


**Yoni Schattner**
**(Weizmann)**

# Strongly correlated materials

*Recurring characteristic:* complex phase diagram
many competing/coexisting types of order



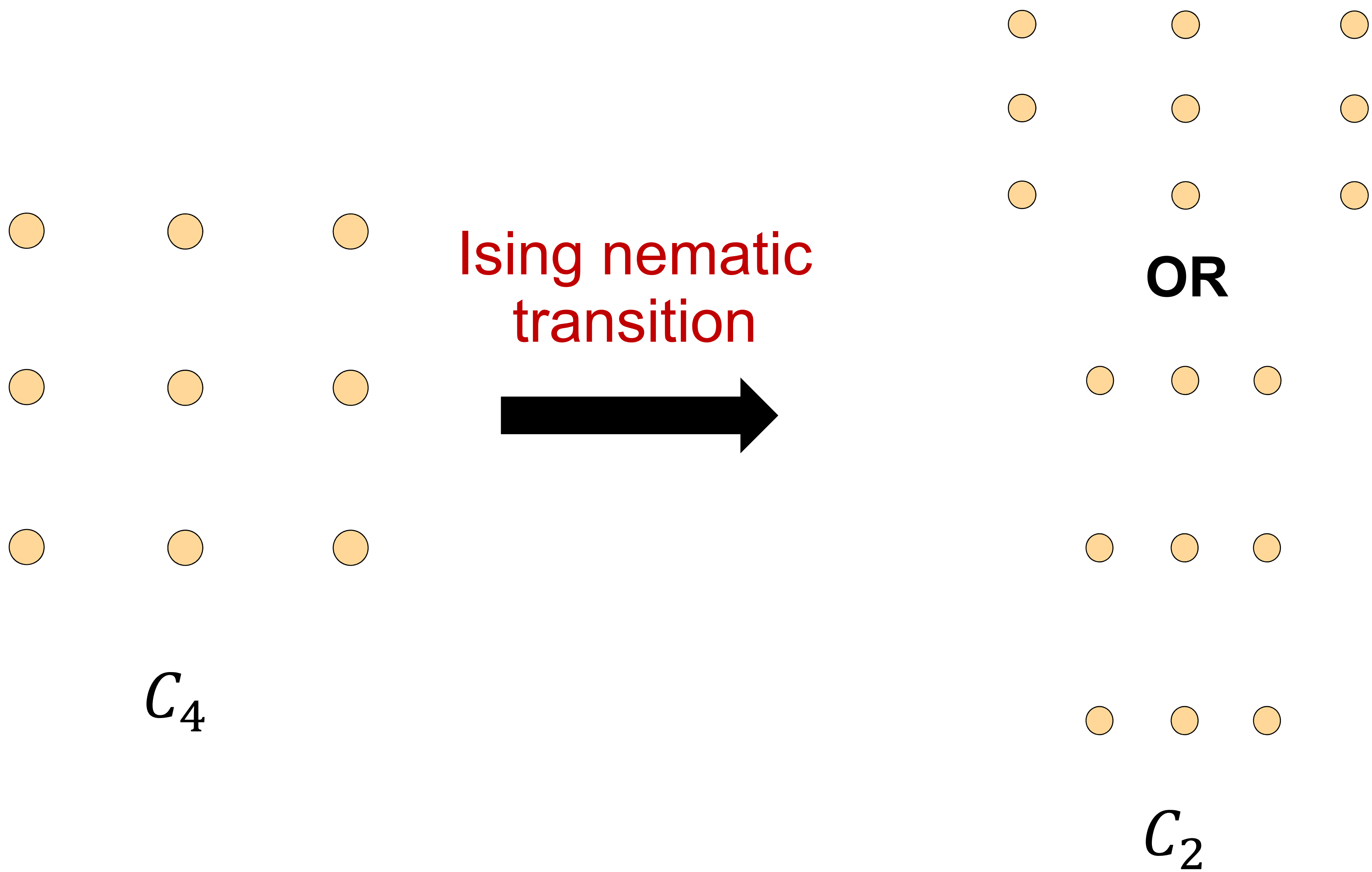

*Role of QCPs?*

K. Hashimoto, K. Cho, T. Shibauchi, S. Kasahara, Y. Mizukami, R. Katsumata, Y. Tsuruhara, T. Terashima, H. Ikeda, M. A. Tanatar, H. Kitano, N. Salovich, R. W. Giannetta, P. Walmsley, A. Carrington, R. Prozorov, and Y. Matsuda, *Science* **336**, 1554 (2012).

# Outline

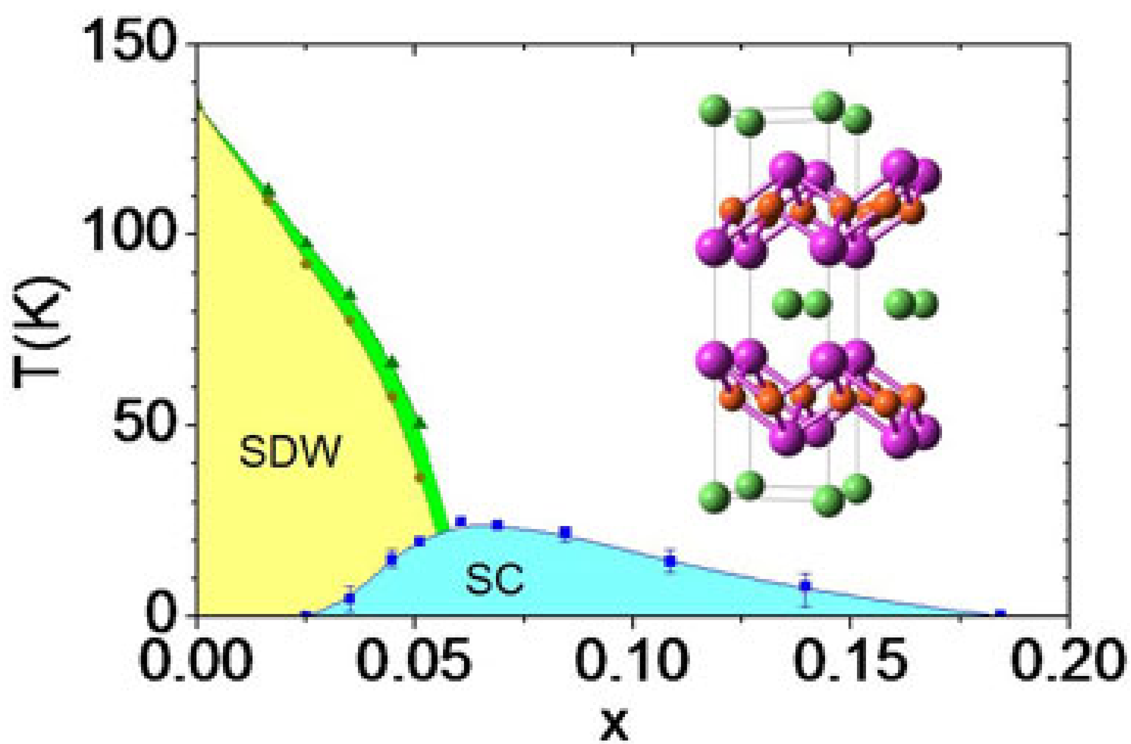
- **The Ising-nematic QCP**
- **Metallic quantum criticality**
- **Lattice model and Numerical QMC results**

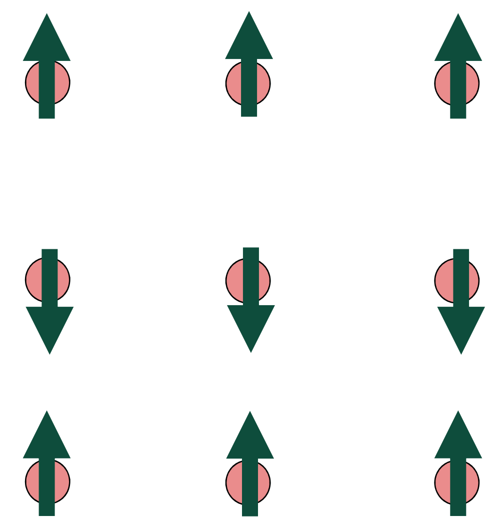
# Ising nematic order



# Electronic Ising nematic in Fe pnictides

$Ba_{1-x}Co_xFe_2As_2$



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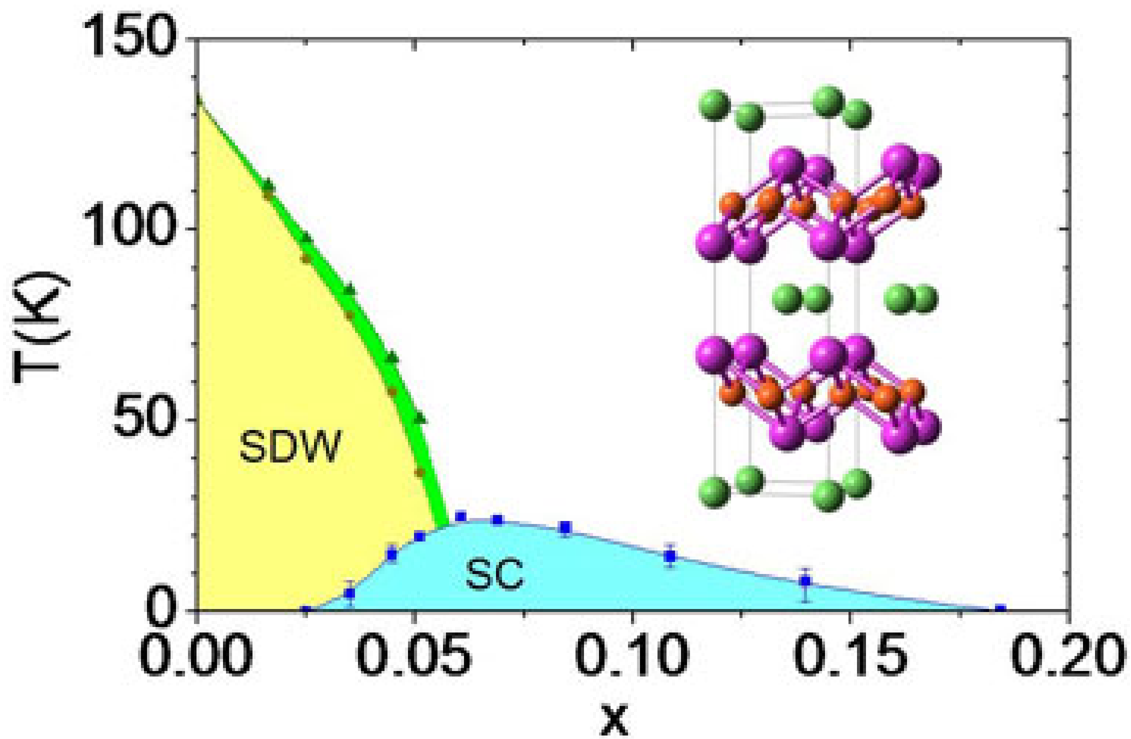
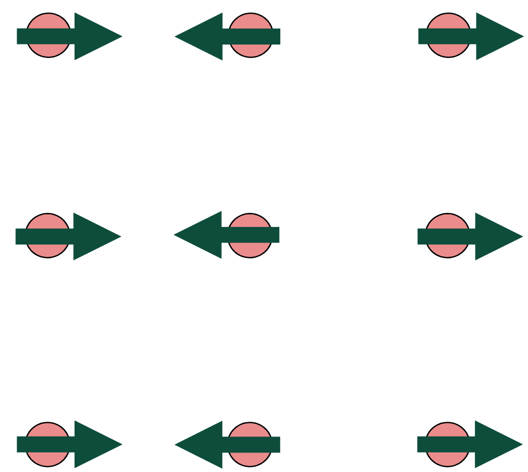


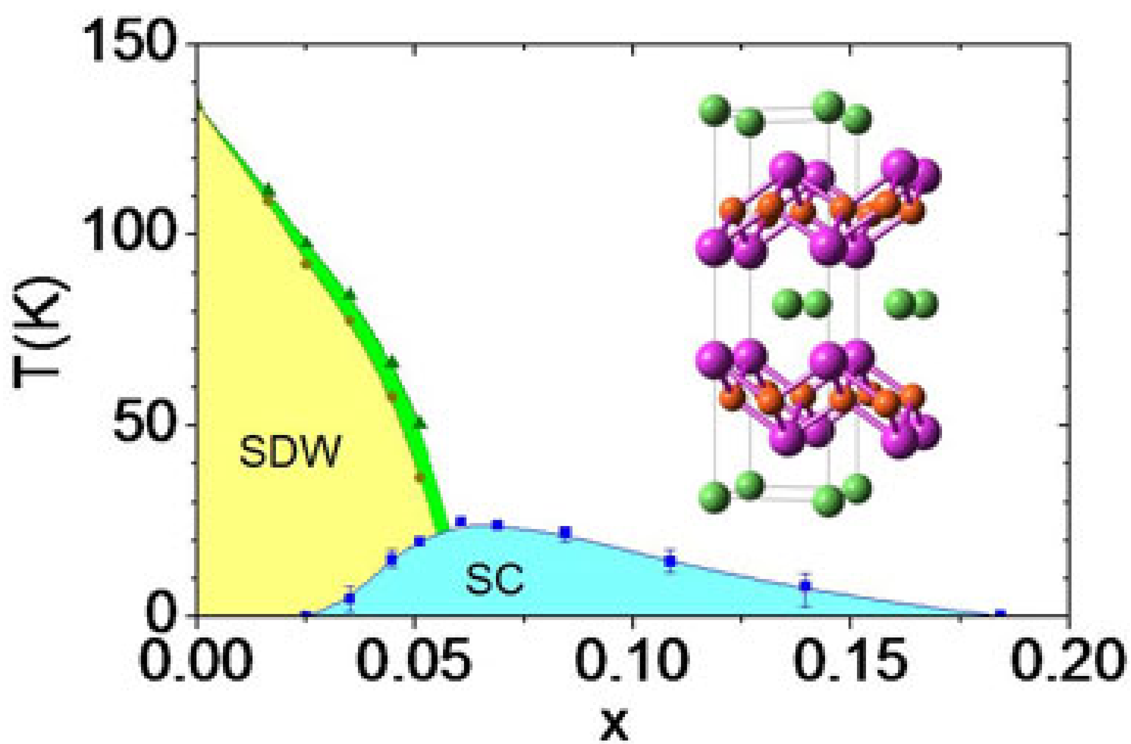
# Electronic Ising nematic in Fe pnictides

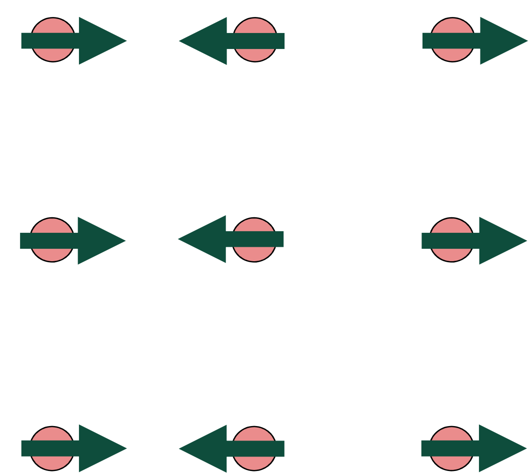
T

Isotropic

Nematic $\langle \vec{S}(\vec{r})\vec{S}(\vec{r}+a\hat{y}) - \vec{S}(\vec{r})\vec{S}(\vec{r}+a\hat{x})\rangle \neq 0$

SDW $\langle \vec{S}(\vec{r})\rangle \neq 0$



# Evidence for nematic critical point in Fe-based SC

Elastoresistive coefficient:

$$m_{66} = \frac{\Delta\rho/\rho}{\varepsilon}$$

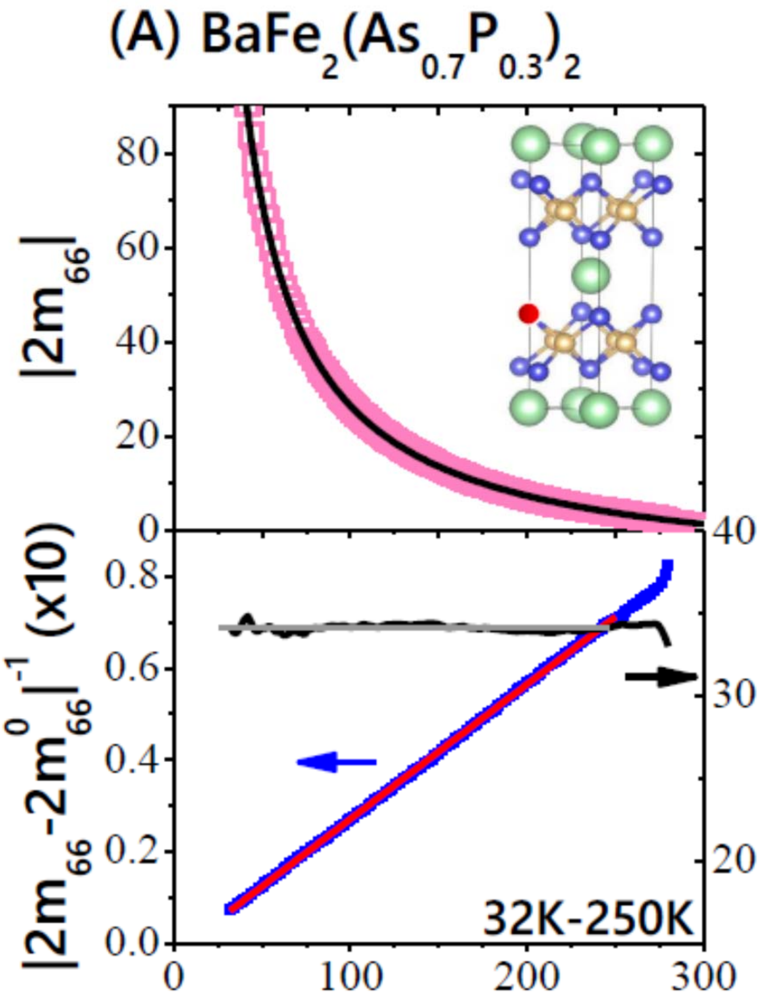
$\propto$ Electron nematic susceptibility

"Curie-Weiss" behavior!

$$m_{66} = m_{66}^{0} + \frac{A}{T - T^{*}}$$

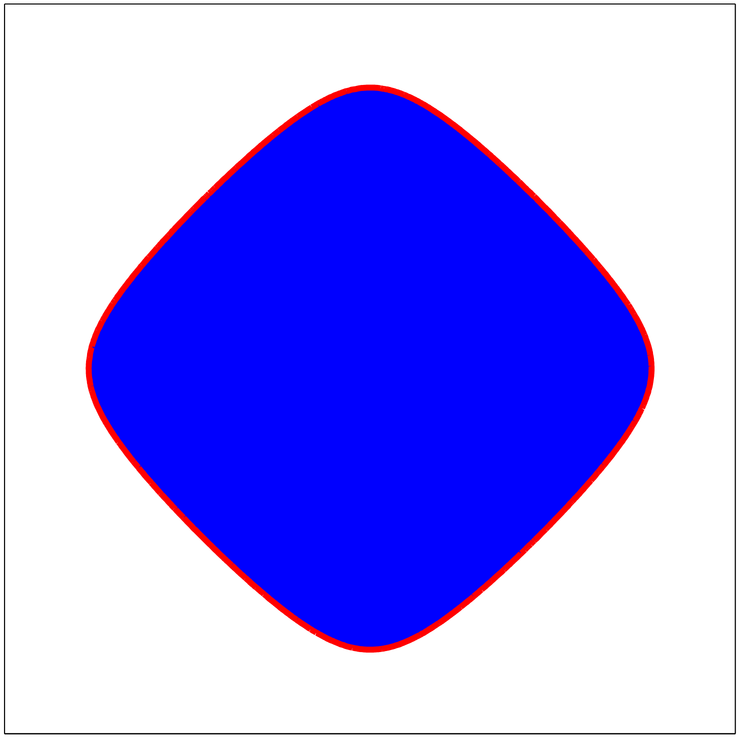
(See also Blumberg's talk)

At putative QCP
(near optimal doping!), $T^{*} \to 0$

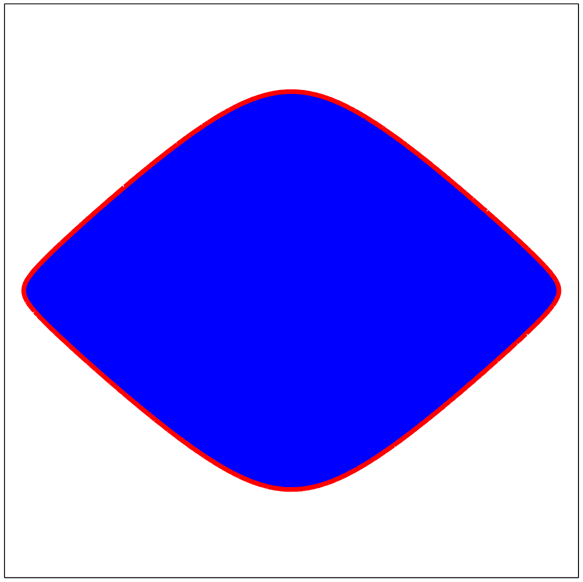


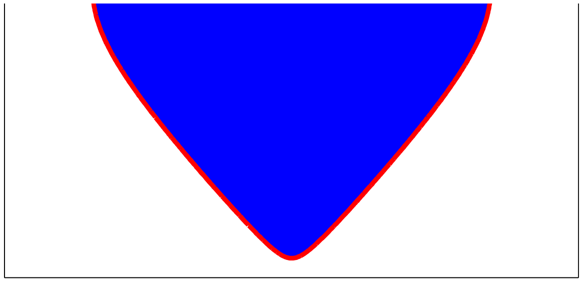

Kuo, Fisher et. al., arXiv: 1503.00402

# Ising-nematic quantum criticality *in a metal*



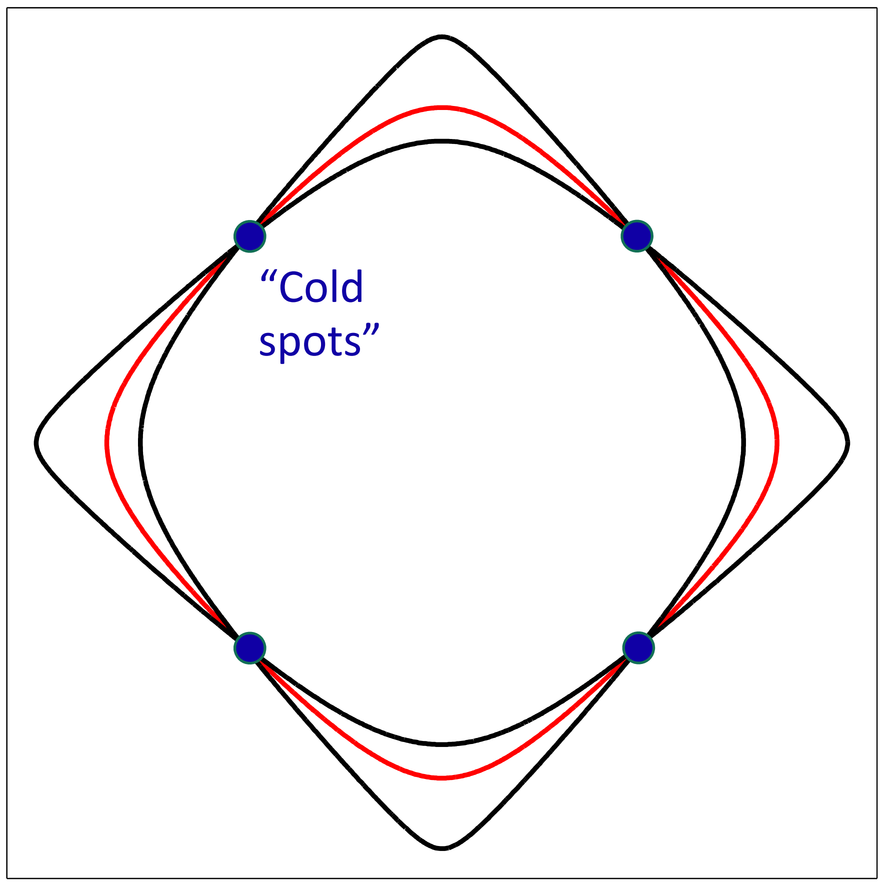
Ising nematic transition





# Ising-nematic quantum criticality *in a metal*

Strong coupling between nematic modes and electrons over the entire FS except at possible "cold spots"



# Open questions

- Critical exponents?
- Destruction of Fermi Liquid theory?
- QCP "masked" by enhanced superconductivity/other order?

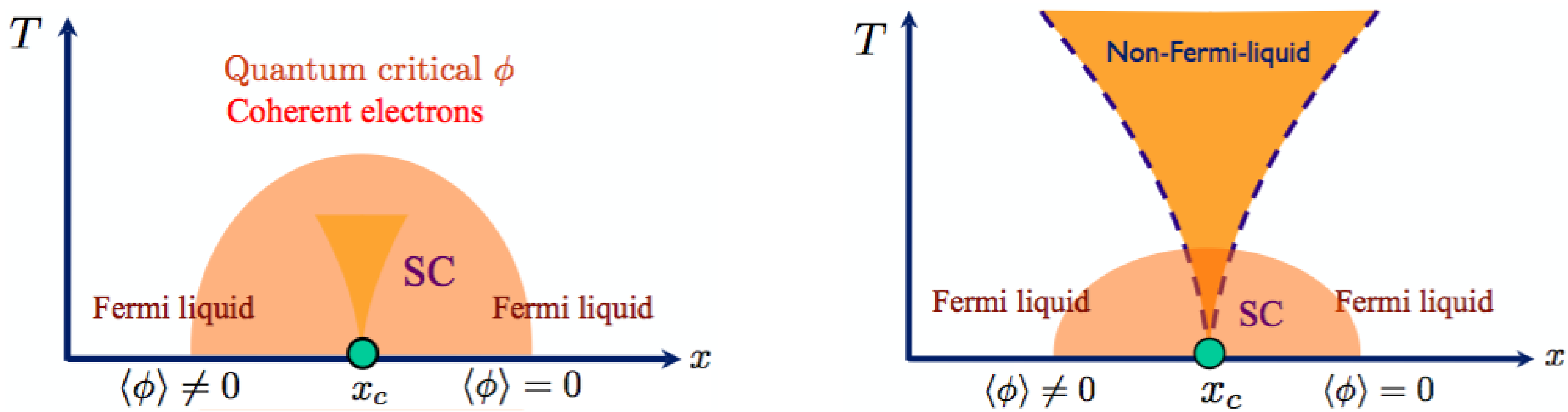



Figure from: Metlitski, Mross et. al. (PRB, 2014)

"Weak coupling" between nematic and electronic degrees of freedom: SC anomalously enhanced *in all channels* near QCP (Lederer, Schattner, EB, Kivelson, PRL 2015)

Properties of the QCP:
Chubukov, Sachdev, Metlitski, Senthil, Raghu, Kachru, Hartnoll, …

# Outline

- The Ising-nematic QCP
- Metallic quantum criticality
- Lattice model
  and Numerical QMC results

# Lattice model for nematic QCP in a metal

$c_{j\sigma}$ – spinful electrons

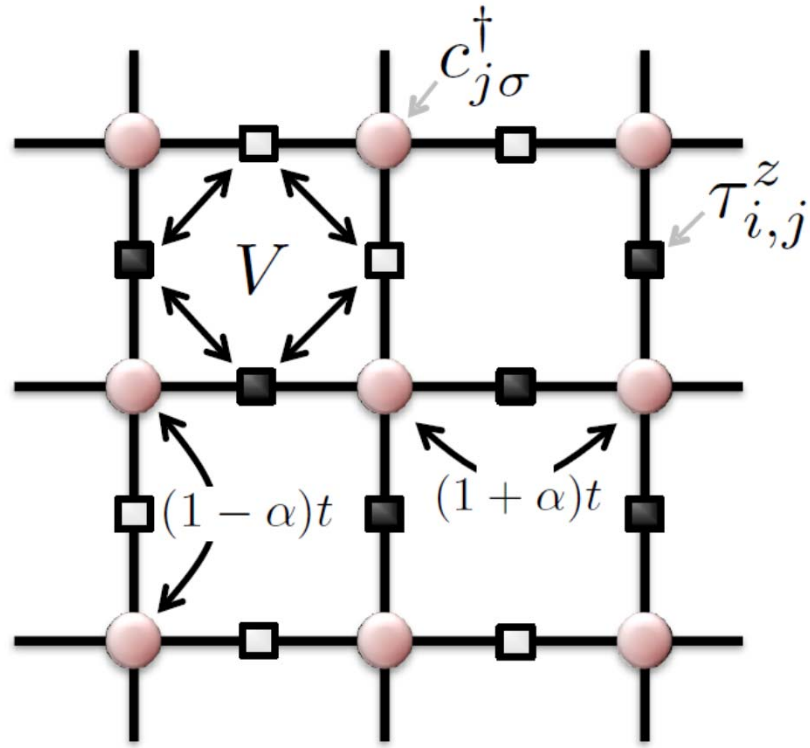
$\tau^z_{i,j}$ – Ising nematic "pseudospins"

$$H = H_f + H_b + H_{\rm int},$$

$$H_f = -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma},$$

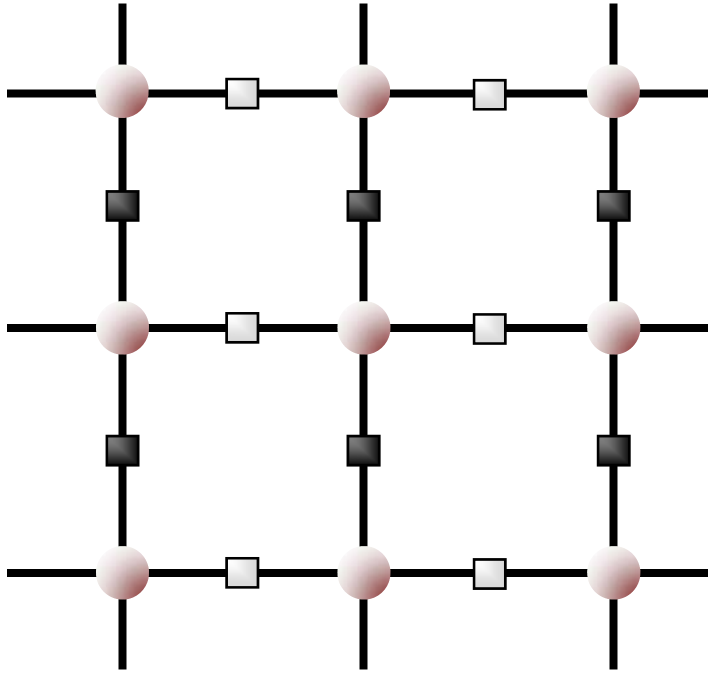
$$H_b = V \sum_{\langle\langle i,j;k,l\rangle\rangle} \tau^z_{i,j}\tau^z_{k,l} - h \sum_{\langle i,j\rangle} \tau^x_{i,j},$$

$$H_{\rm int} = \alpha t \sum_{\langle i,j\rangle,\sigma} \tau^z_{i,j} c^\dagger_{i\sigma} c_{j\sigma}.$$



# Lattice model for nematic QCP in a metal

*Nematic Phase:*



$$H = H_f + H_b + H_{\rm int},$$

$$H_f = -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma},$$

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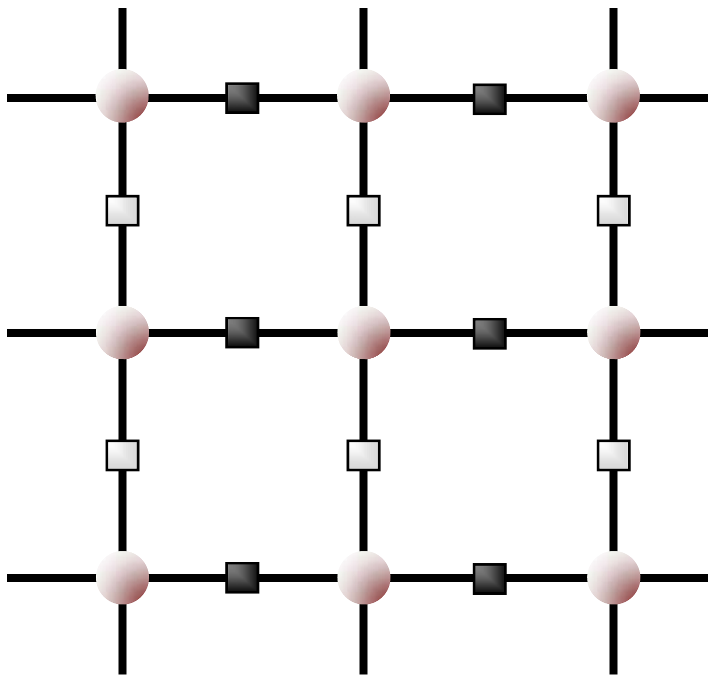
$$H_{\rm int} = \alpha t \sum_{\langle i,j\rangle,\sigma} \tau^z_{i,j} c^\dagger_{i\sigma} c_{j\sigma}.$$

# Lattice model for nematic QCP in a metal

$$H = H_f + H_b + H_{\text{int}},$$

$$\begin{aligned} H_f &= -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma}, \\ H_b &= V \sum_{\langle\langle i,j;k,l\rangle\rangle} \tau^z_{i,j}\tau^z_{k,l} - h \sum_{\langle i,j\rangle} \tau^x_{i,j}, \\ H_{\text{int}} &= \alpha t \sum_{\langle i,j\rangle,\sigma} \tau^z_{i,j} c^\dagger_{i\sigma} c_{j\sigma}. \end{aligned}$$

*Nematic Phase:*



$\alpha = 0$:
Wilson-Fisher d=2+1 QCP
+ free fermions

$\alpha \neq 0$:
Metallic Ising-nematic QCP?

# Determinant Quantum Monte Carlo (QMC)

Formulate problem as path integral, integrate out fermions.

Effective bosonic action: $e^{-S_{\text{eff}}} = e^{-S_0} \det(M_\uparrow) \det(M_\downarrow)$

If coupling of bosonic modes to ↑ and ↓ spins the same and the action is real: $\det(M_\uparrow)\det(M_\downarrow) = |\det(M_\uparrow)|^2 \geq 0$

No sign problem!

Larger class of fermionic problem can be simulated

C. Wu and S-C. Zhang, PRB (2005)

In particular, *SDW* quantum critical points in metals

EB, Metlitski, Sachdev, Science (2012)

# Determinant Quantum Monte Carlo (QMC)

- Unbiased, numerically exact
(sources of error: statistical sampling errors, Trotter errors: both controlled)

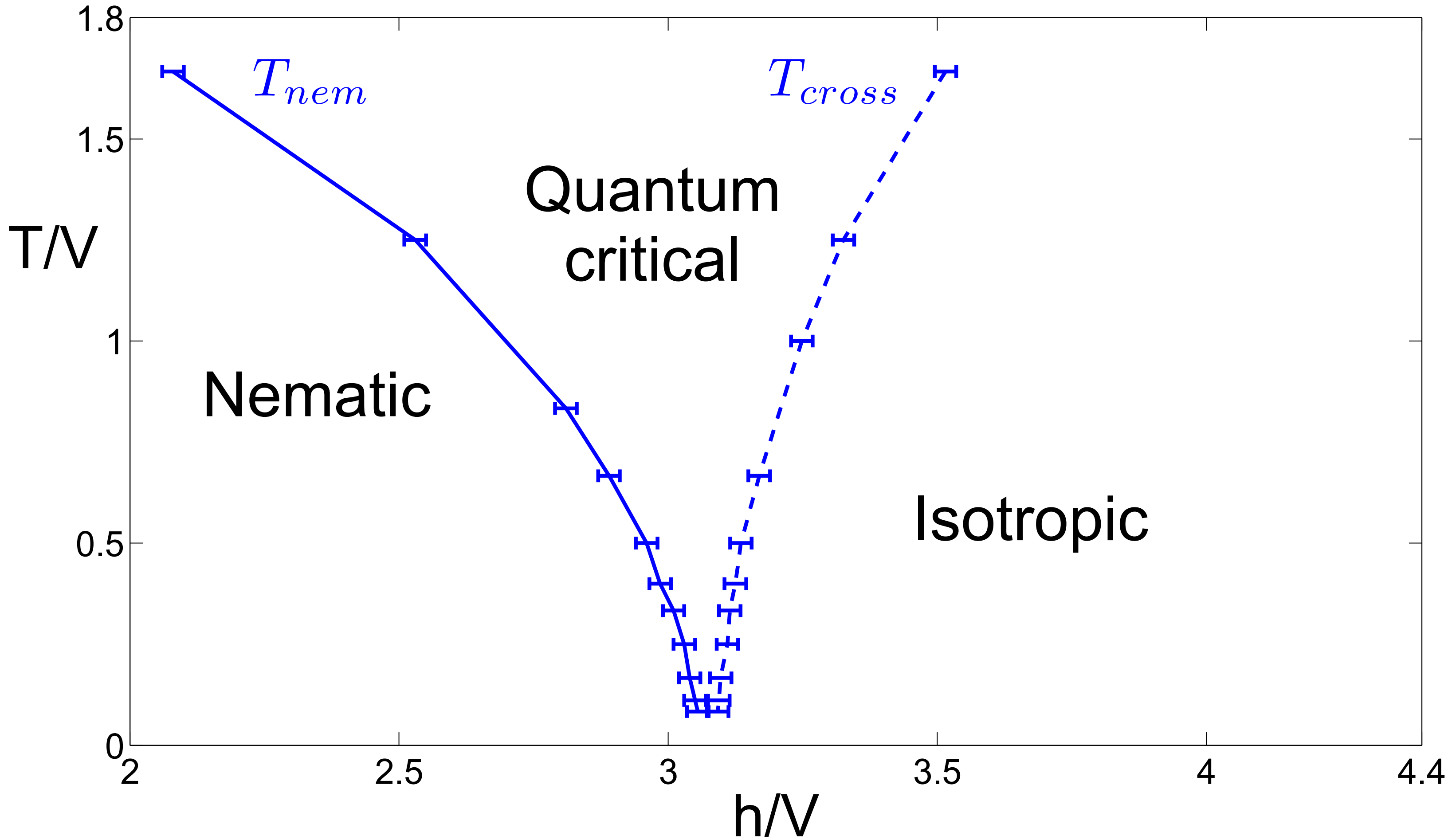
- Finite systems (here $L \leq 24$)

- Finite temperatures (here $\mathrm{T} \geq 0.05t \approx E_F/80$)

- Thermodynamic quantities, imaginary time/Matsubara frequency correlations (real frequency: requires analytic continuation)

# QMC results: Phase diagram

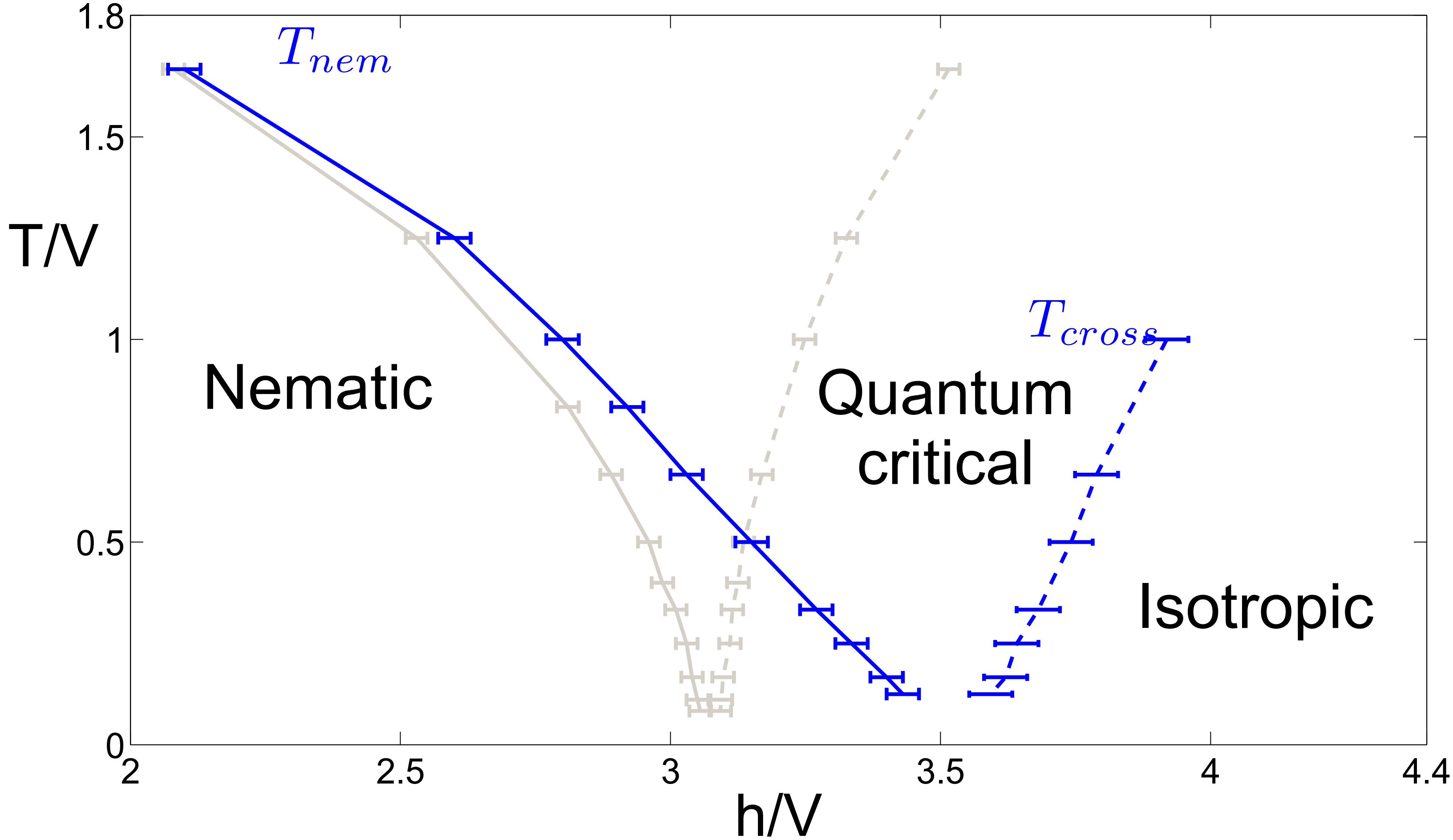
$\alpha = 0$: Decoupled fermions and nematic modes




Lederer, Schattner, Kivelson, and EB (to appear)

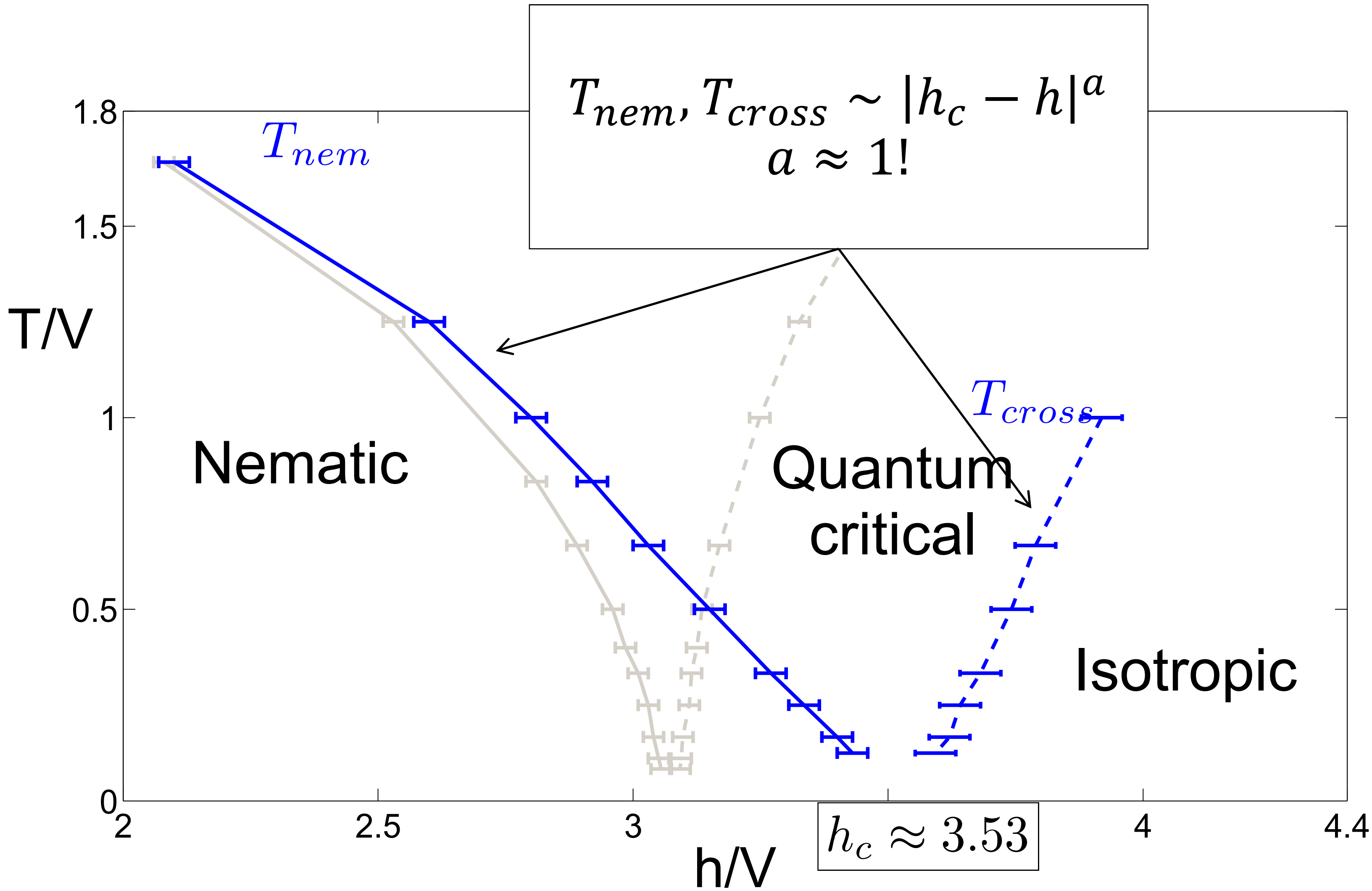
# QMC results: Phase diagram

$\alpha = 0.5$



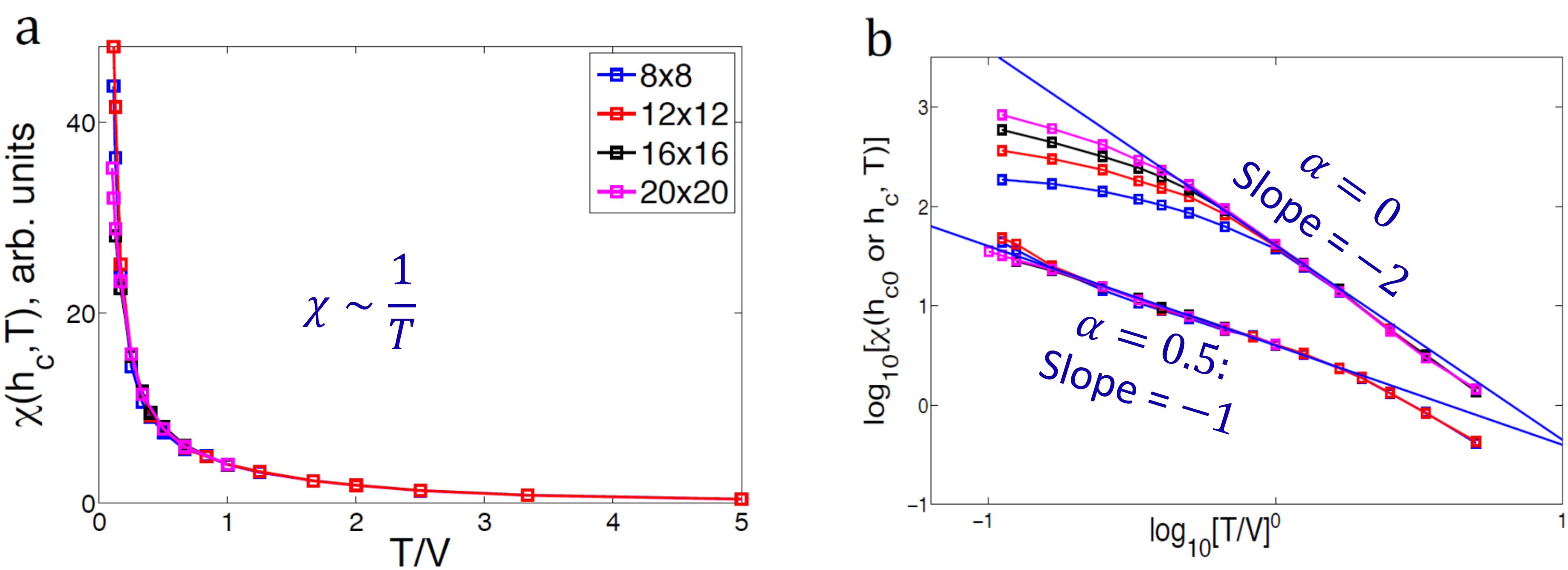

Lederer, Schattner, Kivelson, and EB (to appear)

# QMC results: Phase diagram



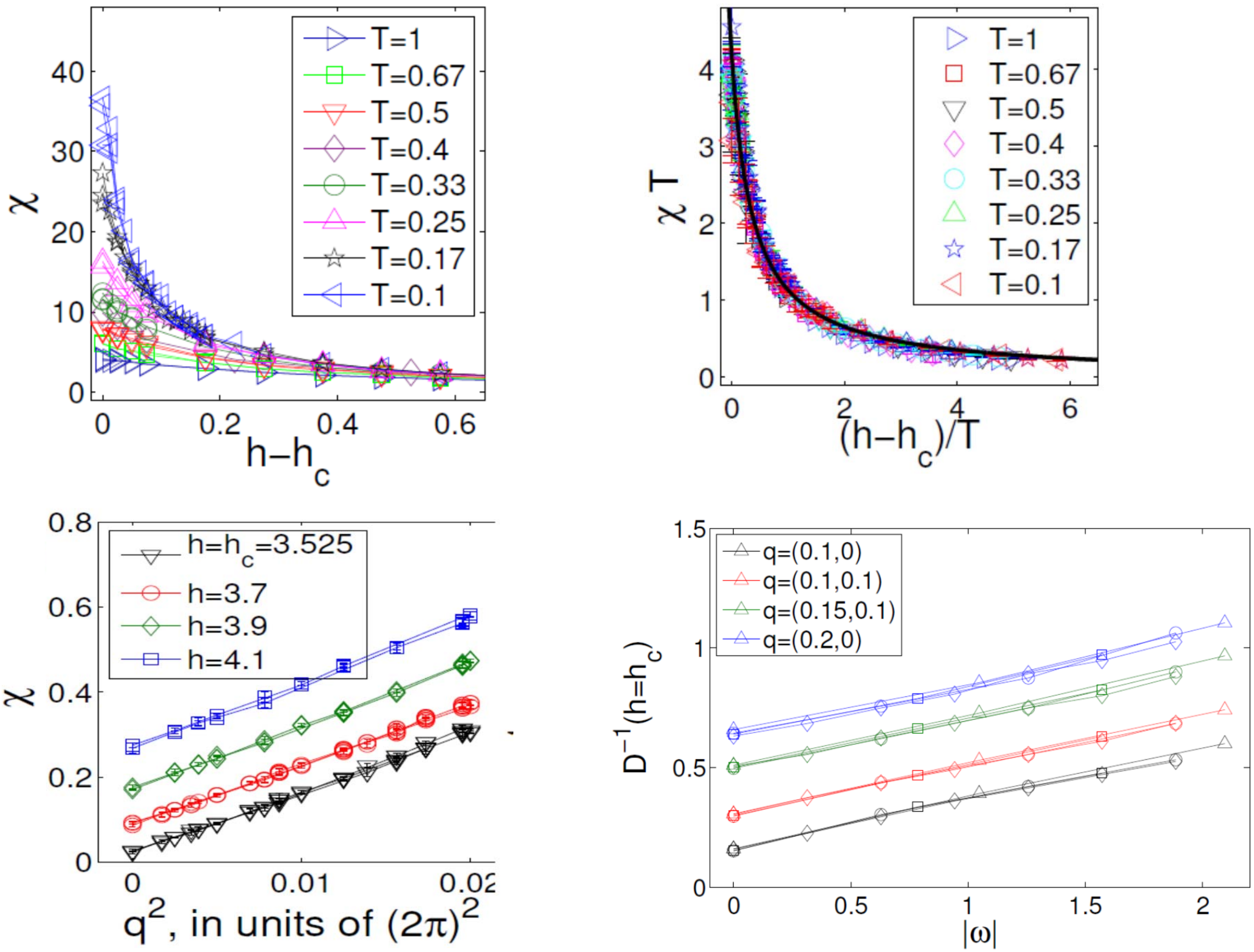

Lederer, Schattner, Kivelson, and EB (to appear)

# Nematic susceptibility at criticality

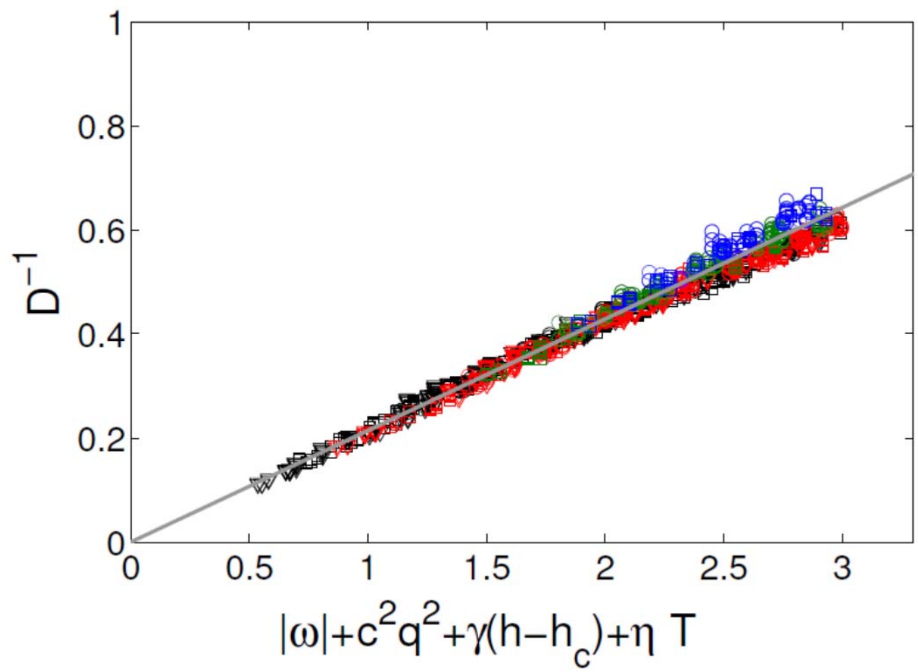



Lederer, Schattner, Kivelson, and EB (to appear)

# Nematic susceptibility at criticality



# Nematic susceptibility at criticality: data collapse




$$\chi(q,h,T,i\omega_n) = \frac{A}{T + B(h-h_c) + Cq^2 + \gamma|\omega_n|}$$

In particular, "Curie-Weiss" law for $\chi(q=0,h,T)$!

Dynamical critical exponent $z = 2$??

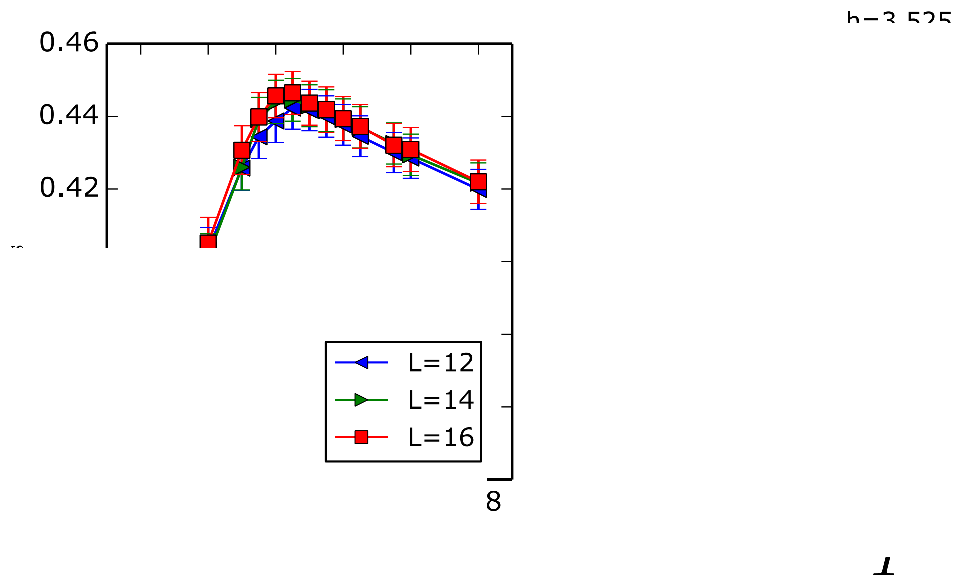
# What are the fermions doing?

Are they superconducting?

*Not above $T = 0.05t \approx E_F/80$.*

*(Superfluid density = 0)*

*s-wave superconducting susceptibility is enhanced near QCP:*



# What are the fermions doing?

Are they a Fermi liquid?

*Down to* $T \geq 0.1t \approx E_F/40$: possible marginal/weak non-FL…

Direct information about fermion spectral function $A(\mathbf{k},\omega)$:

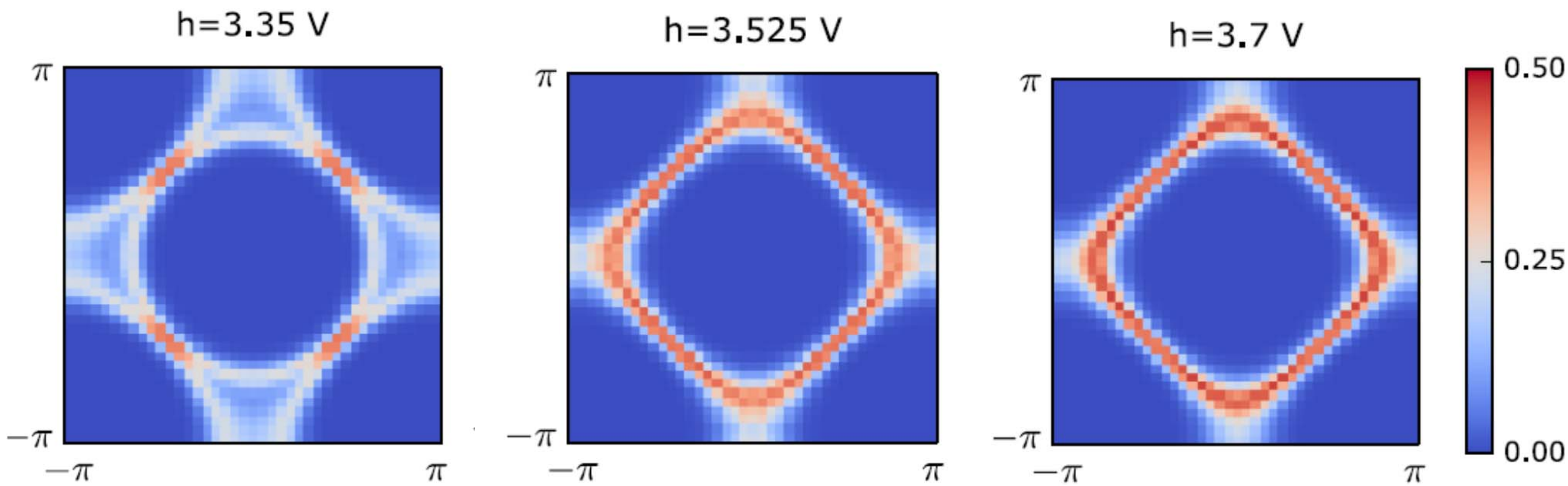
$$G\left(\mathbf{k},\tau=\frac{\beta}{2}\right)=\int d\omega\,\frac{A(\mathbf{k},\omega)}{2\cosh\left(\frac{\beta\omega}{2}\right)}$$

$$\approx \frac{1}{2}\int_{-T}^{T} d\omega\, A(\mathbf{k},\omega)$$

Trivedi, Randeria PRL (1995)

# Fermi surface

$$G\left(\mathbf{k}_F, \tau = \frac{\beta}{2}\right) = \int d\omega \frac{A(\mathbf{k}, \omega)}{2\cosh\left(\frac{\beta\omega}{2}\right)}$$

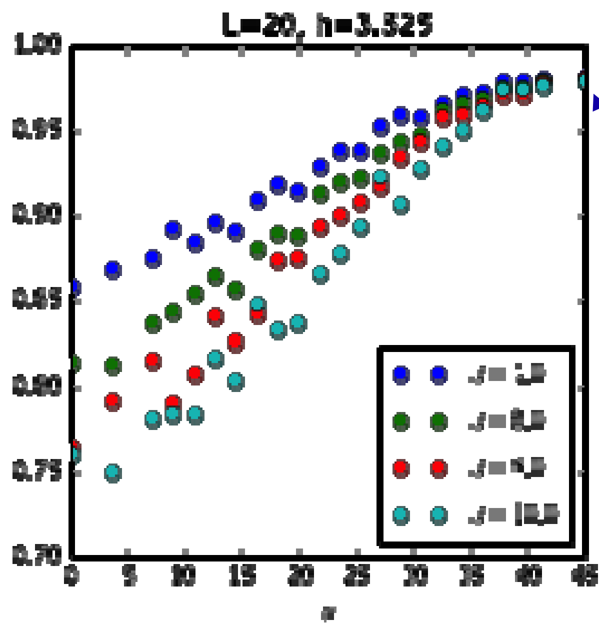



*ordered* *QCP* *disordered*

# Quasi-particle properties

*Assume* FL form of $A(\mathbf{k},\omega)$:

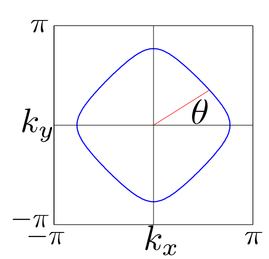
$$G\left(\mathbf{k}_F, \tau = \frac{\beta}{2}\right) = \int d\omega \, \frac{A(\mathbf{k},\omega)}{2\cosh\left(\frac{\beta\omega}{2}\right)} \approx Z_{\mathbf{k}_F}$$

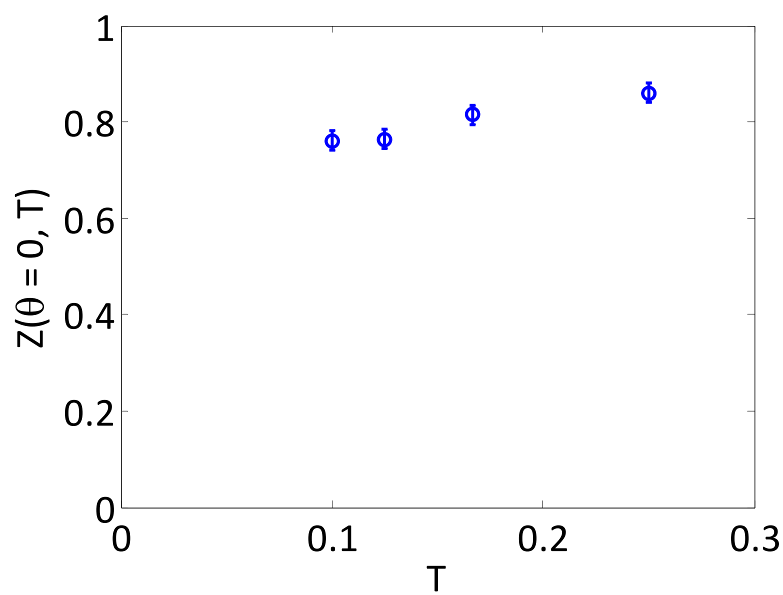



"Hot region"
$Z \approx 0.75$

"Cold spot"
$Z \approx 1$

$Z(\theta)$
at QCP




$Z(\theta = 0, T)$
at QCP

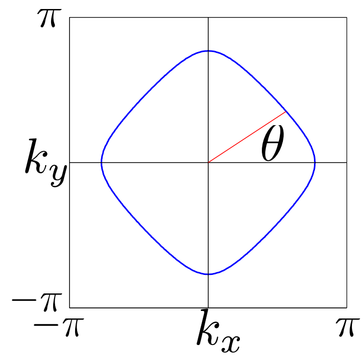
$E_{NFL} \leq 0.1t \approx E_F/40$

# Quasi-particle properties

*Assume* FL form of $A(\mathbf{k},\omega)$:

$$G\left(\mathbf{k}_F, \tau = \frac{\beta}{2}\right) = \int d\omega \frac{A(\mathbf{k},\omega)}{2\cosh\left(\frac{\beta\omega}{2}\right)} \approx Z_{\mathbf{k}_F}$$

- *Also*: strongly angle-depedent effective mass renormaliztion
- $m^*$ increases towards approaching $h_c$ but doesn't seem to diverge…



# Conclusions

- **Ising nematic QCP in a $d = 2 + 1$ metal:** strong deviations from Wilson-Fisher
- Nematic susceptibility follows **Curie-Weiss law** over wide range of temperature and tuning parameter!
- **No superconductivity** in this range (although the pairing susceptibility is enhanced at QCP – probably ground state **is** a SC)
- **Possible marginal FL/weak non-FL** at low $T$ – Still under investigation…

# Preliminary results, future directions

- Larger $\alpha$: superconductivity near QCP (detailed results coming…)

- Frequency dependence of the nematic susceptibility $\chi(q, i\omega_n)$, inconsistent with Herz-Millis theory… $z = 2$!
  Needs theoretical understanding!

- Other types of metallic QCP (AFM, CDW, …)

**Thank you.**