Lattice vs Continuum (And 2 vs 3 Species) in the BCS-BEC Crossover

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S-Y Chang, A. Daley, S. Diehl, M. Baranov (IQOQI Innsbruck)

21.04.2011 INT Seattle

Layout of the Seminar

- Lattice Vs Continuum
  - Dilute Gases
  - Lattice Systems
  - Dilute Limit: MF & DMFT
  - Take-Home Message 1

- From 2 to 3 species
  - SU(3) symmetric case
  - Lithium Case
  - Take-Home Message 2

Part 1

Lattice vs Continuum

A. Privitera, M. Capone and C. Castellani, PRB 81, 014523 (2010)

A. Privitera and M. Capone (in preparation)

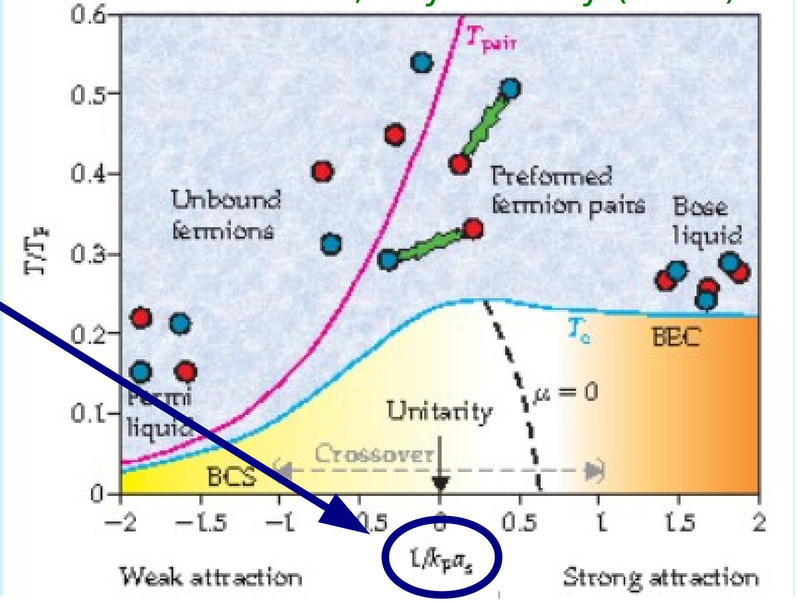
Crossover in Dilute Gases

- Dilute Fermi gas (e.g. ultracold gases)

$$k_F b \to 0 \longrightarrow (k_F a_s)^{-1} = \eta$$

BCS-BEC crossover in dilute Fermi gases

Sa De Melo, Phys. Today (2008)



Universal

Crossover in Dilute Gases

- Dilute Fermi gas (e.g. ultracold gases)

$$k_F b \to 0 \longrightarrow (k_F a_s)^{-1} = \eta$$

BCS-BEC crossover in dilute Fermi gases

- Diverging $a_s \longrightarrow \eta \to 0$

k_F **only length in the system**

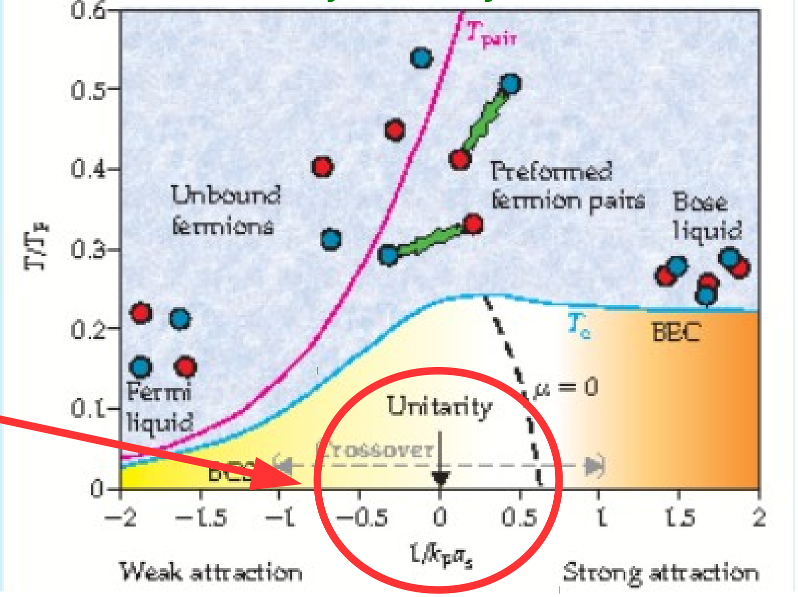
$$\frac{E_{UFG}}{E_0} = \frac{E_{UFG}}{3/5N\varepsilon_F} = \xi_s = \frac{\mu}{\varepsilon_F}$$

Universal Parameters

$$\xi_s = \frac{\mu}{\varepsilon_F}, \quad \tilde{\Delta} = \frac{\Delta}{\varepsilon_F}, \quad \gamma = \frac{T_c}{\varepsilon_F}$$

e.g. the same for different atomic species

Sa De Melo, Phys. Today 61 45 (2008)



Requires Simultaneously:

- **Diluteness condition**
- **Diverging Scattering Length**

Open Theoretical Issues ?

Non perturbative problem

- Analytical approaches
  (not controlled)

- Numerical approaches
  (Finite-Size + Finite-Range/-Density + Sign problem)

- **Qualitative Level**: **General Agreement**

  (crossover, no transition)

- **Quantitative Level:** **Open Problems ?**

  (e.g. ξ_s , γ , pseudogap for $\eta = 0$)

Crossover in a (Specific) Lattice Model

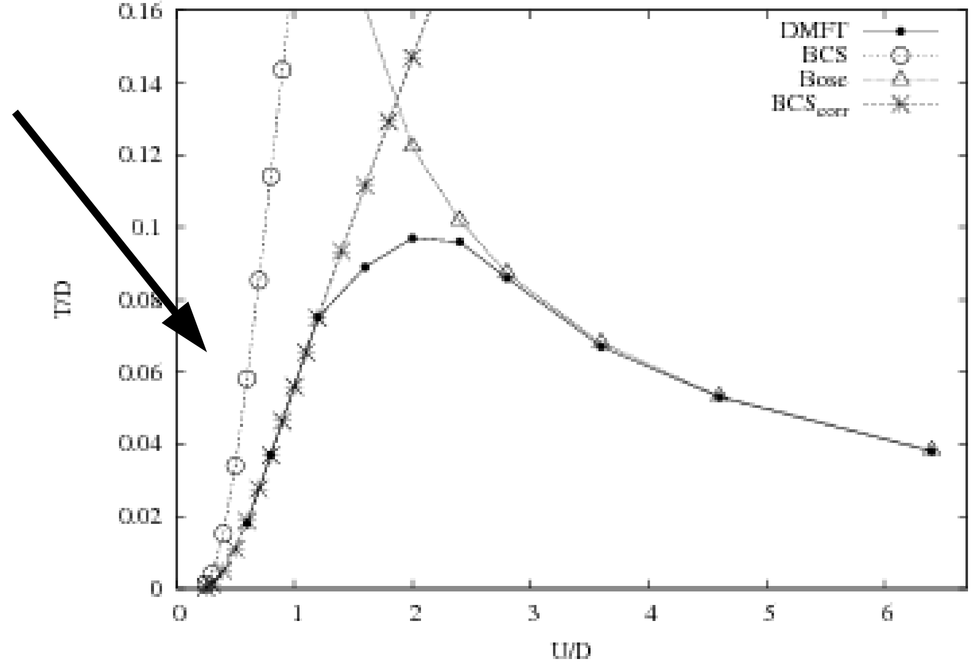
Attractive Hubbard Model

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sum_{\sigma=\uparrow,\downarrow} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \qquad (U < 0)$$

(DMFT $n = 0.75 = \mathcal{O}(1)$)

- **BCS Regime** $|U| \ll J$

$T_c \propto \Delta_0 \ll D_s \qquad (\xi_0 \gg l)$



A. Toschi et al. , PRB (2005)

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- **BCS Regime** $|U| \ll J$

$$T_c \propto \Delta_0 \ll D_s \qquad (\xi_0 \gg l)$$

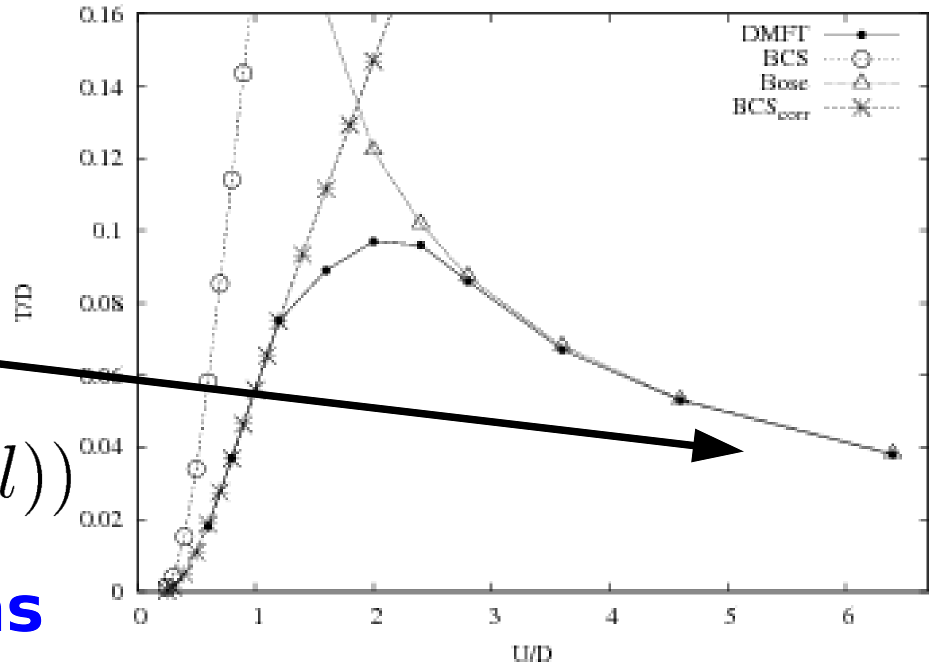
- **BEC Regime** $|U| \gg J$

$$T_c \propto D_s \propto |U|/J \ll \Delta_0$$

$$m_B \propto |U|/J \gg m_e \, (\xi_0 = \mathcal{O}(l))$$

(Heavy) Hard-Core Bosons

(DMFT $n = 0.75 = \mathcal{O}(1)$)



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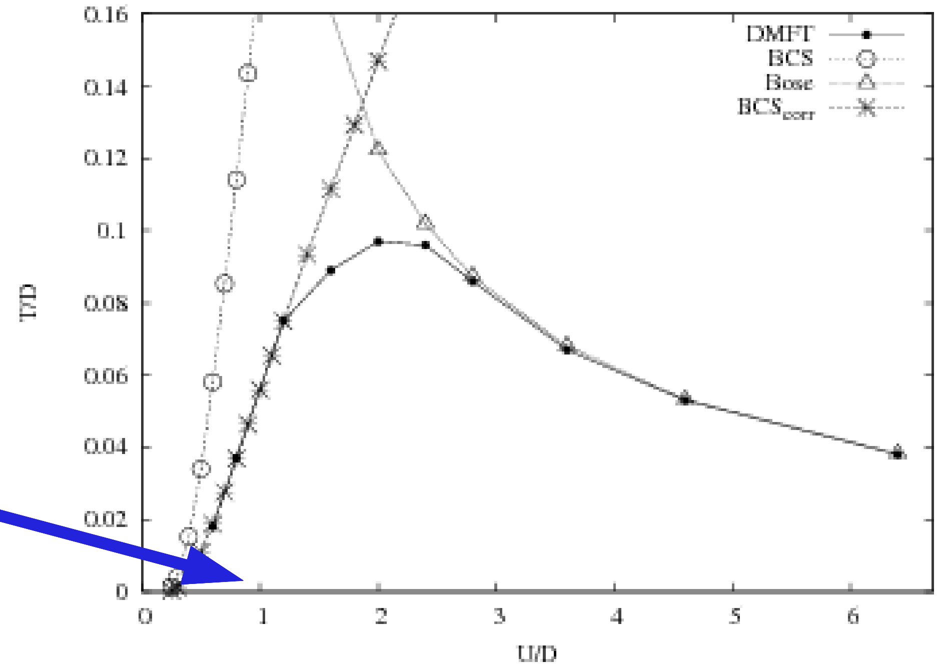
- **BCS Regime** $|U| \ll J$
- **BEC Regime** $|U| \gg J$
- **Unitary Point ??**

$U_c = -D \quad a_s = \infty$

(DMFT $n = 0.75 = \mathcal{O}(1)$)



A. Toschi e. al. , PRB 72, 235118 (2005)

Dilute Limit of the Lattice Model

A. Privitera et al. ,PRB 2010
A. Privitera and M. Capone (in prep.)

Are these scenarios connected ?

- Well Defined Recipe..

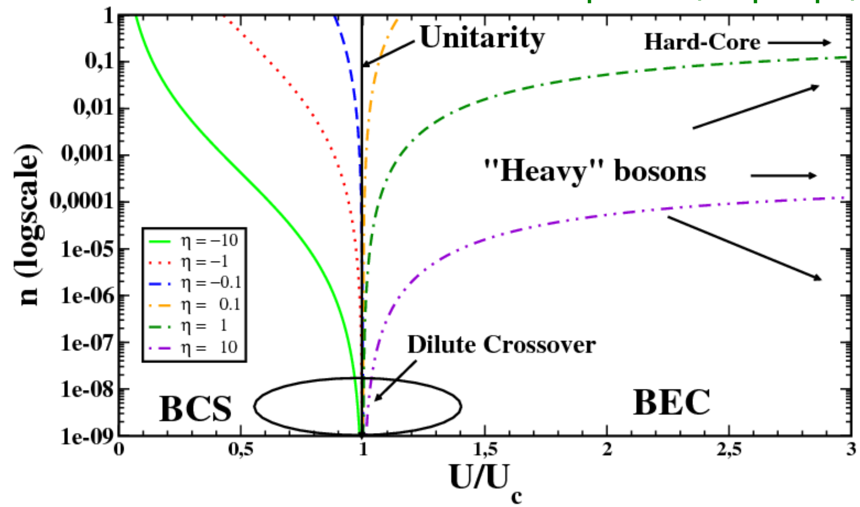
$$\lim_{n\to 0} \text{Lattice Model}_{|\eta} = \text{Dilute Fermi Gas}_{|\eta}$$

$$(U, n) \to (a_s, k_F)$$

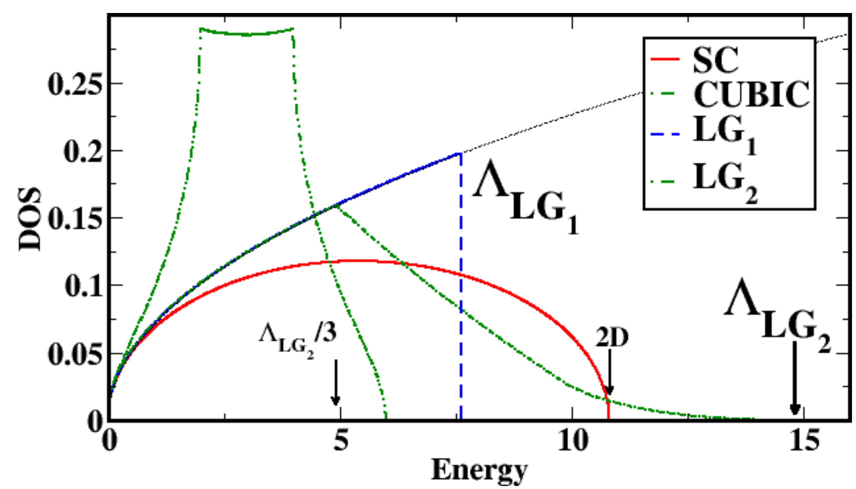
$$a_s^{latt}(U) = \frac{m_e l^3}{4\pi\hbar^2} \frac{1}{U^{-1} - U_c^{latt}}$$

$$U_c^{latt} = \left[-\int_0^\Lambda d\epsilon \frac{D_{latt}(\epsilon)}{2\epsilon} \right]^{-1}$$

$$E_F = \frac{\hbar^2 k_F^2}{2m} \qquad k_F = \left[3\pi^2 \left(\frac{n}{l^3} \right) \right]^{\frac{1}{3}}$$



$$\frac{U}{U_c^{latt}} = \frac{1}{1 - C_{latt}\eta n^{1/3}}$$



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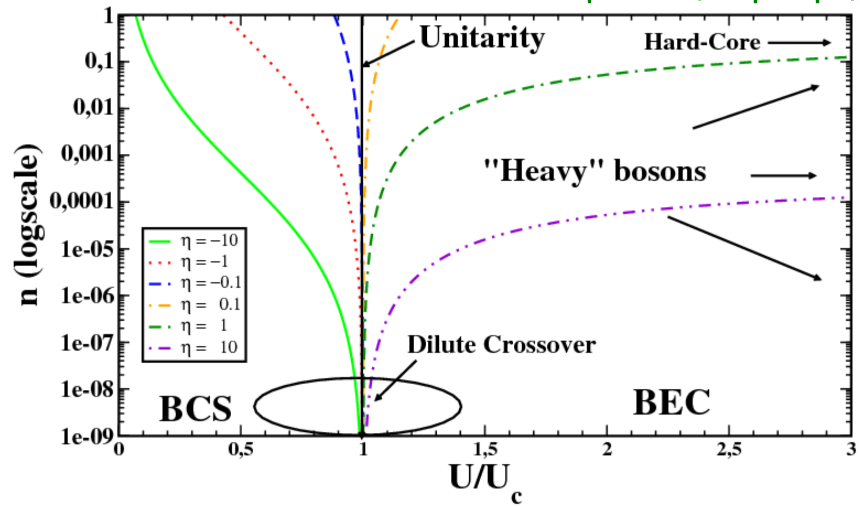
- Tells us nothing about the convergence speed...

Every Non-Universal Feature has to disappear...



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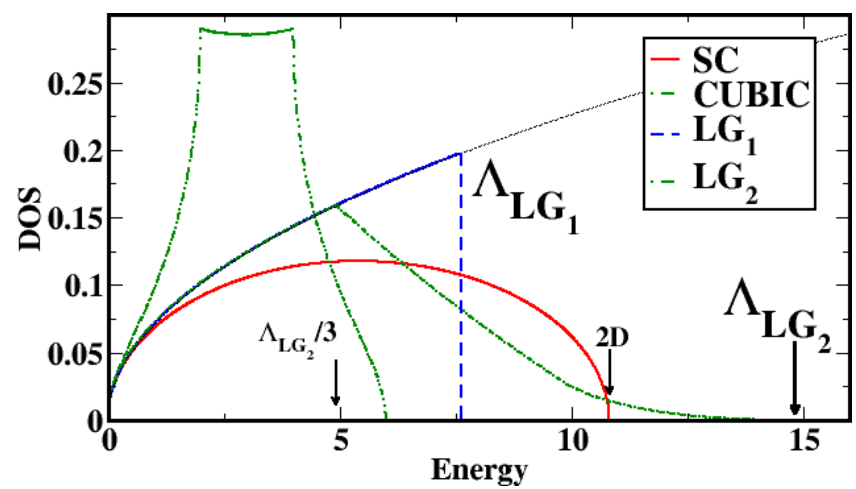

From Nozieres To Leggett

Static Mean-Field

- Exact in Both Limits at T=0
- Thermodynamic (no Finite Size)
- No limitation in density
- Lattice and Continuum
- Easy
- No Fluctuations

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$$n = \frac{1}{N_s}\sum_{\mathbf{k}}\left(1 - \frac{\eta_{\mathbf{k}}}{E_{\mathbf{k}}}\right)$$

$$\frac{1}{|U|} = \frac{1}{N_s}\sum_{\mathbf{k}}\frac{1}{2E_{\mathbf{k}}}$$

$$\eta_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu' \quad \mu' = \mu - (Un/2)$$

$$E_{\mathbf{k}} = \sqrt{\eta_{\mathbf{k}}^2 + \Delta^2}$$

$$(U,n) \rightarrow (a_s, k_F) \quad \forall n$$

$$\frac{4}{3} = \int_0^{\Lambda/E_F} dx\ \tilde{D}(x)\left[1 - \frac{(x-\tilde{\mu}')}{\sqrt{(x-\tilde{\mu}')^2 + \tilde{\Delta}^2}}\right]$$

$$\eta = \frac{1}{\pi}\int_0^{\Lambda/E_F} dx\ \tilde{D}(x)\left[\frac{1}{x} - \frac{1}{\sqrt{(x-\tilde{\mu}')^2 + \tilde{\Delta}^2}}\right]$$

$$\tilde{\mu} = \frac{\mu}{E_F} \quad \tilde{\Delta} = \frac{\Delta}{E_F} \quad \tilde{D}(x) = \frac{D_{latt}(E_F x)}{D_{free}(E_F)}$$

Nozieres & Schmitt-Rink (1985)

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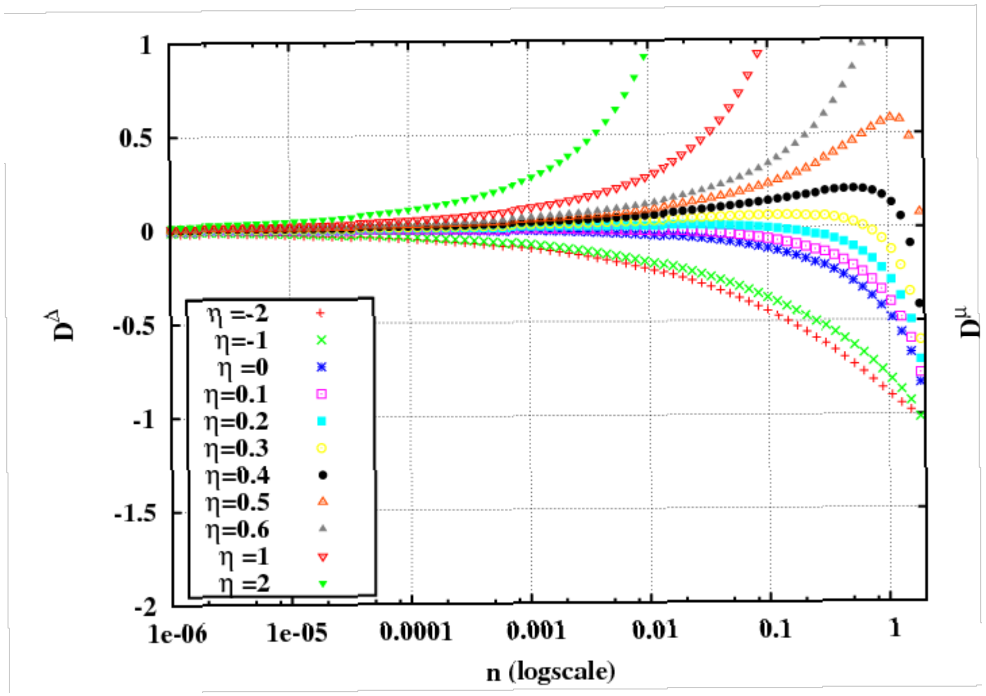
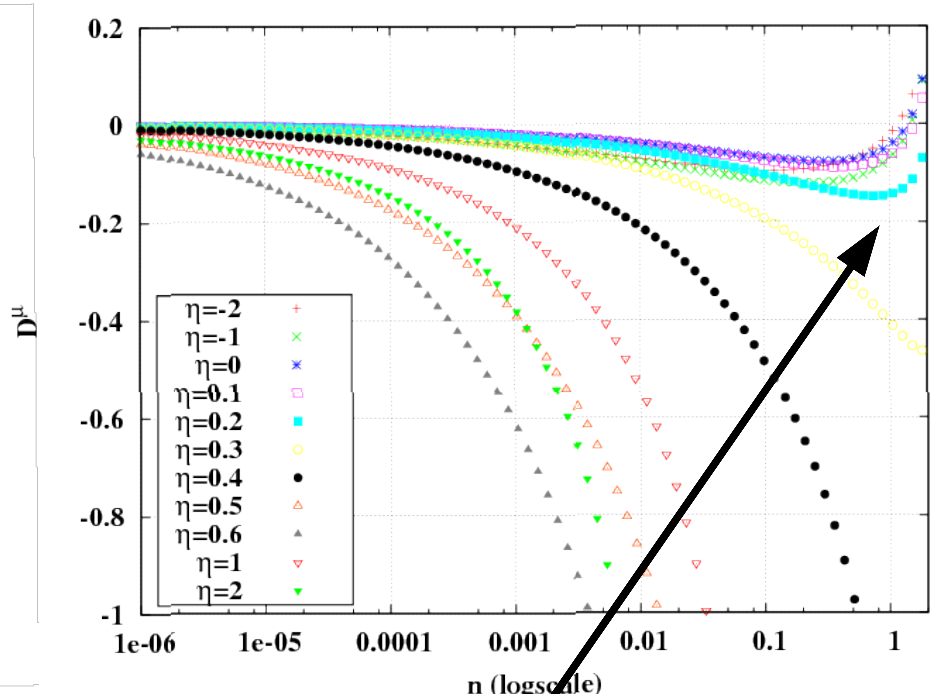
$$\lim_{n\rightarrow 0} = \mathrm{Leggett}(1980)$$

Finite n ?

Hartree, DOS, Cut-Off

Mean-Field Results 1



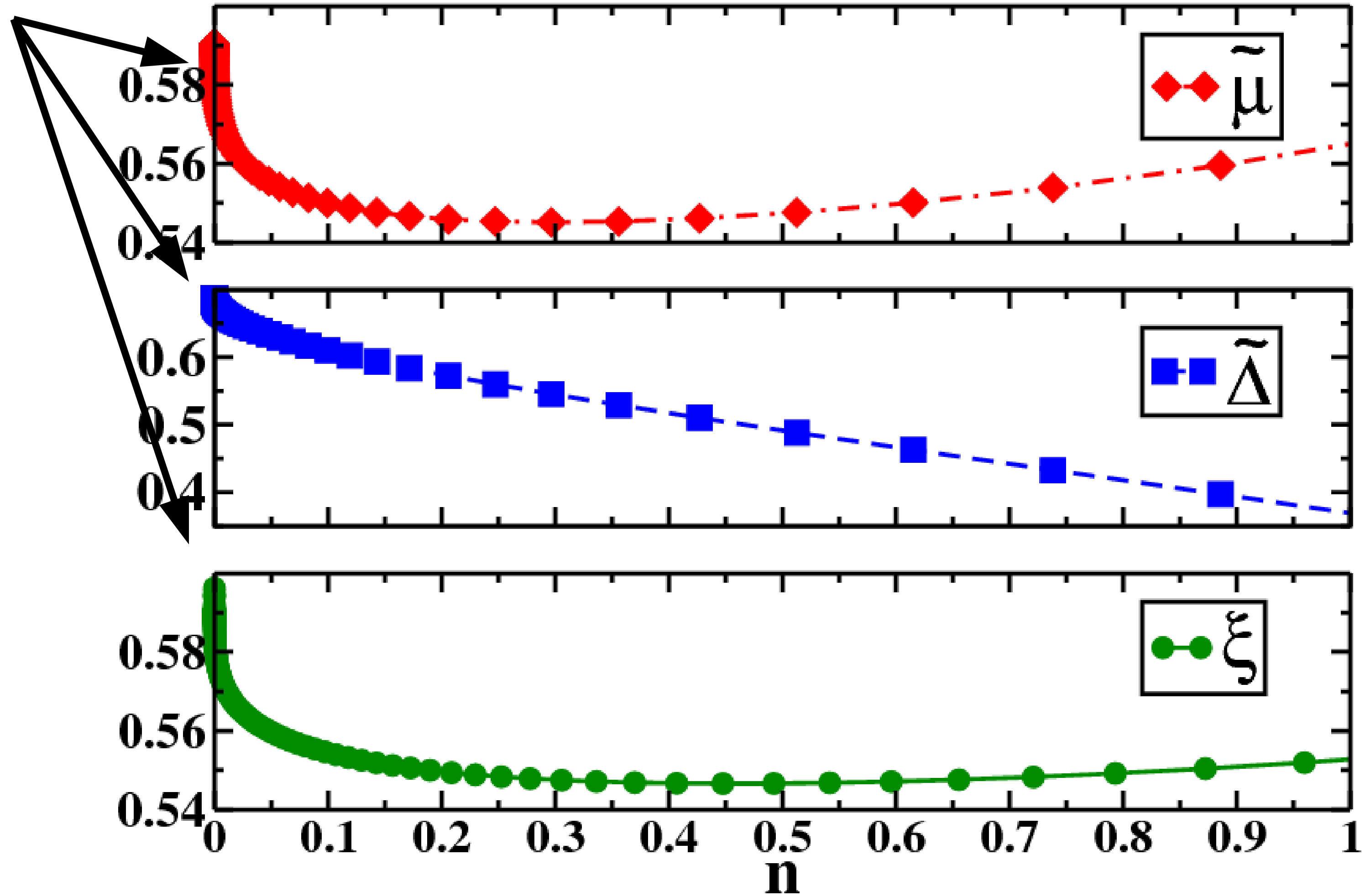


- Very Slow Convergence !!
- Non-Monotonic (Lattice-Dependent) Corrections
- Universal Power-Law Behavior Asymptotically $k_F l \propto n^{1/3}$

Hartree-Shift $\delta\tilde{\mu} = \dfrac{-|U(n)|_\eta n}{2E_F} \propto k_F l \propto n^{1/3}$

Mean-Field Results 2 (Unitary)

- Divergent Slope..

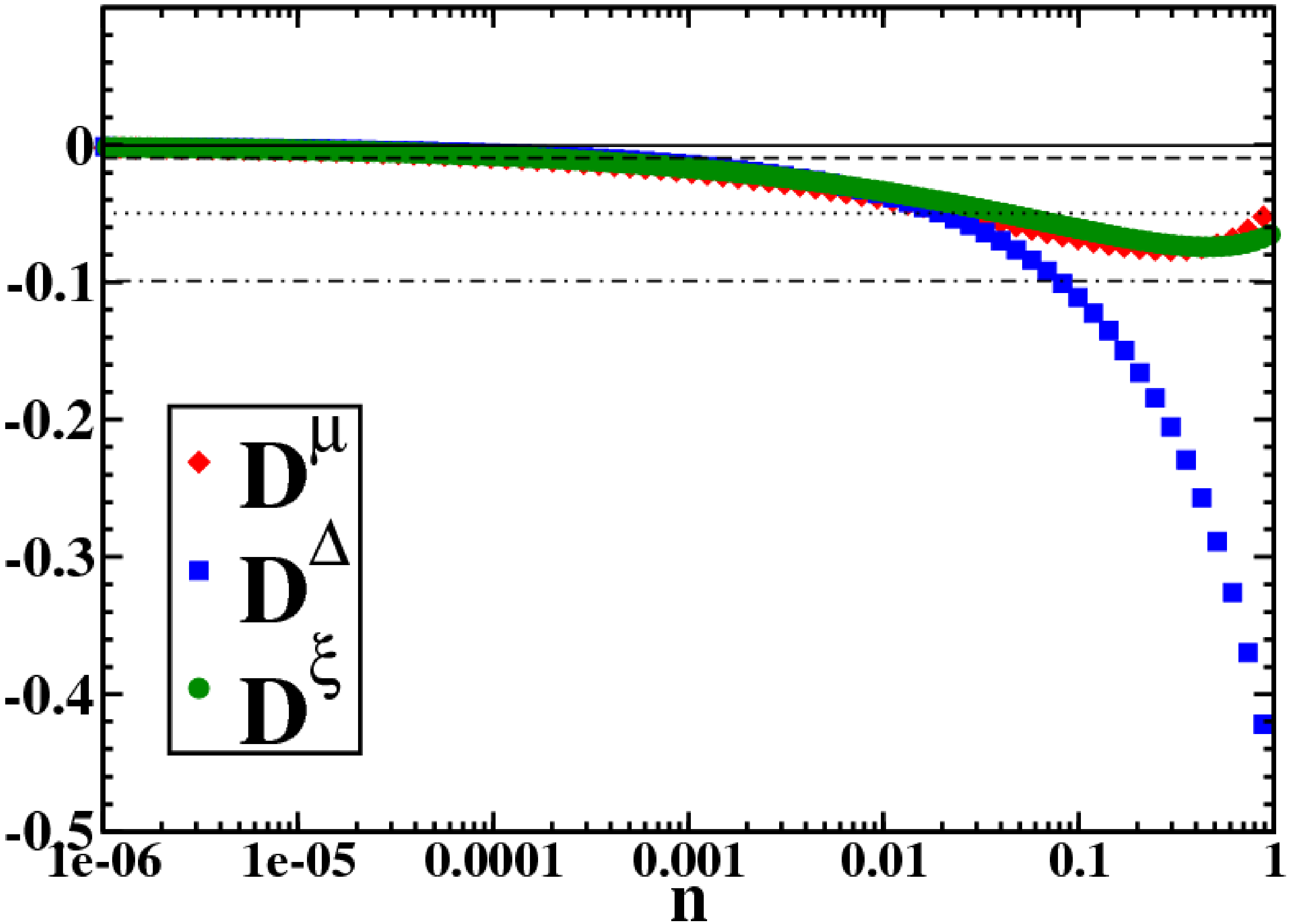


Mean-Field Results 2 (Unitary)

- Divergent Slope..
- $D < 0.01$

  only for

  $n \neq 10^{-6}$



Mean-Field Results 2 (Unitary)

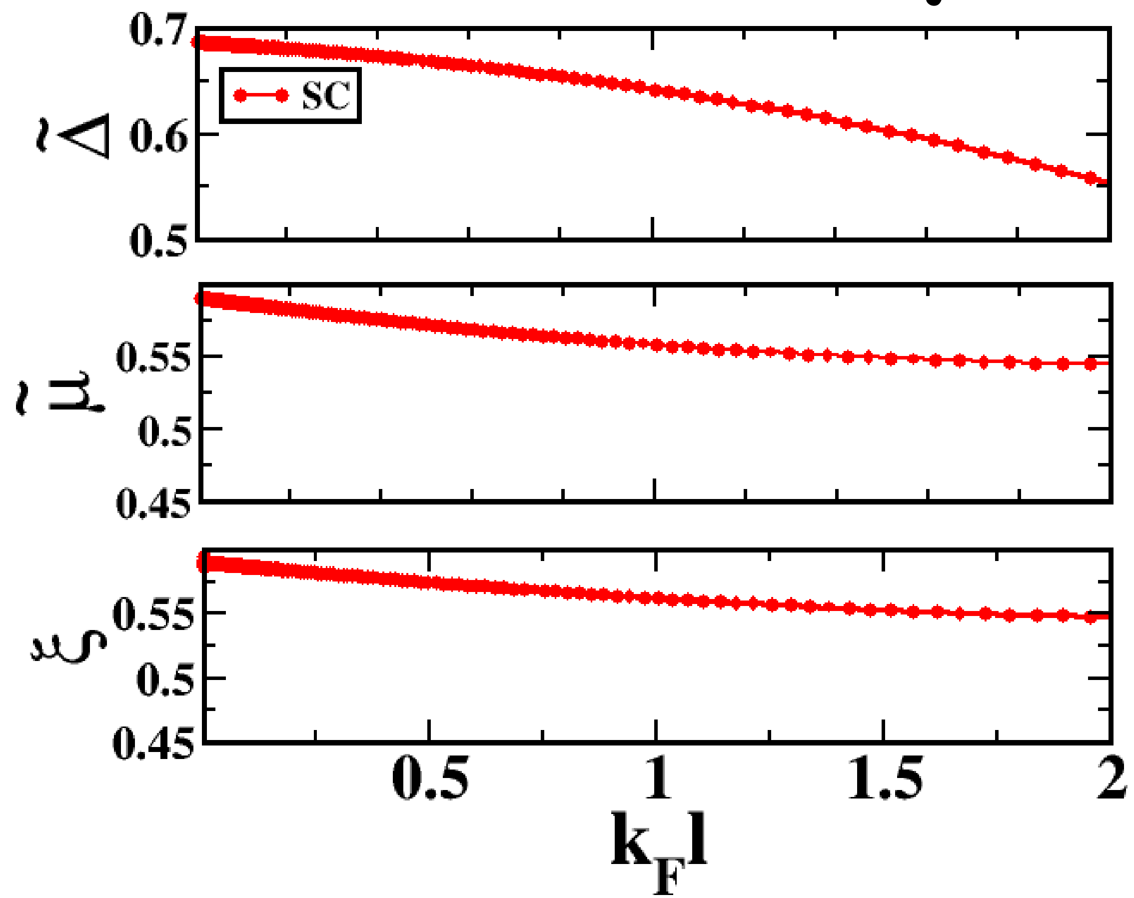
- Best Fit (low n)

$$\tilde{\mu}(k_F l)_{SC} \approx \tilde{\mu}_L + a_{SC}\ (k_F l)$$

$$\tilde{\Delta}(k_F l)_{SC} \approx \tilde{\Delta}_L + b_{SC}\ (k_F l)$$

$$\xi(k_F l)_{SC} \approx \xi_L + c_{SC}\ (k_F l)$$

(Mean-Field)



$$(a = -0.040, b = -0.028, c = -0.034)$$

$$\delta\tilde{\mu}_{SC} = \frac{U_c^{SC} n}{2E_F} = -0.182(k_F l)$$

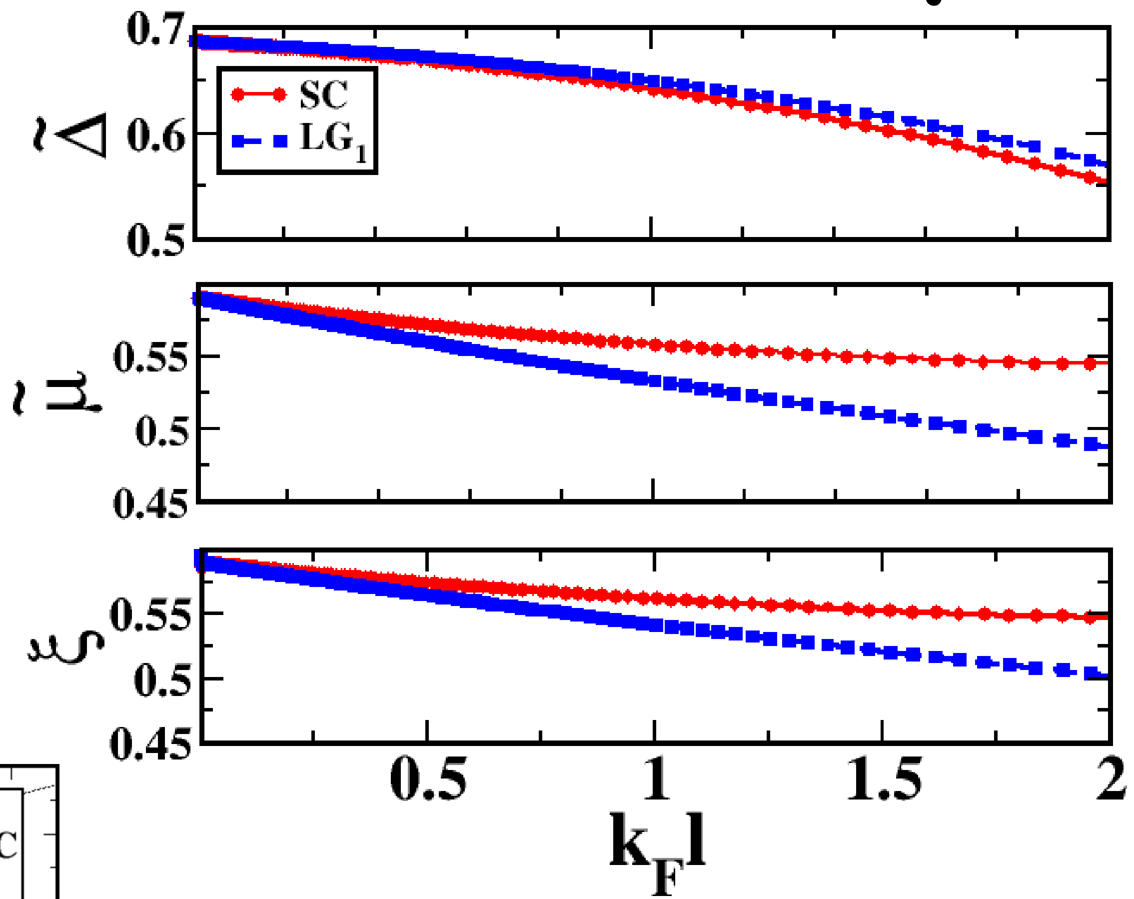
Where do the other corrections come from ?

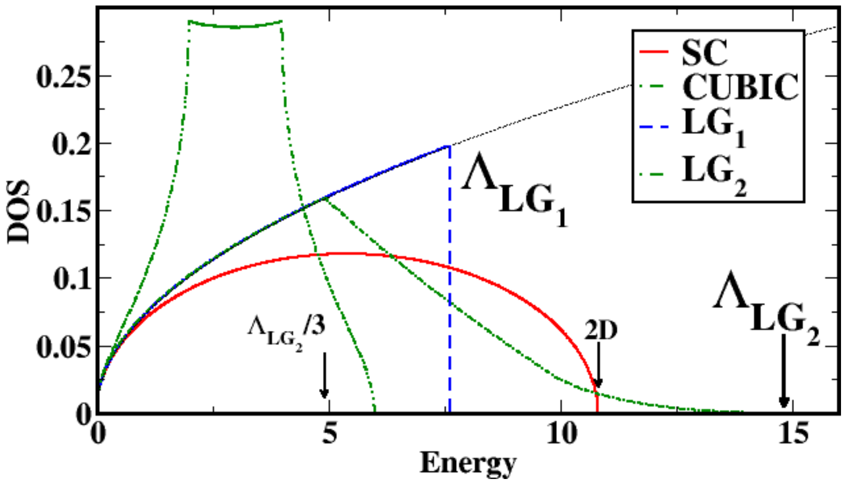
Mean-Field Results 2 (Unitary)

Semicircular
Vs
Lattice Gas

$$a_{LG_1} = -0.063$$

$$\delta\tilde{\mu}_{LG_1} = \frac{U_c^{LG_1} n}{2E_F} = -0.171(k_F l)$$





Take-Home Message:
Cut-Off Matters !
(Lattice Intrinsic)

From Static to Dynamical Mean-Field

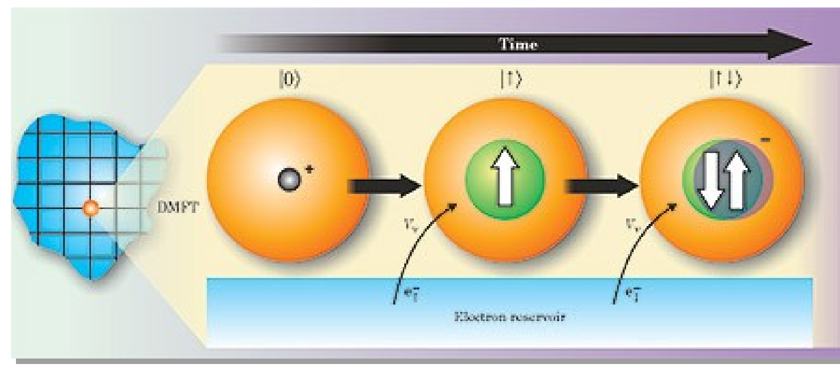
Dynamical Mean-Field Theory

- Exact in Both Limits at T=0
- Thermodynamic (no Finite Size)
- (almost) No limitation in density
- Includes Fluctuations :-)
- Non-Perturbative in U
- Lattice Approach
- Not So Easy

- Interacting Lattice Model

Self-consistent local problem

- Exact solution in $d = \infty$



Kotliar & Vollhardt, PT (2004)

For systems in 3d

$$\Sigma(\mathbf{k}, i\omega_n) \rightarrow \Sigma(i\omega_n) \rightarrow \Sigma$$

Exact — DMFT — Static MF

Dynamical Mean-Field Theory

- Interacting Lattice Model

  ↓

  Self-consistent local problem

- Exact solution in $d = \infty$

For systems in 3d

$$\Sigma(\mathbf{k}, i\omega_n) \longrightarrow \Sigma(i\omega_n) \longrightarrow \Sigma$$

Exact — DMFT — Static MF

(N) $$G(i\omega_n) = G_{latt}(i\omega_n) \equiv \int_{-\infty}^{\infty} d\epsilon\ D(\epsilon)\ \frac{z^* - \epsilon}{|z-\epsilon|^2 + S^2}$$

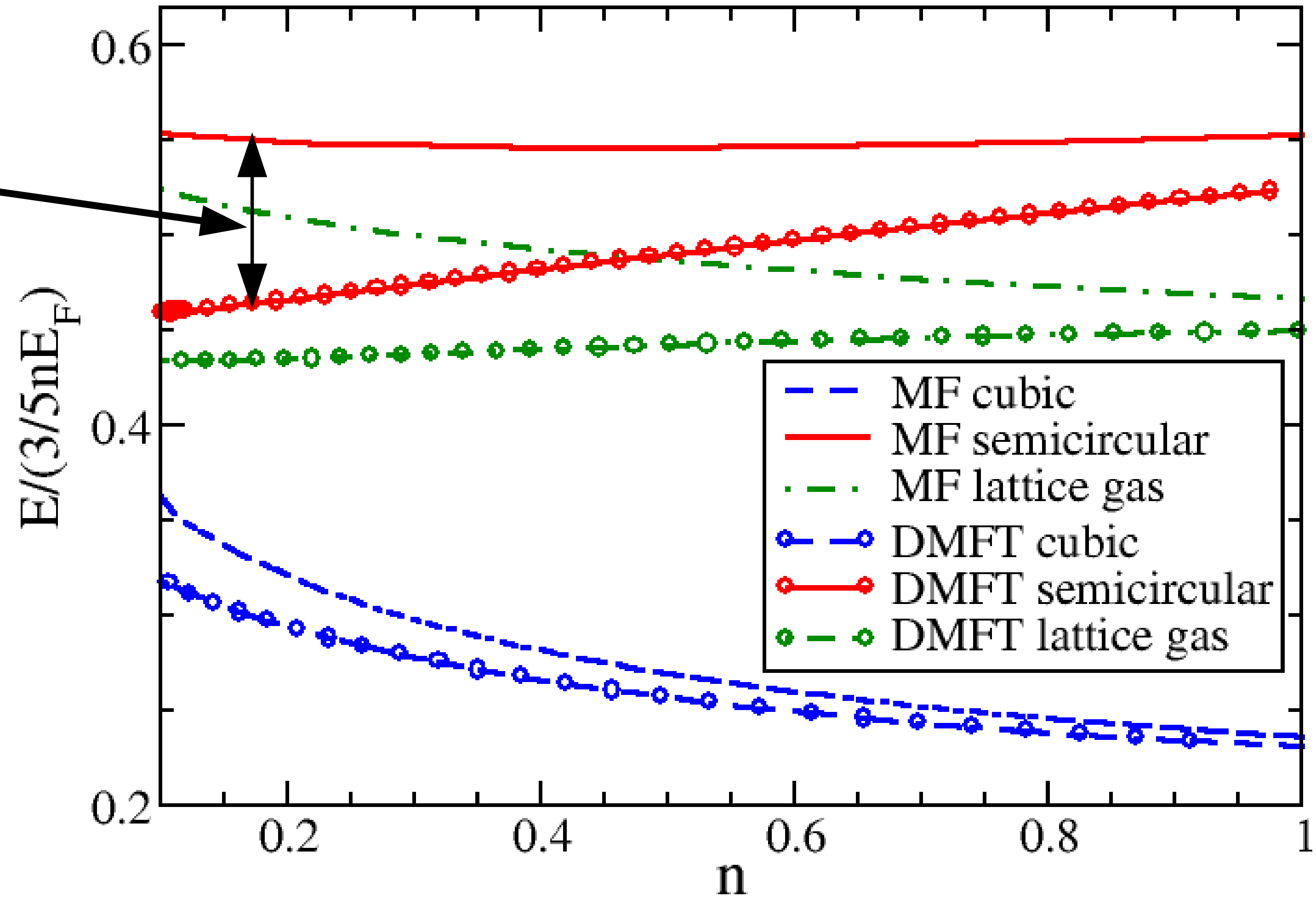
(A) $$F(i\omega_n) = F_{latt}(i\omega_n) \equiv \int_{-\infty}^{\infty} d\epsilon\ D(\epsilon)\ \frac{-S(i\omega_n)}{|z-\epsilon|^2 + S^2}$$

- where G, F, Σ, S come from the solution of a self consistent Anderson Impurity Model

$$z = i\omega_n + \mu - \Sigma(i\omega_n)$$

DMFT Results n > 0.1

- Relevance of Fluctuations Increases for Decreasing Density

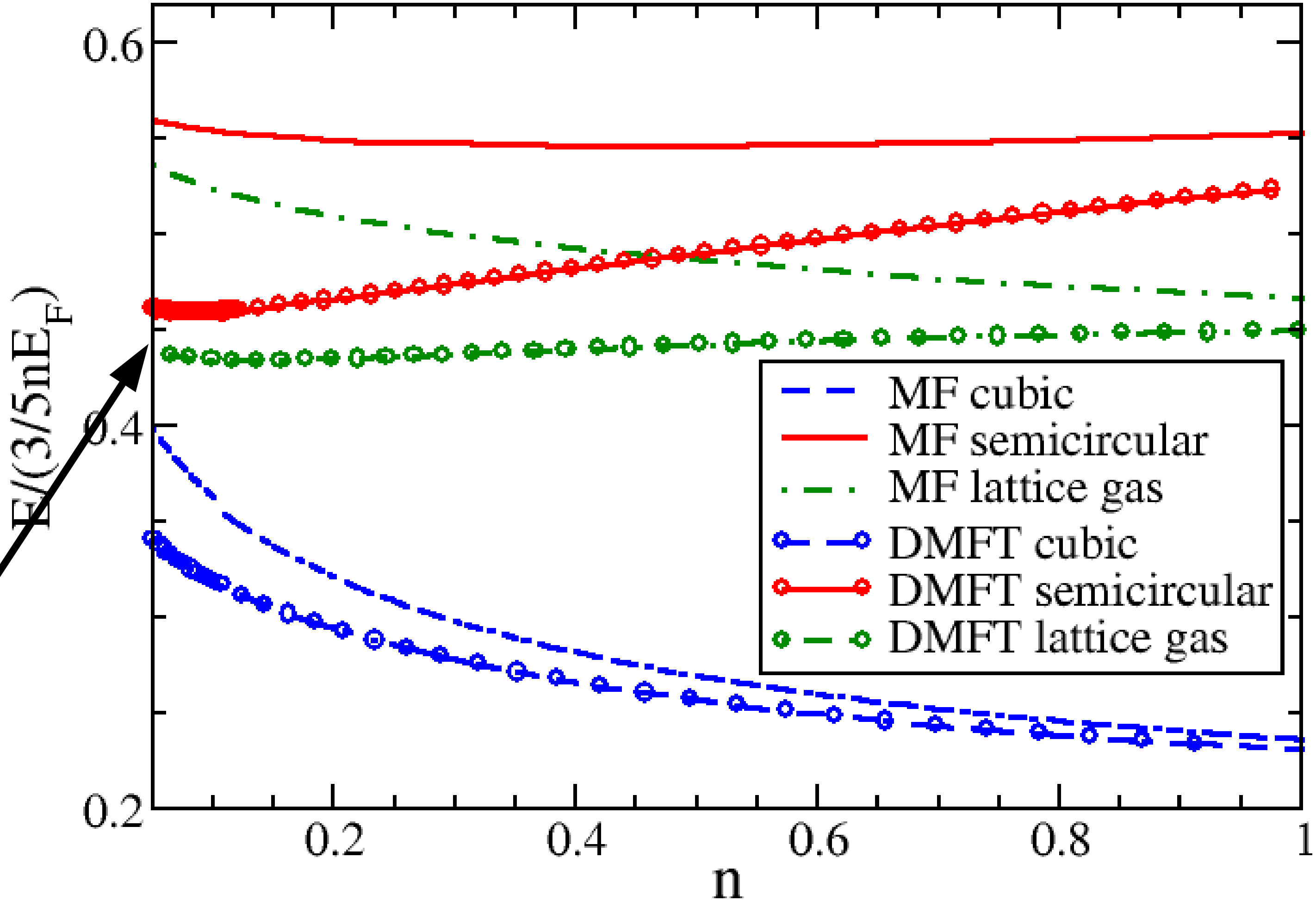


- Fairly Good Agreement
  with previous Lattice approaches (QMC and DMFT at the same n)

Not Yet Universal

DMFT Results n > 0.05

- Seems to Saturate..



The Asymptotic Slope should Diverge..

$$n_{min}^{QMC} \approx 0.01 - 0.1$$

Not Yet Universal

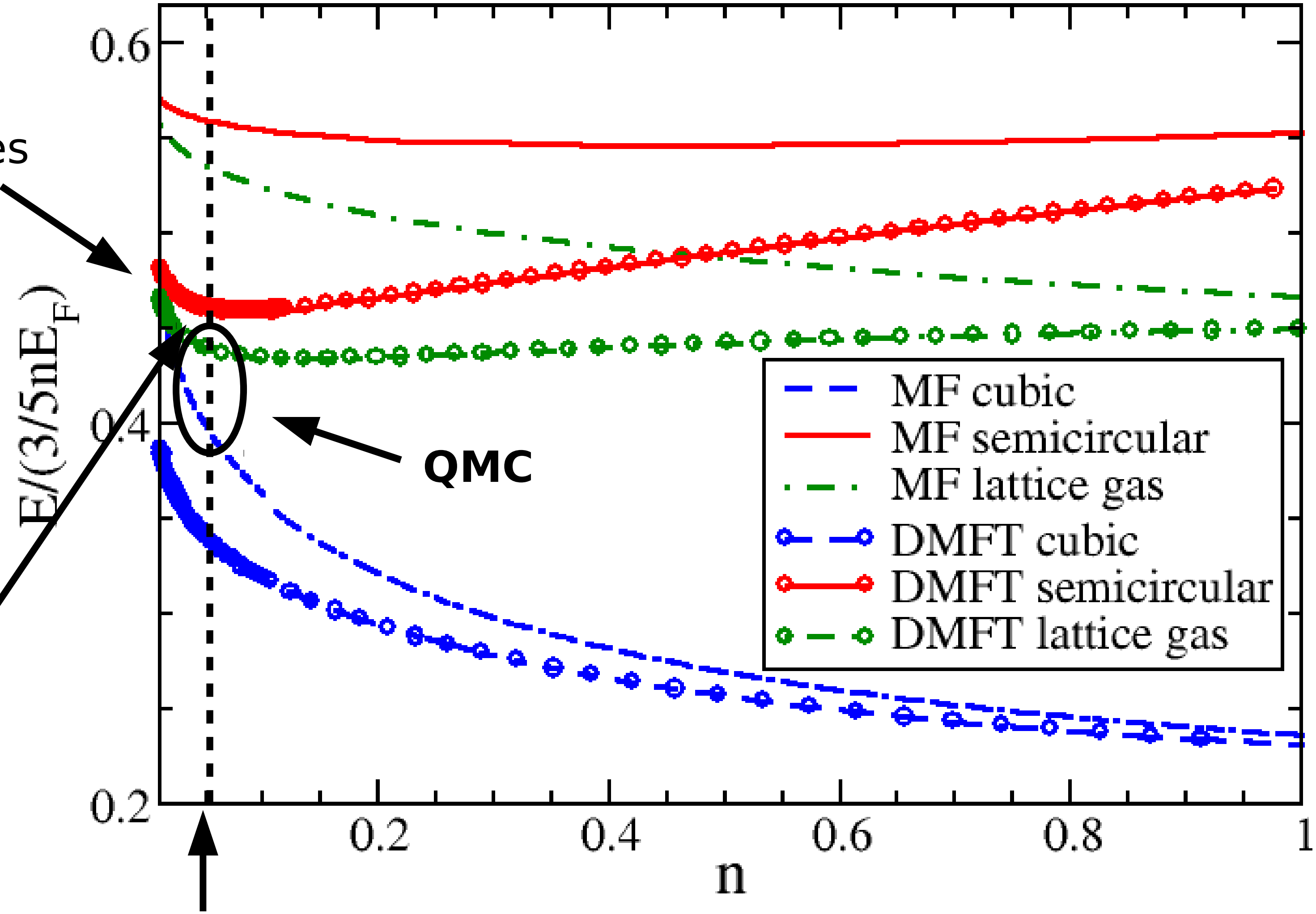
DMFT Results n > 0.01

- Everything changes at Lower Densities

- Fake Universality

For $n = \bar{n}$

$$\frac{E}{3/5nE_F} = \frac{\mu}{E_F}$$



$n_{min}^{QMC} \approx 0.01 - 0.1$

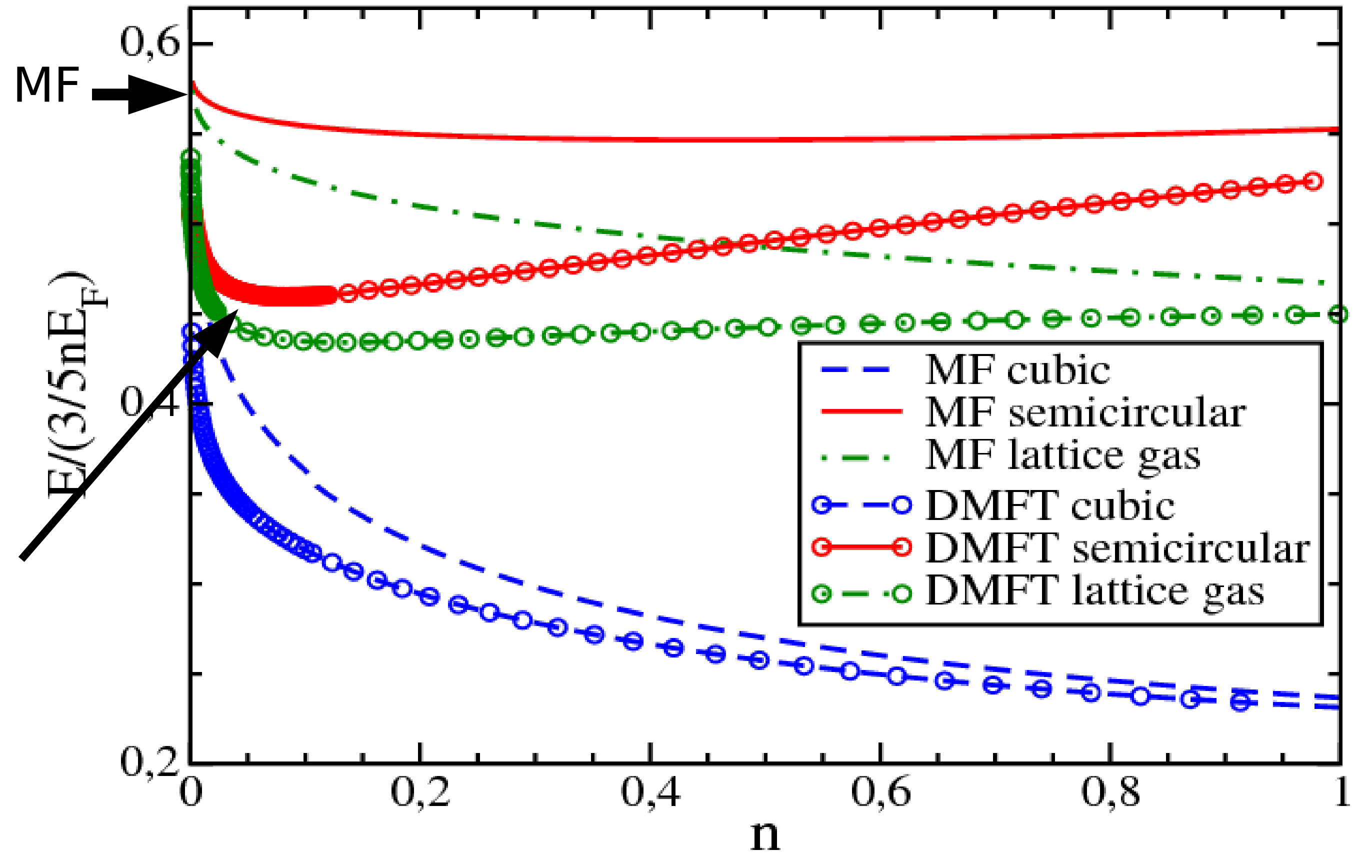
Not Yet Universal

DMFT Results full

- DMFT → MF

  for

  $n < n_{MF} \approx 10^{-3}$



- Is the existence of this minimum only due to this effect ?

Minima within MF are real..

DMFT Results full

- DMFT → MF

for

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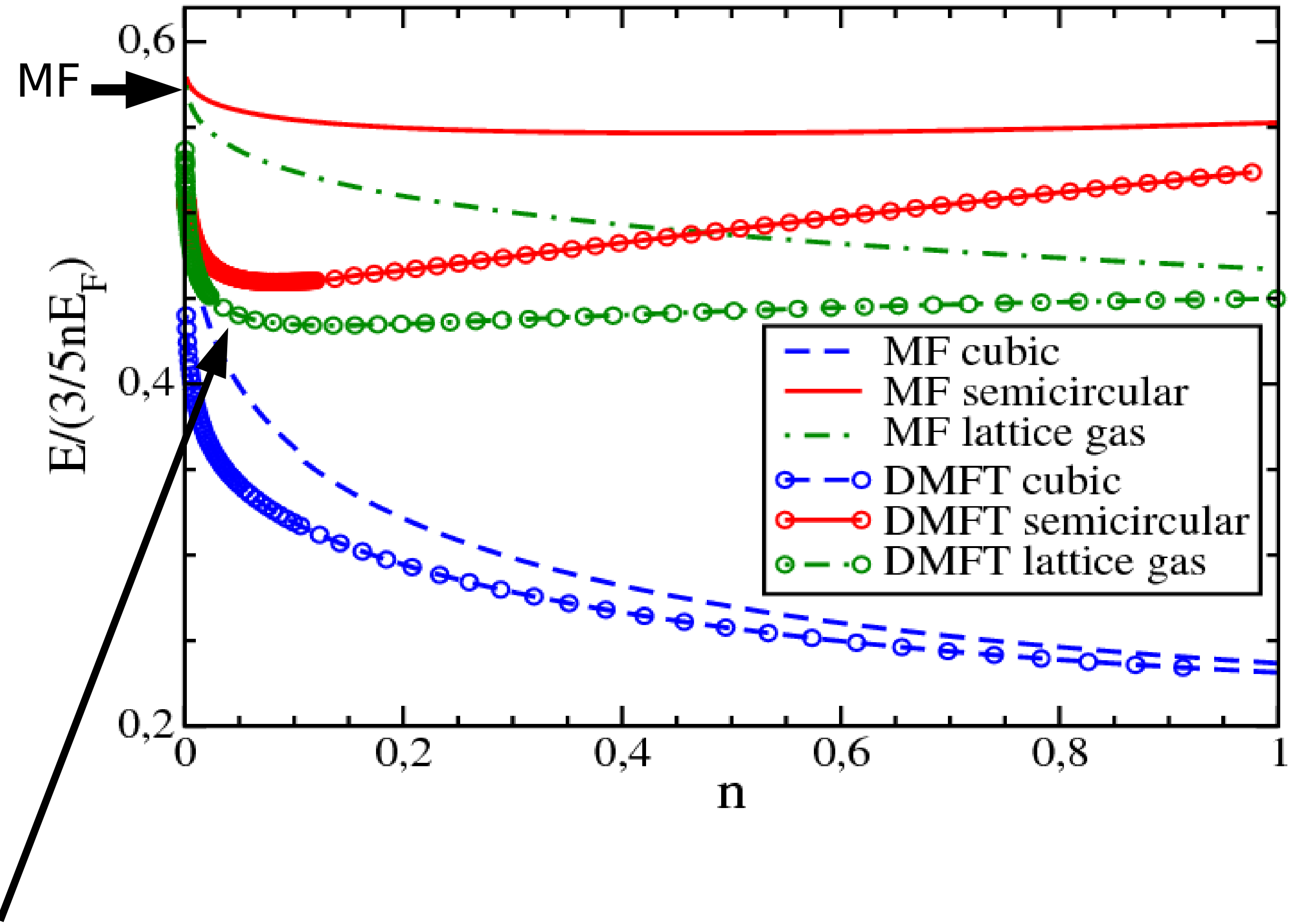

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Minima within MF are real..

- <u>Relevance of fluctuation increases</u>

$\forall n > n_{MF}$

DMFT Results full

- DMFT → MF

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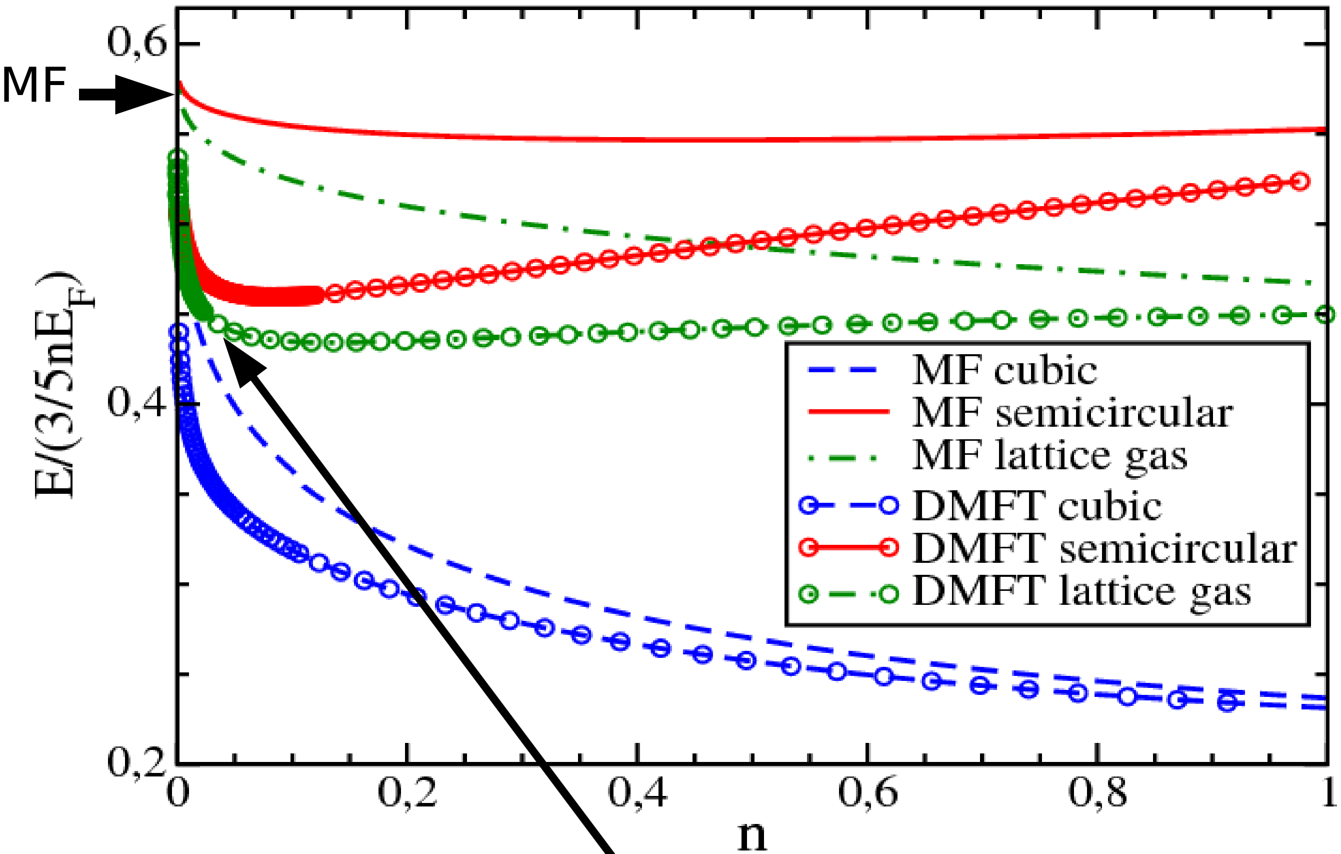
MF →



- Is the existence of this minimum only due to this effect ?

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$\forall n > n_{MF}$

At the lowest densities not trivially MF different lattices are still not-equivalent

NON-UNIVERSAL REGIME

Take-Home Message 1

- Extrapolation very tricky!

Estimates for the asymptotic slope are needed

- Cubic Lattice is the worst choice

Lattice Gas is better but not that much

CUT-OFF is intrinsical to a lattice model..

Safe extrapolation of UFG properties requires probably very low densities...

Part 2

N=2 vs N=3

I. Titvinidze & al. , New Journal of Physics 13 035013 (2011)

A. Privitera & al. , Arxiv:1010.0114

Motivation: From N=2 to N=3

- Within Ultracold Gases

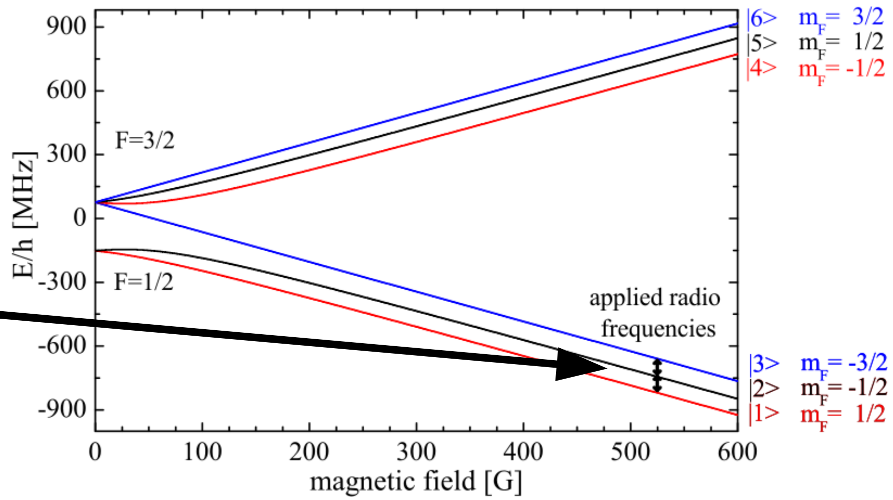
$$\sigma = \uparrow, \downarrow \longrightarrow \sigma = 1, 2, \cdots, N$$

3 Hyperfine States of Fermions

$^{6}\mathrm{Li}$ or ^{173}Yb

Loaded in a Optical Lattice

Ottenstein et. al. PRL 101,203202 (2008)



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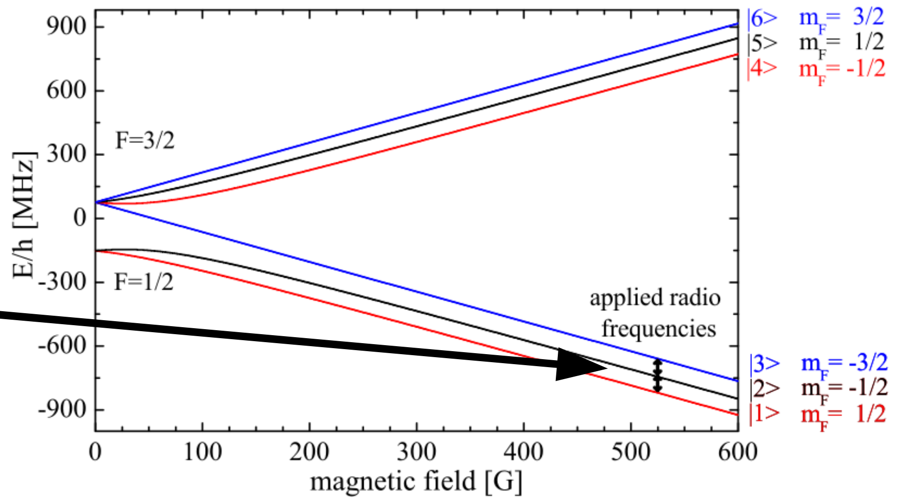
Loaded in a Optical Lattice

3 Species of Fermions in a lattice with local attractive interactions

Ottenstein et. al. PRL 101,203202 (2008)



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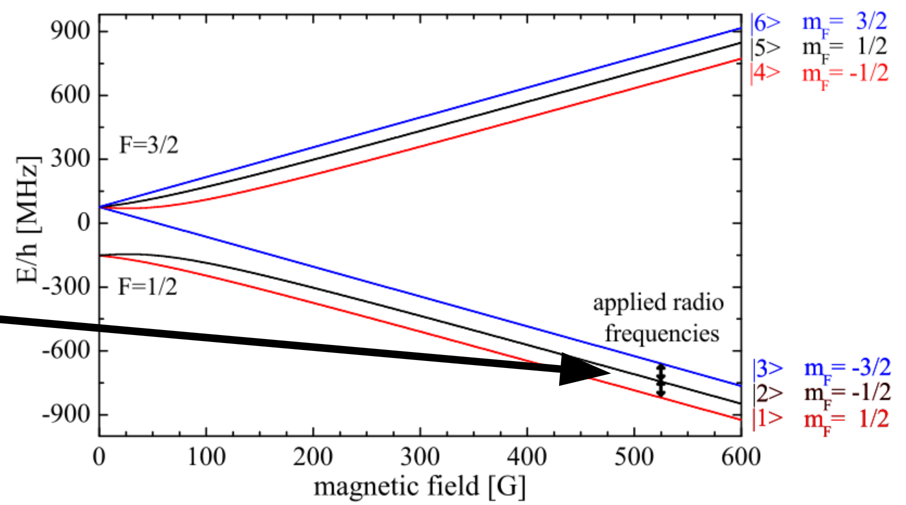
Loaded in a Optical Lattice

- **SU(2)** ⟶ **SU(3)**

BCS-BEC crossover ⟶ **trionic transition**

Ottenstein et. al. PRL 101,203202 (2008)



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3 Hyperfine States of Fermions

$^{6}\mathrm{Li}$ or ^{173}Yb

Loaded in a Optical Lattice

- **SU(2) ⟶ SU(3)**

- **Connection with the transition between**

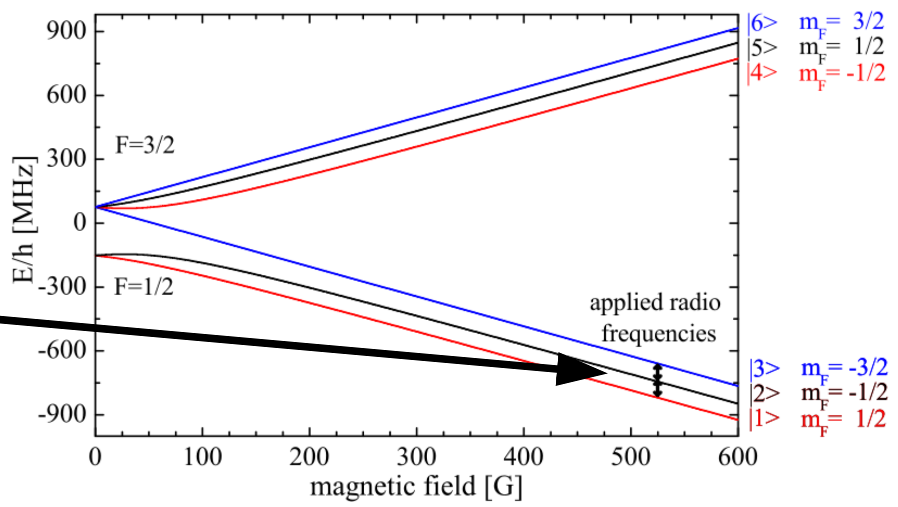
Quark SF ⟶ Barionic phase

in

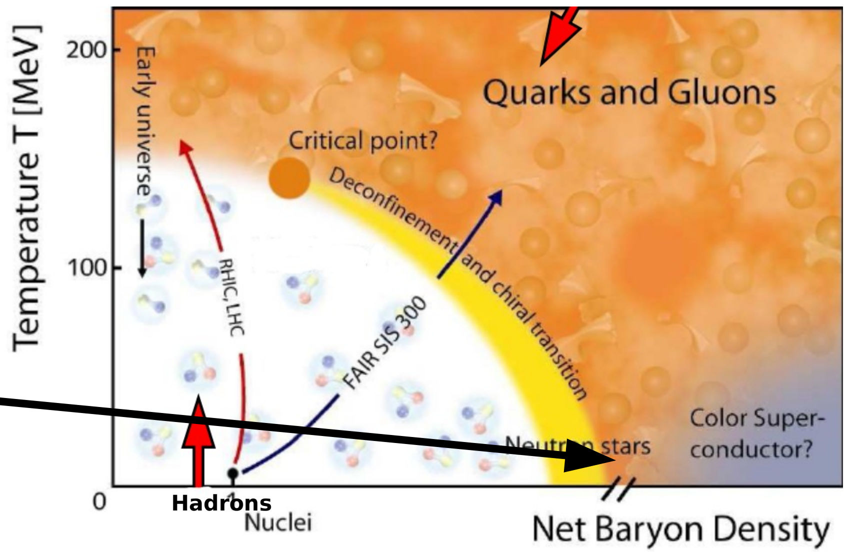
Quantum Chromo Dynamics

F. Wilczek, Nature Physics 2007

Ottenstein et. al. PRL 101,203202 (2008)

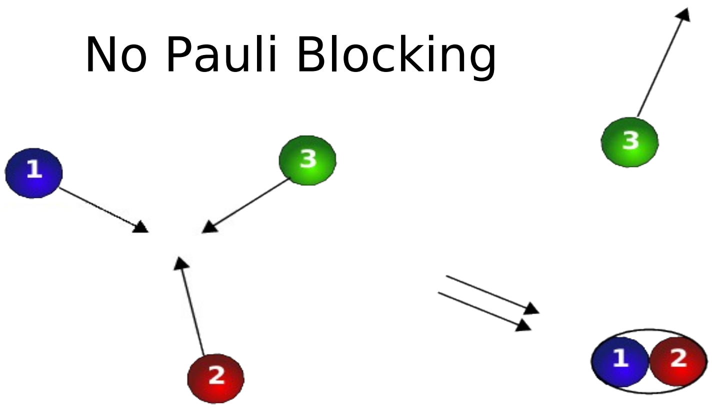


QCD phase diagram (FAIR, www.gsi.de)



3-body losses

No Pauli Blocking



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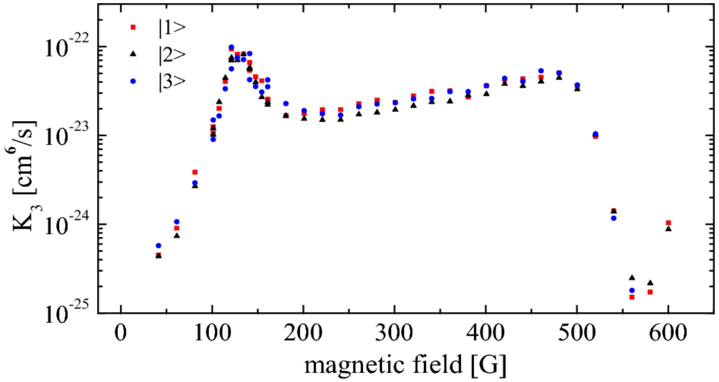
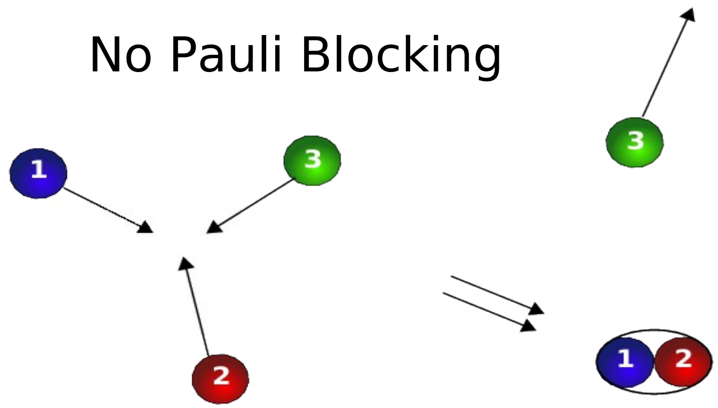
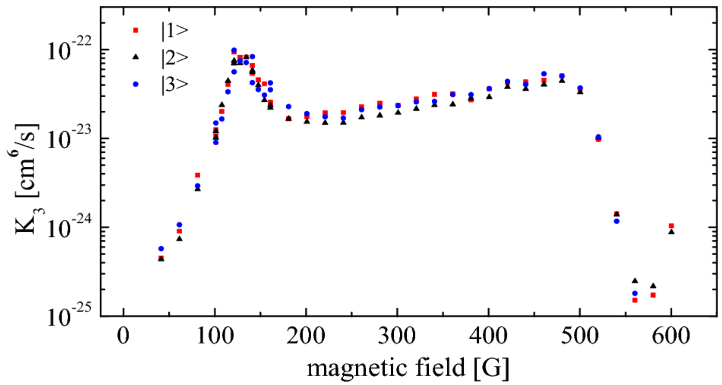


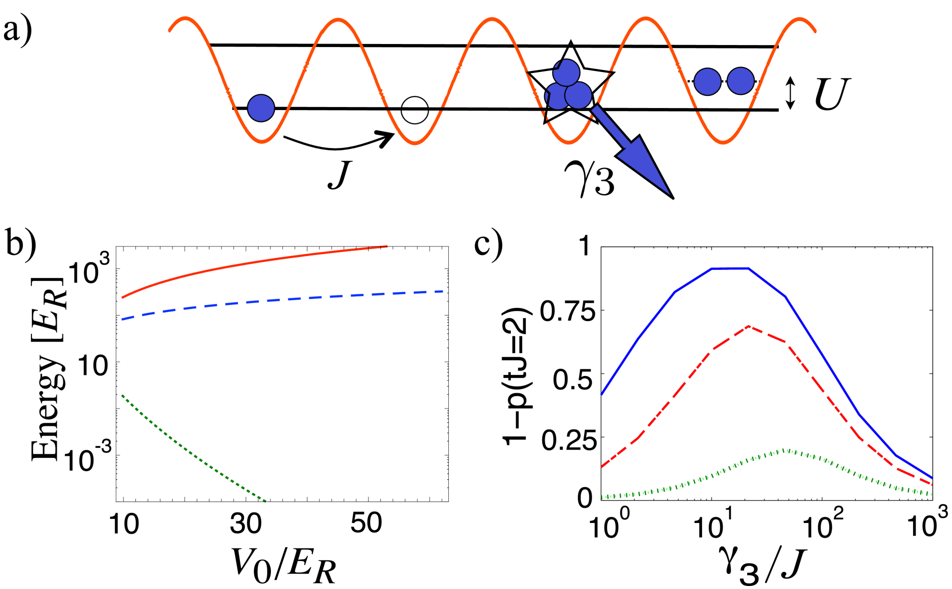
3-body losses

No Pauli Blocking



Ottenstein et. al. PRL 101,203202 (2008)





Daley et. al. PRL 102, 040402 (2009)

Strong losses regime
In a lattice

$\gamma_3/J \gg 1$

- Strong suppression of triple occupancies
- Effective strong three-body repulsion

$V n_1 n_2 n_3 \qquad V \to \infty$

Kantian et. al. PRL 103, 240401 (2009)

Model & Method

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sum_{\sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \sum_{i} \sum_{\sigma \neq \sigma'} \frac{U_{\sigma\sigma'}}{2} \hat{n}_{i\sigma} \hat{n}_{i\sigma'} - \sum_{i} \sum_{\sigma} \mu_{\sigma} \hat{n}_{i\sigma}$$

$$+V \sum_{i} \hat{n}_{i1} \hat{n}_{i2} \hat{n}_{i3}$$

$\sigma = 1, 2, 3$
$U_{\sigma\sigma'} < 0$
$V = 0, \infty$

For $U_{\sigma\sigma'} = U, \mu_{\sigma} = \mu$

SU(3) Hubbard Model

Model & Method

$$\mathcal{H} = -J\sum_{\langle ij\rangle}\sum_{\sigma}\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \sum_{i}\sum_{\sigma\neq\sigma'}\frac{U_{\sigma\sigma'}}{2}\hat{n}_{i\sigma}\hat{n}_{i\sigma'} - \sum_{i}\sum_{\sigma}\mu_{\sigma}\hat{n}_{i\sigma}$$

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$\sigma = 1,2,3$
$U_{\sigma\sigma'} < 0$
$V = 0, \infty$

For $U_{\sigma\sigma'} = U, \mu_{\sigma} = \mu$

SU(3) Hubbard Model

DMFT Self-consistency equations

$$\zeta_{\sigma} = i\omega_n + \mu_{\sigma} - \Sigma_{\sigma}(i\omega_n)$$

$$G_{\sigma}(\tau) = -\langle T_{\tau}c_{\sigma}(\tau)c^{\dagger}_{\sigma}\rangle$$

(n)

$$G_1(i\omega_n) = \int_{-\infty}^{\infty} d\varepsilon D(\varepsilon)\frac{\zeta_2^* - \varepsilon}{(\zeta_1 - \varepsilon)(\zeta_2^* - \varepsilon) + \Sigma_{SC}^2(i\omega_n)}$$

$$G_2(i\omega_n) = \int_{-\infty}^{\infty} d\varepsilon D(\varepsilon)\frac{\zeta_1^* - \varepsilon}{(\zeta_2 - \varepsilon)(\zeta_1^* - \varepsilon) + {\Sigma_{SC}^*}^2(i\omega_n)}$$

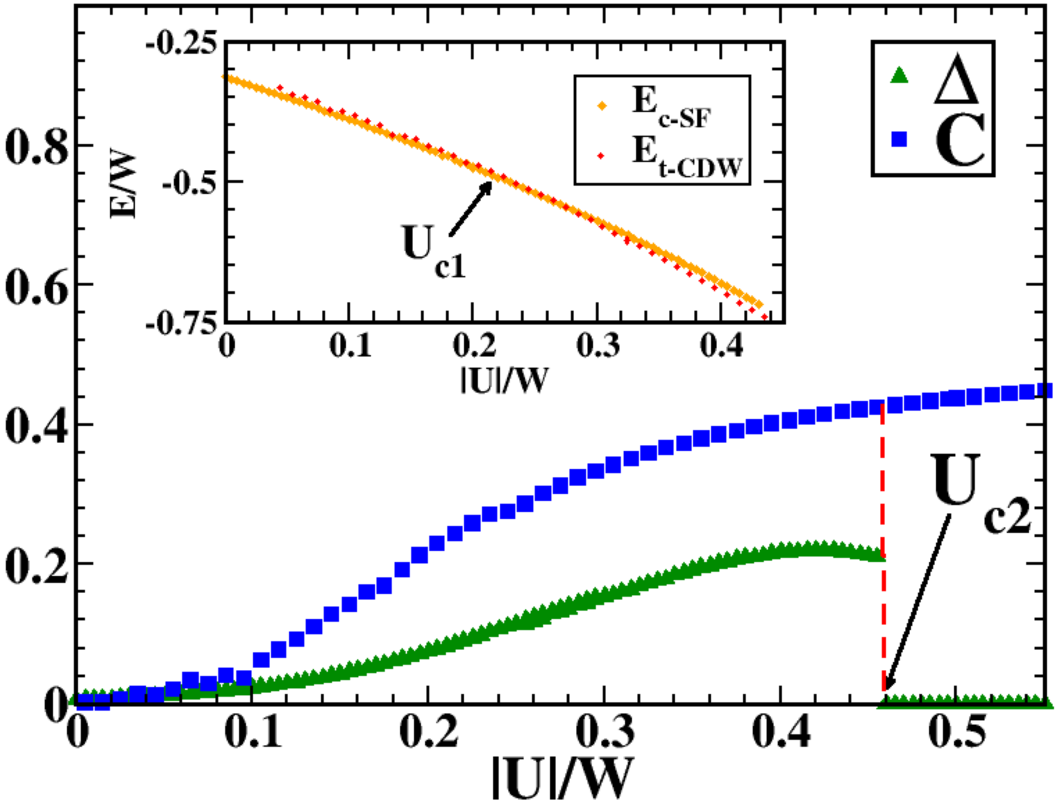
(a)

$$F(\tau) = -\langle T_{\tau}c_1(\tau)c_2\rangle$$

$$F(i\omega_n) = -\int_{-\infty}^{\infty} d\varepsilon D(\varepsilon)\frac{\Sigma_{SC}(i\omega_n)}{(\zeta_1 - \varepsilon)(\zeta_2^* - \varepsilon) + \Sigma_{SC}^2(i\omega_n)}$$

$$G_3(i\omega_n) = \int_{-\infty}^{\infty} d\varepsilon D(\varepsilon)\frac{1}{\zeta_3 - \varepsilon}$$

SU(3) Symmetric Case T=0



$$\Delta = \langle c_1 c_2 \rangle$$
$$m = n_{1,2} - n_3$$
$$C = |n_{A,B} - 1/2|$$

- Small $|U|/J$?

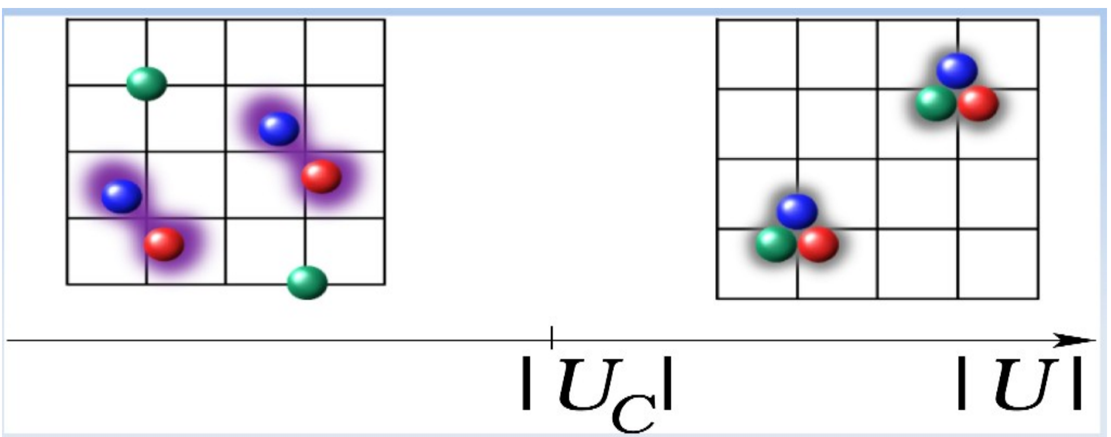
  Color Superfluid (SU(N) BCS)

  Honerkamp PRL (2004)

- Large $|U|/J$?

Transition to *trionic phase*

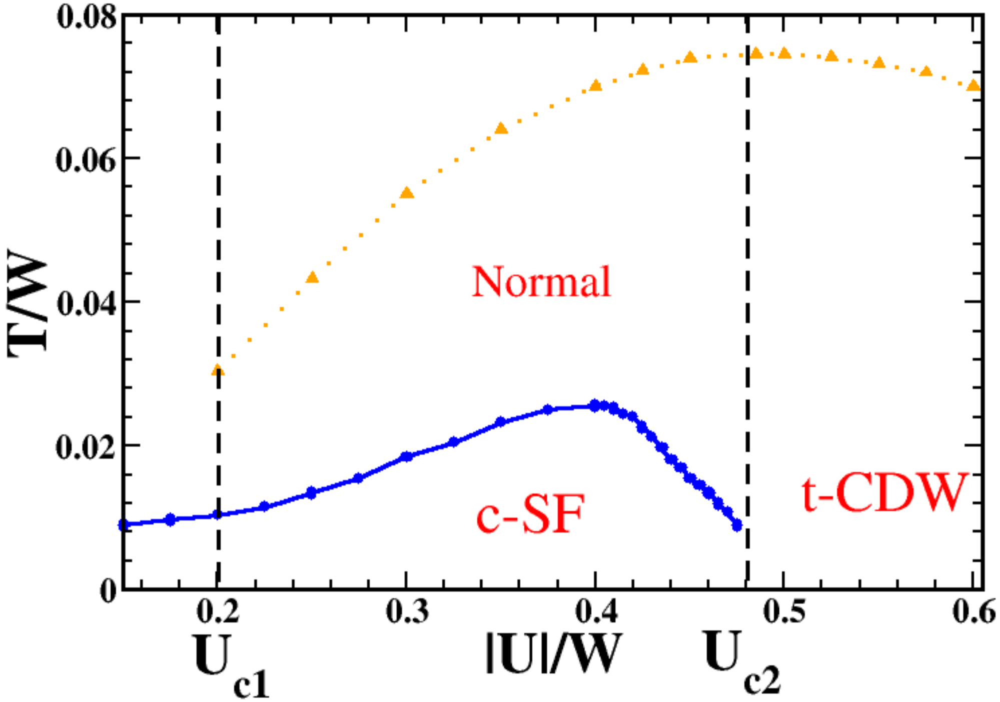
Rapp. et. al. ,PRB (2008)



(Gutzwiller) II order → *(DMFT)* I order

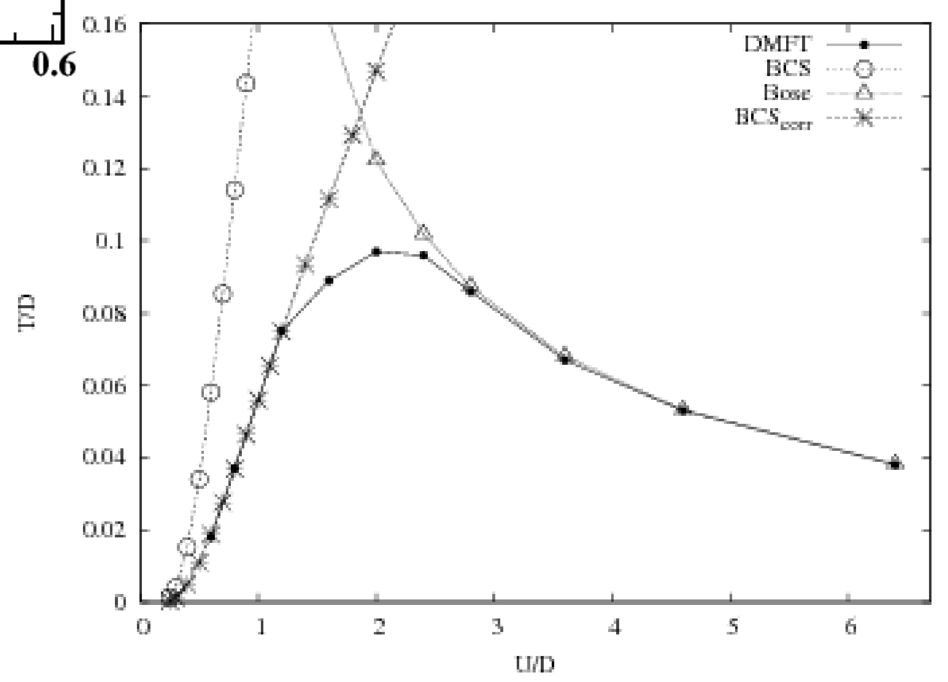
$$m = 0$$

SU(3) Case Finite T



(Confirmed by QMC simulations)

3-Species
Vs
2-Species



Phase diagram

- SF to normal (2ndorder)
- CDW to normal (2ndorder)
- Coexistence region
  (1st order transition)

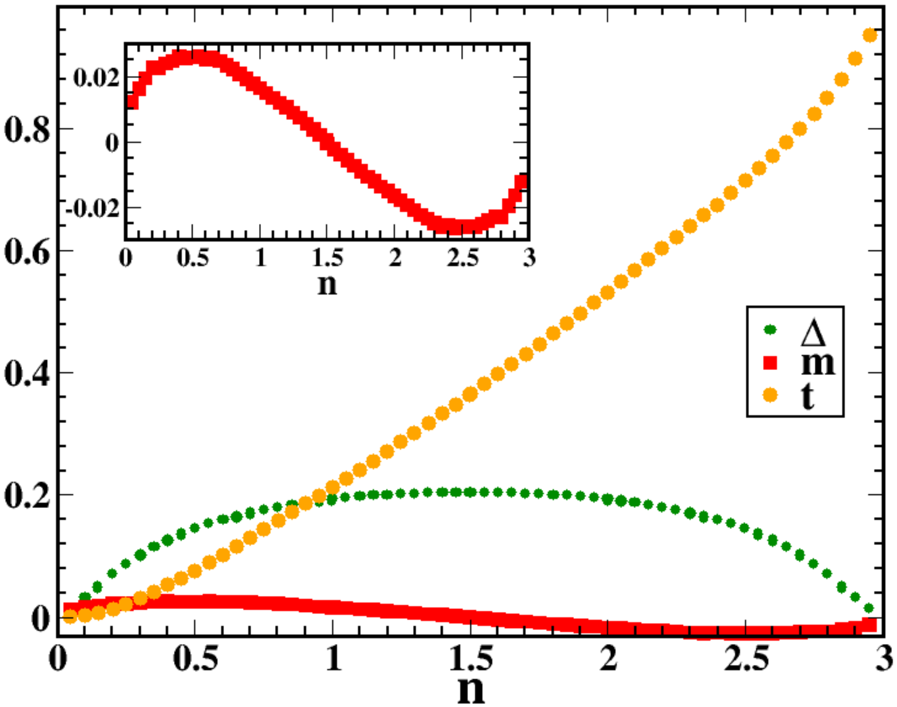
Uncommensurate Density

3d Cubic Lattice

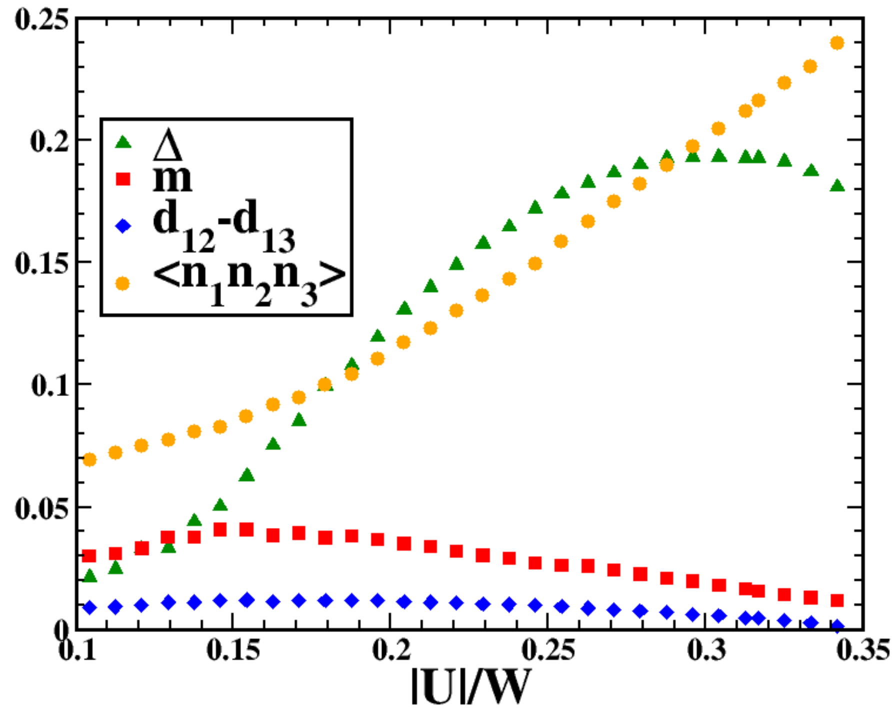
$$m = n_{1,2} - n_3$$

- c-SF is MAGNETIZED
- Non-Monotonic Magnetization

$$U = -0.312W$$



$$n_{tot} = 1$$



Including 3-Body Constraint

DMFT 3D Cubic lattice
$n_{tot} = 0.48, V = 1000J$

No Trionic Phase

Always c-SF with finite m

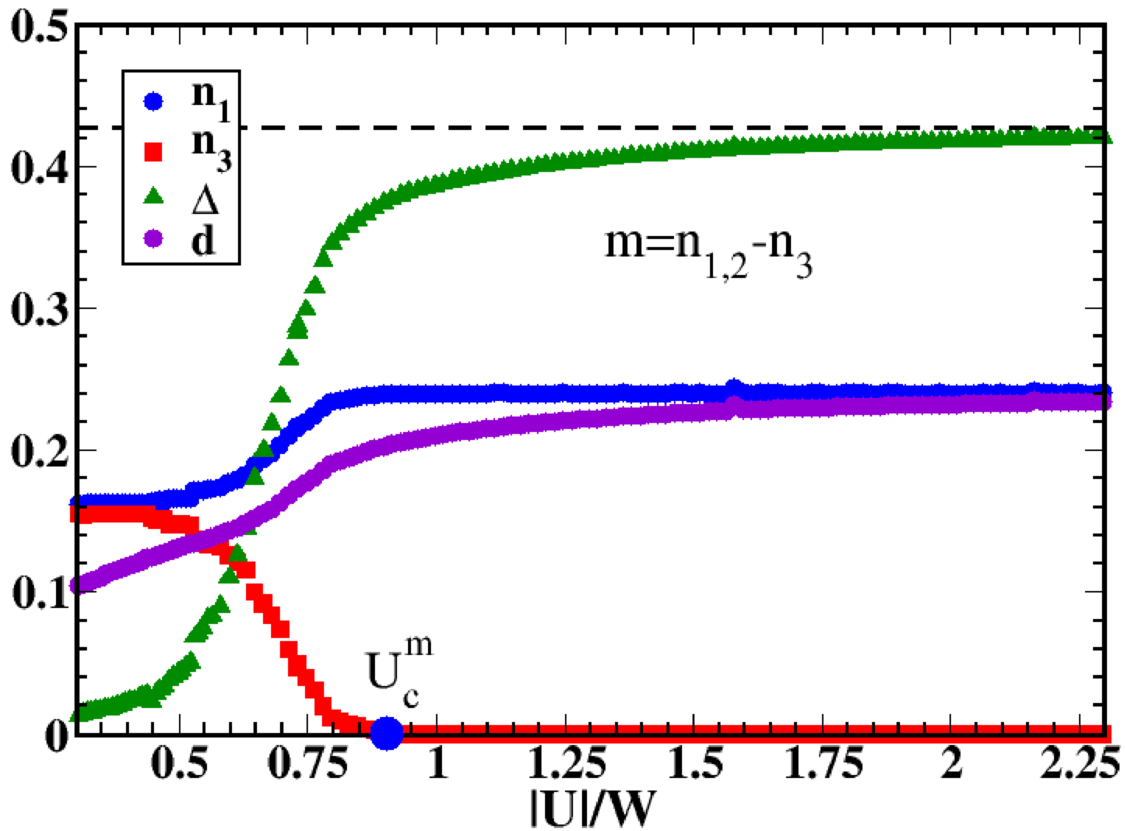
$(T = 0, W = 12J)$

- For $U > U_c^m$ system fully polarize $n_3 \longrightarrow 0$

- SU(2) limit

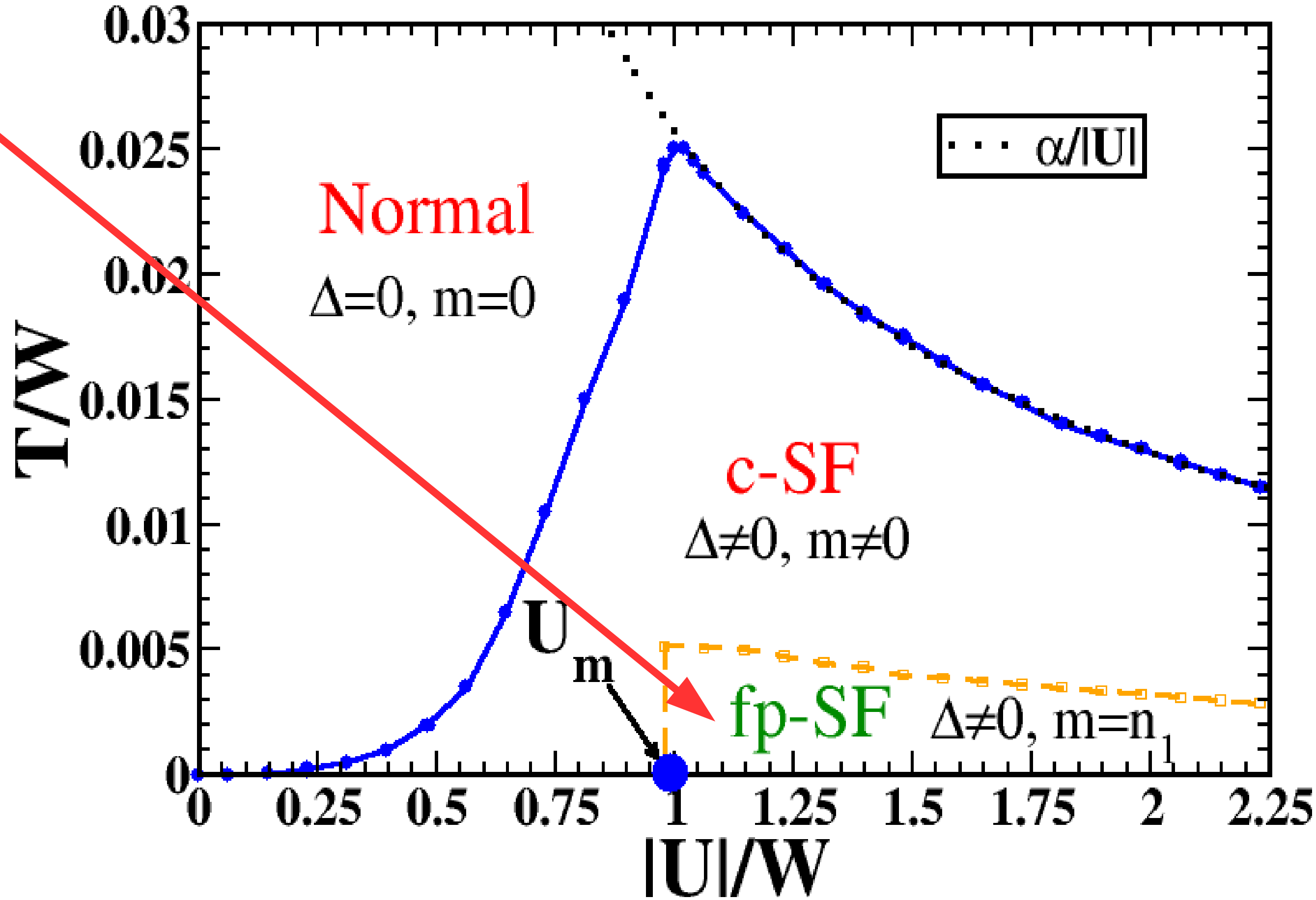
$$\lim_{|U|/W \to \infty} \Delta(U) = \Delta^{atom}_{SU(2)}$$

$$\Delta^{atom}_{SU(2)} = \frac{1}{2}\sqrt{n_1(2 - n_1)}$$



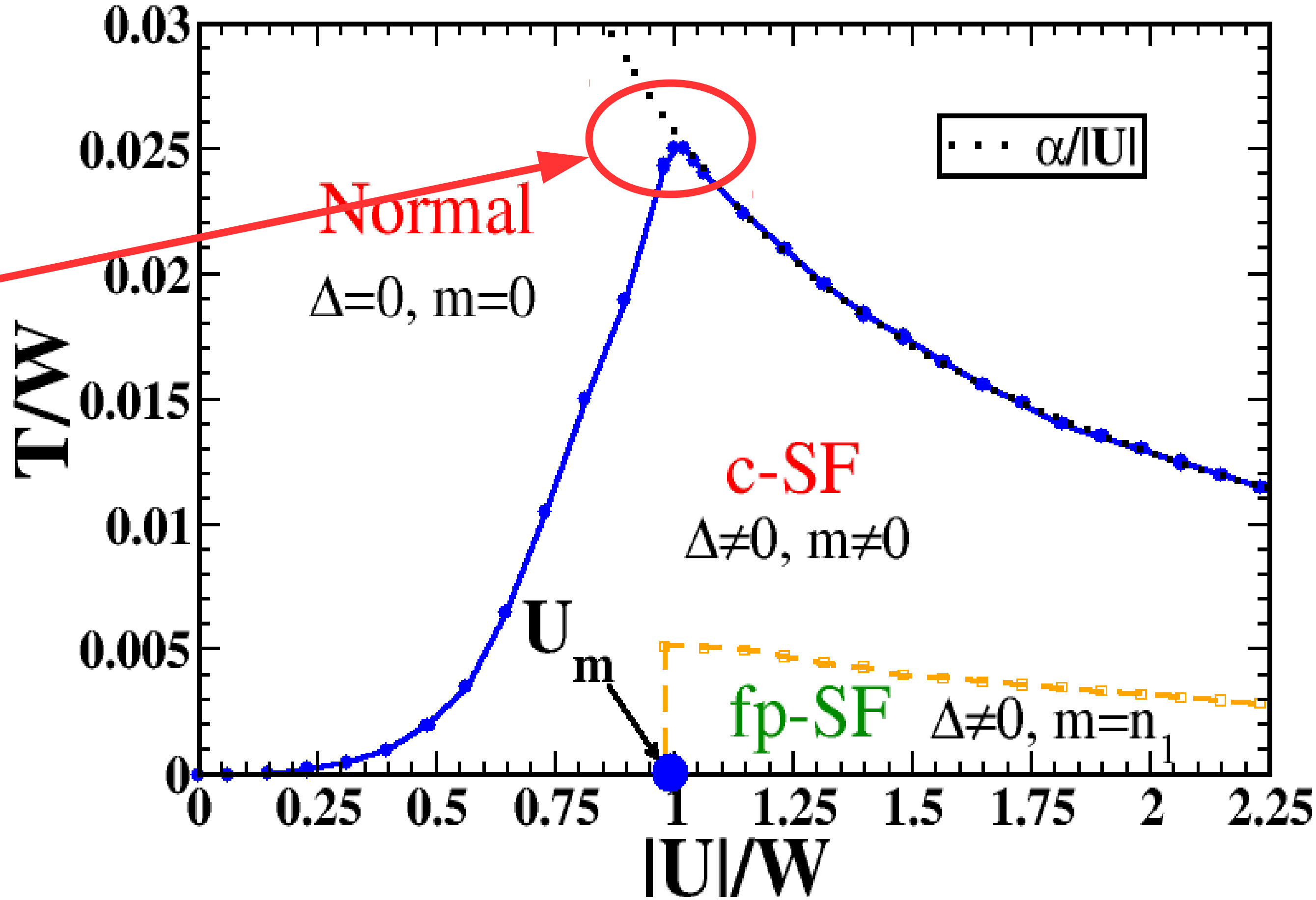
Phase Diagram

- Fully polarized superfluid for $U > U_c^m$



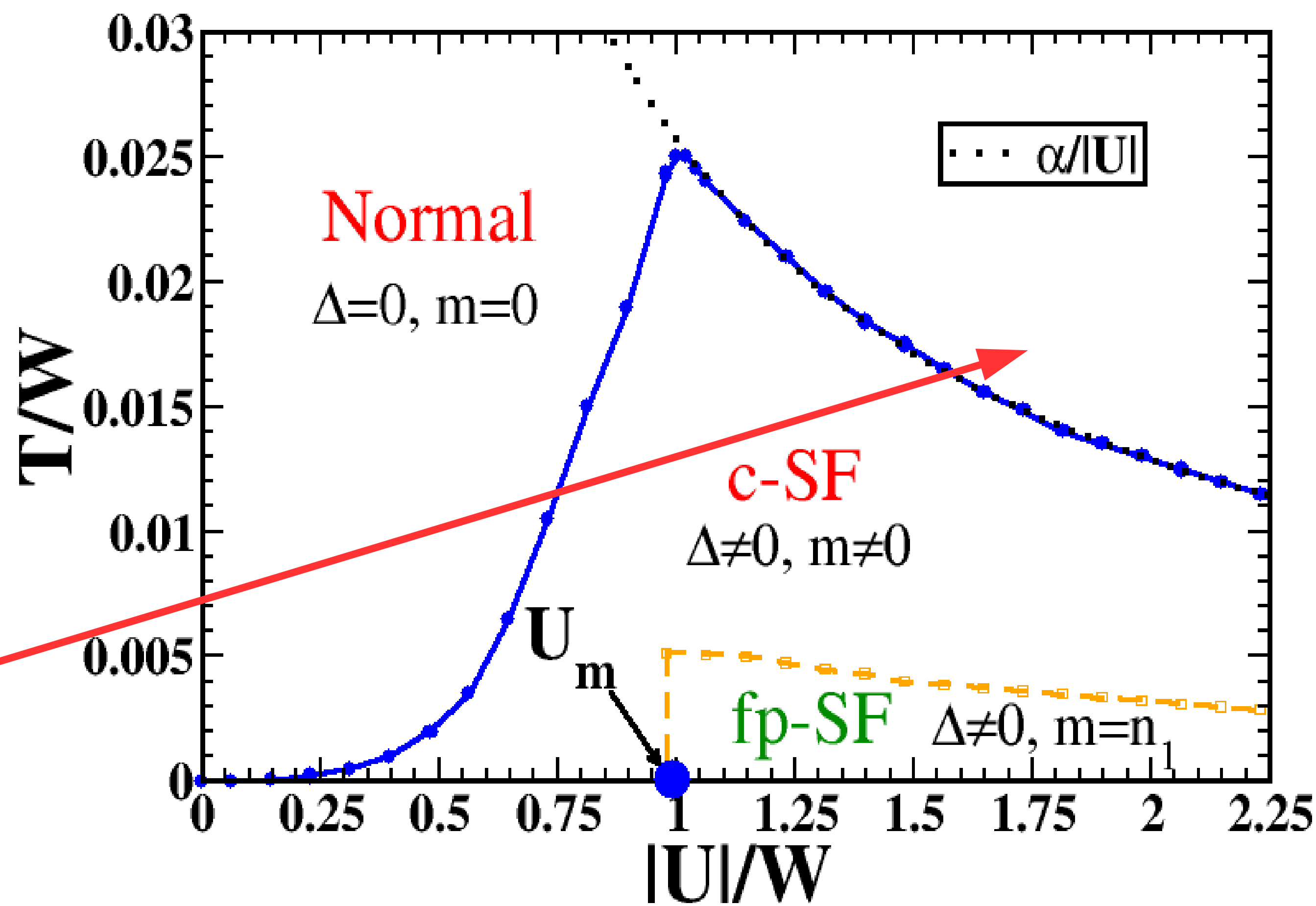
Phase Diagram

- Fully polarized superfluid for $U > U_c^m$
- Cusp in T_c ?
  Different from SU(2)
  (smooth evolution)



Phase Diagram

- Fully polarized superfluid for $U > U_c^m$
- Cusp in T_c ? Different from SU(2) (smooth evolution)
- Full SU(3) physics recovered at the transition ($m = 0$)



Magnetism & Phase Separation

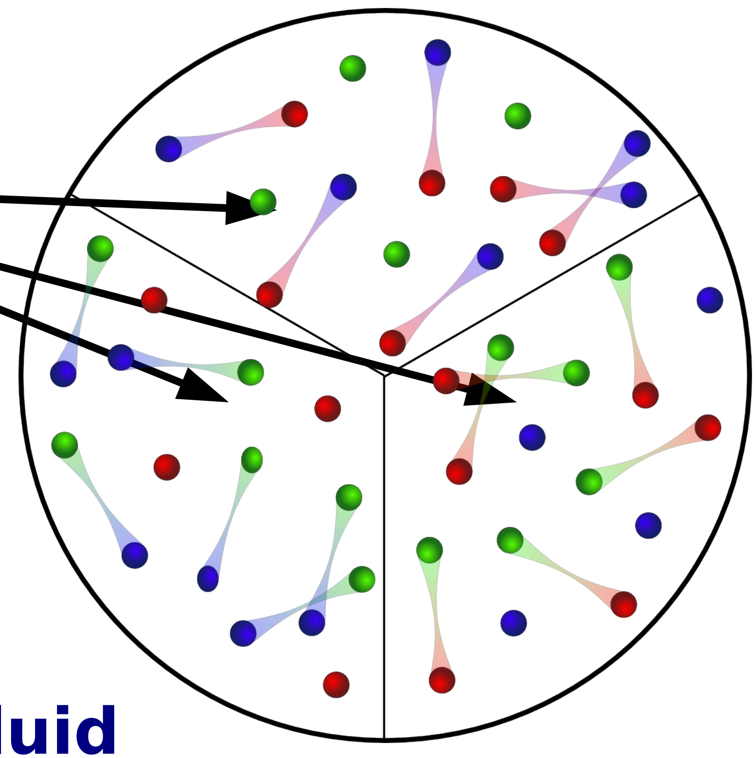
Out of half-filling → $m = n_{1,2} - n_3 \neq 0$

Color-Superfluidity always triggers magnetism

For Fixed $N_\sigma = N$? **Phase Separation**

DMFT + QMC

- Many polarized domains
- Globally non-polarized system



Oversimplified..

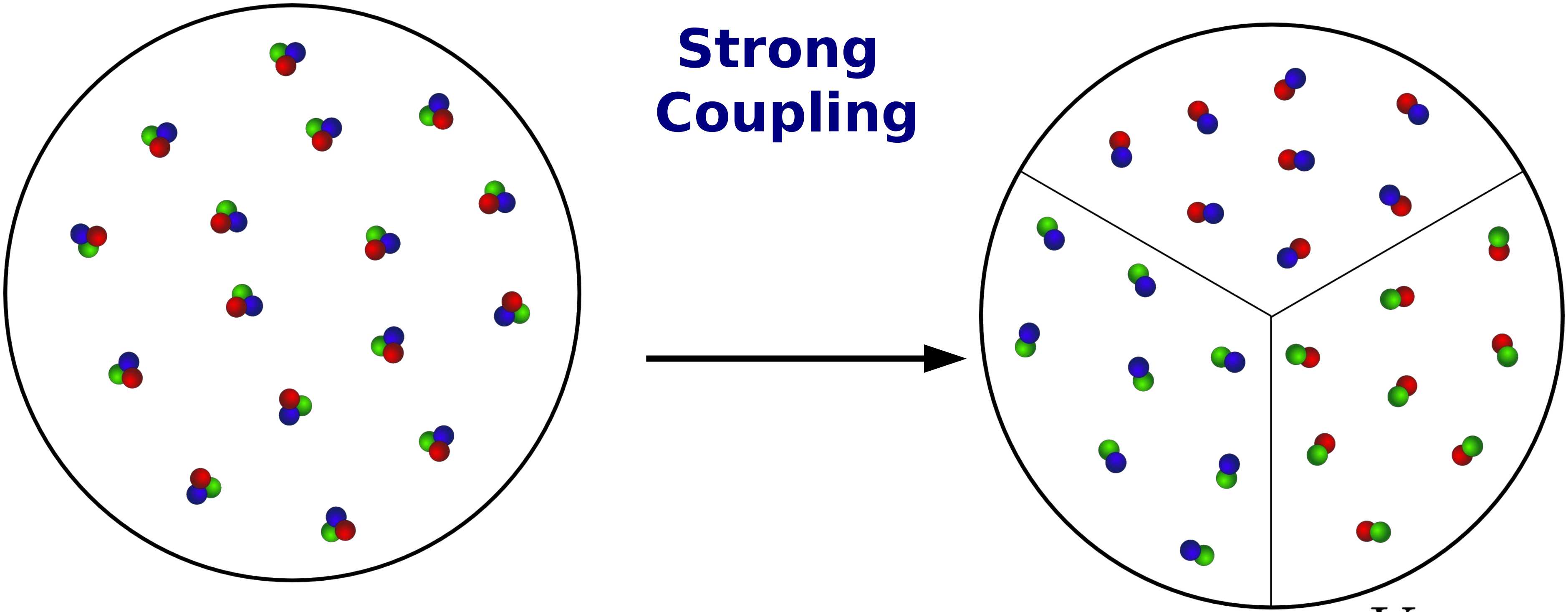
Small Coupling Color-Superfluid

Magnetism & Phase Separation

Out of half-filling → $m = n_{1,2} - n_3 \neq 0$

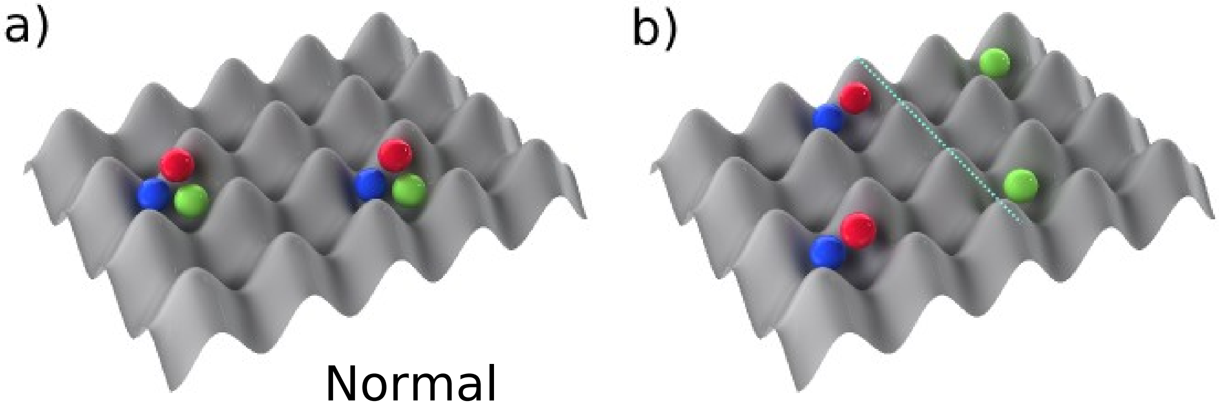
Color-Superfluidity always triggers magnetism

For Fixed $N_\sigma = N$? **Phase Separation**



$V = 0$ (No Losses) (Strong Losses) $V = \infty$

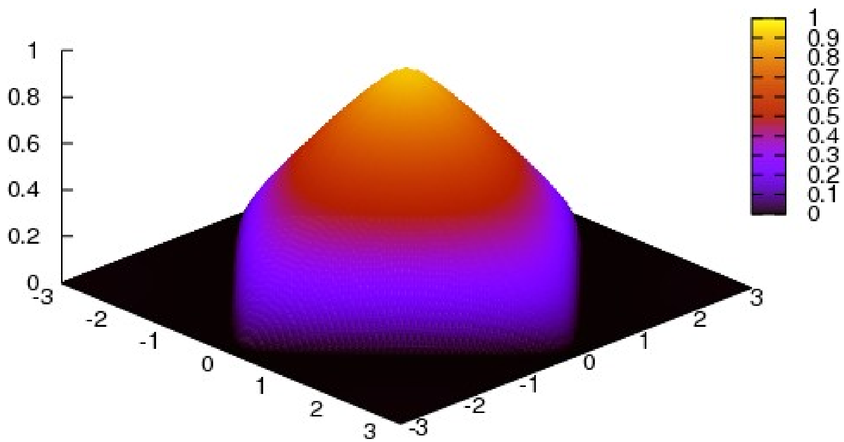
Lithium Case

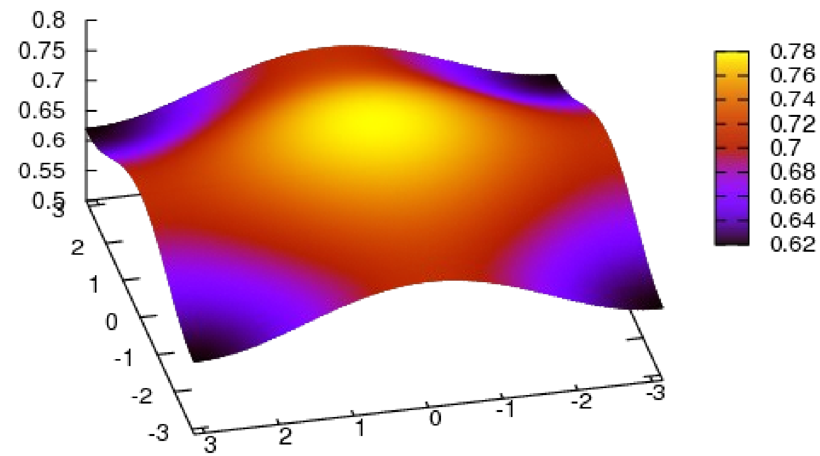


$$\bar{n}(k_x, k_y) = \int \frac{dk_z}{2\pi} n(\mathbf{k})$$

Normal

Superfluid





- Strong coupling superfluid $n^{SF}(k_x, k_y) \simeq const$
- Normal component $n^{norm}(k_x, k_y) = 0$ for large $\mathbf{k}$

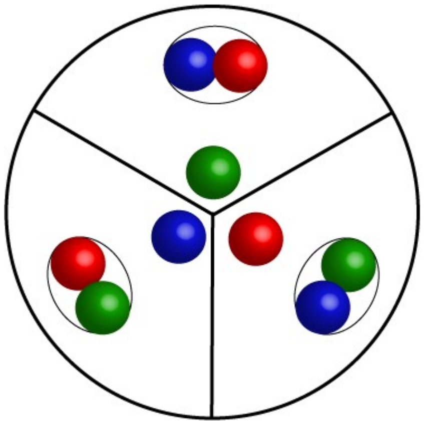
Take-Home Message 2

- Without constraint $(V = 0)$:
  Phase Transition c-SF ⟶ trionic phase

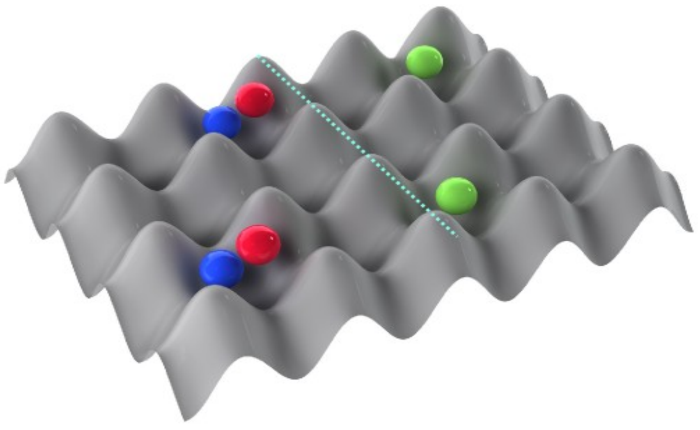
- Effect of three-body losses:
  No Trionic Phase; Fully Polarized c-SF for large $|U|$

- C-SF vs Magnetization: Phase Separation

$SU(3)$



$^6\mathrm{Li}$



Effective Range