QUANTUM PHASE TRANSITIONS IN ITINERANT FERMION SYSTEMS

Pawel Jakubczyk
MPI Stuttgart

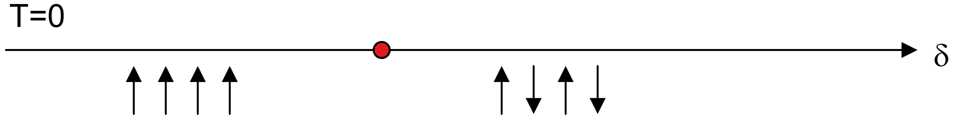
Outline

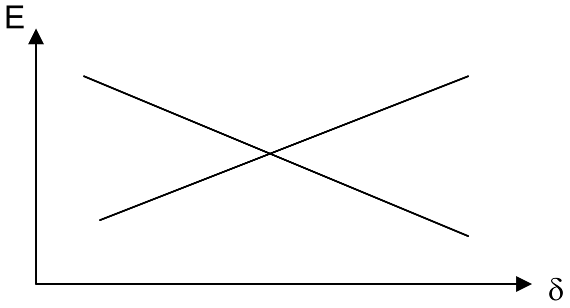
- Quantum phase transitions – generalities
- Standard treatment (Hertz – Millis theory)

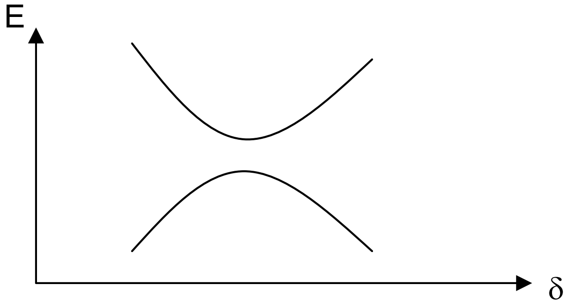
- Criticisms and possible improvements
- Our contributions so far …

Quantum phase transitions

Hamiltonian H(δ)







Transverse-field Ising model

Quantum Ising Hamiltonian

$$H_I = -J\delta \sum_i \sigma_i^x - J \sum_{<ij>} \sigma_i^z \sigma_j^z \qquad (J, \delta > 0)$$

For δ=*0* this is the classical Ising Hamiltonian

Influence of magnetic field: $\sigma_i^x = |\uparrow\rangle_i \langle\downarrow|_i + |\downarrow\rangle_i \langle\uparrow|_i$

The limit $\delta << 1$

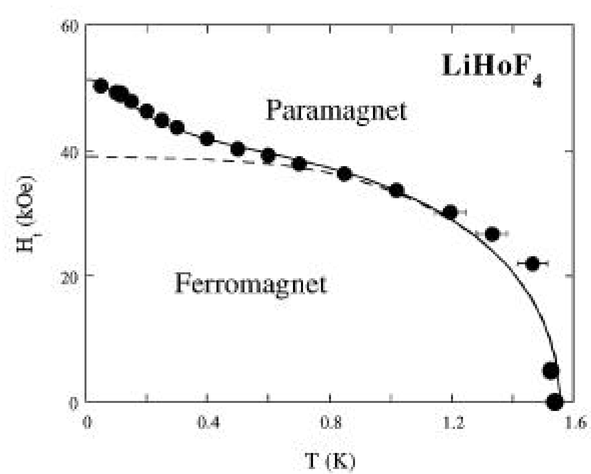
$$\left|\uparrow\right\rangle = \prod_i \left|\uparrow\right\rangle_i$$

$$\left|\downarrow\right\rangle = \prod_i \left|\downarrow\right\rangle_i$$

The limit $\delta >> 1$

$$|0\rangle = \prod_i |\rightarrow\rangle_i$$

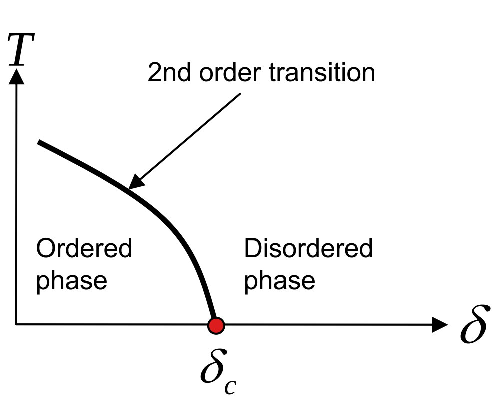
$$|\rightarrow\rangle_i = \left(|\uparrow\rangle_i + |\downarrow\rangle_i\right)/\sqrt{2}$$

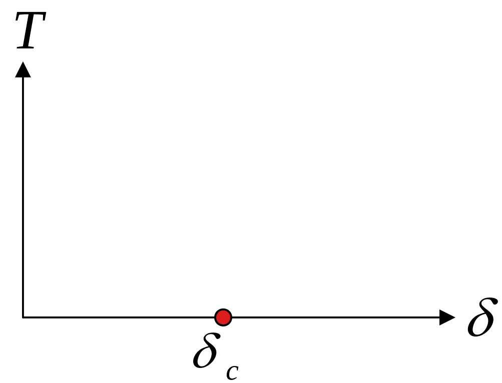


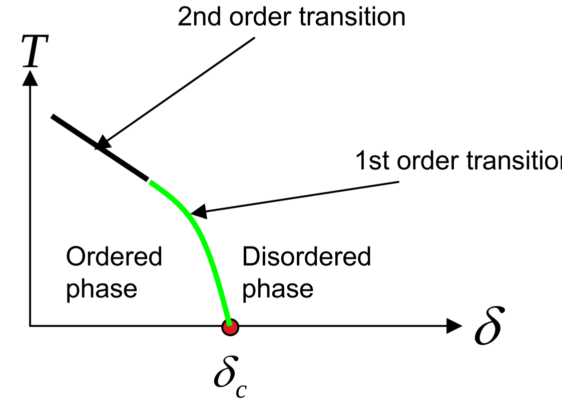
(Bitko et. al. 1996)

A phase transition occurs at $\delta = \delta_c > 0$

Possible phase diagrams:







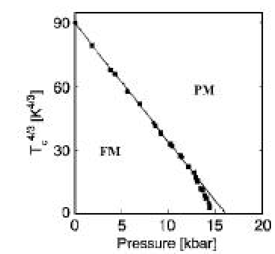
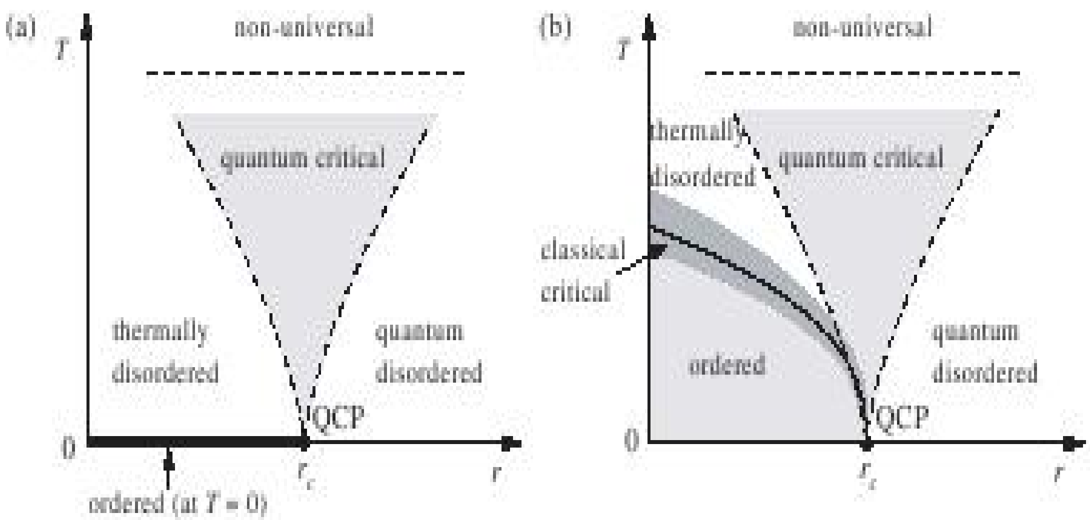
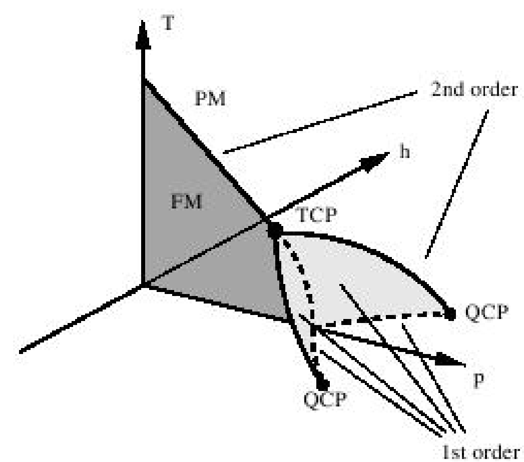


FIG. 18. Phase diagram of MnSi. These are the same data as in Fig. 14, scaled to display the relation given in Eq. (4.19). The tricritical point separating second- and first-order transitions coincides with the point at which the scaling breaks down. Adapted from Pfleiderer *et al.*, 1997.





Where‘s the difference?

$$Z = \exp(-\beta H)$$

$$H = H_{kin} + H_{pot}$$

$$Z = Z_{kin} Z_{pot}$$

-only for classical systems

QPT in systems of itinerant fermions

Hertz (1976)

- effective action ‚derived‘ from a microscopic model
- critical behaviour at T=0

Millis (1993)

- extension (and correction) of Hertz for T>0
- scaling regimes in the disordered phase

Hertz (1976)

Partition function:

$$Z = \int D[\psi^*\psi]\exp\left[-\int_0^\beta d\tau L(\psi^*,\psi)\right]$$

$$L(\psi^*,\psi) = \sum_{i,\sigma}\psi^*_{i,\sigma}(\partial_\tau - \mu)\psi_{i,\sigma} - \sum_{i,i',\sigma} t_{i-i'}\psi^*_{i,\sigma}\psi_{i',\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow} \qquad n_{i\sigma} = \psi^*_{i\sigma}\psi_{i\sigma}$$

$$U\sum_i n_{i\uparrow}n_{i\downarrow} = \frac{U}{4}\sum_i\left[\xcancel{(n_{i\uparrow}+n_{i\downarrow})^2} - (n_{i\uparrow}-n_{i\downarrow})^2\right]$$

charge　　　　spin

$$1 = \sqrt{\frac{U}{4\pi}}\int_{-\infty}^{\infty} d\varphi \exp\left[-\frac{U}{4}(\varphi - m_i)^2\right]$$

$$Z = \int D[\psi^*\psi]\int D\varphi \exp\left[-\int_0^\beta d\tau L(\psi^*,\psi,\varphi)\right]$$

$$L(\psi^*,\psi,\varphi) = \sum_{i,\sigma}\psi^*_{i,\sigma}(\partial_\tau - \mu)\psi_{i,\sigma} - \sum_{i,i',\sigma} t_{i-i'}\psi^*_{i,\sigma}\psi_{i',\sigma} + \frac{U}{4}\sum_i\varphi_i^2 + \frac{U}{2}\sum_i\varphi_i(n_{i\uparrow}-n_{i\downarrow})$$

Integrating the fermions out:

$$\int \prod_i d\psi_i^* d\psi_i \exp\left(-\psi_i^* H_{ij} \psi_j\right) = \det H$$

$$Z = \int D\varphi \exp\left[-\left(\frac{U}{4} \int_0^\beta d\tau \sum_i \varphi_i^2 - Tr \log M \right) \right]$$

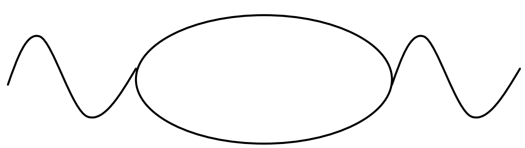
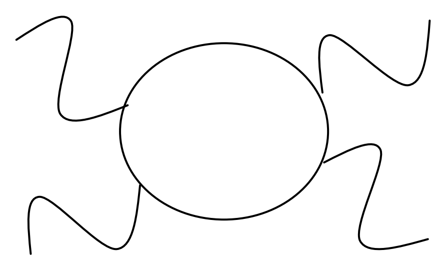
In momentum-frequency representation:

$$M_{(\bar{k},\omega_n,\sigma),(\bar{k}',\omega_{n'},\sigma')} = -G_0^{-1}(\bar{k},\omega_n) + V(\sigma, \bar{k}-\bar{k}', \omega_n - \omega_{n'})$$

where

$$G_0^{-1}(\bar{k},\omega_n) = i\omega_n - (\varepsilon_{\bar{k}} - \mu)$$
$$V(\sigma, \bar{k}-\bar{k}', \omega_n - \omega_{n'}) \propto \sigma\varphi(\bar{k}-\bar{k}', \omega_n - \omega_{n'})$$

$$Tr \log M = Tr \log(-G_0^{-1} + V) = Tr \log(-G_0^{-1}) + Tr \log(1 - G_0 V) = Tr \log(-G_0^{-1}) - \sum_{n=1}^{\infty} \frac{1}{n} Tr(G_0 V)^n$$

$Tr \log M =$  +  + $\cdots$

The effective action up to quadratic order:

$$S_{eff}^{(2)} = \sum_{\bar{q},\omega_n} \frac{U}{4}\left(1 - U\chi_0(\bar{q},\omega_n)\right)\varphi(\bar{q},\omega_n)\varphi(-\bar{q},-\omega_n)$$

where $\chi_0(\bar{q},\omega_n) = \frac{1}{N}\sum_{\bar{k}} \frac{f(\xi_{\bar{k}+\bar{q}}) - f(\xi_{\bar{k}})}{i\omega_n - \xi_{\bar{k}+\bar{q}} + \xi_{\bar{k}}}$ (the Matsubara sums were done using contour integrals)

and $\xi_{\bar{k}} = \varepsilon_{\bar{k}} - \mu$

$$S_{eff}^{(2)} \approx \sum_{\bar{q},\omega_n} \frac{U}{4}\left[1 - U\chi_0(\bar{q},0) + C\frac{|\omega_n|}{v_F q'}\right]\varphi(\bar{q},\omega_n)\varphi(-\bar{q},-\omega_n)$$

$$q' = \begin{cases} q & \text{ferromagnet} \\ 1 & \text{antiferromagnet} \end{cases}$$

- For the ferromagnet put $\chi_0(\bar{q},0) \approx \chi_0(0,0) - aq^2$
- For the antiferromagnet: $\chi_0(\bar{q},0) \approx \chi_0(\bar{Q},0) - aq^2$

Leading to $S_{eff}^{(2)} \approx \sum_{\bar{q},\omega_n}\left[q^2 + \delta + \frac{|\omega_n|}{q'}\right]\varphi(\bar{q},\omega_n)\varphi(-\bar{q},-\omega_n)$

For the quartic coupling one just puts a constrant (i.e. evaluates it at *q=0* or *q=Q).*

Millis (1993)

$$S_{eff} \approx \sum_{\bar{q},\omega_n} \left[q^2 + \delta + \frac{|\omega_n|}{q'} \right] \varphi(\bar{q},\omega_n)\varphi(-\bar{q},-\omega_n) + u\int_0^\beta d\tau \int d^d r \left[\varphi(\bar{r},\tau)\right]^4$$

Parameters specifying the model: δ, u, T and the cutoffs Λ , Γ

RG procedure:

- integrate out modes from the shell $\Lambda / b \leq q \leq \Lambda$ and sum over frequencies
- rescale momenta to restore the cutoff to the original value, field and temperature to keep the coefficient in the propagator constrant
- linearize around the (unstable) Gaussian fixed point *T*=δ=*u*=*0*
- deduce the phase diagram from the bahaviour of *T* and *u* under scaling

$$\frac{dT(b)}{d\log b} = zT(b)$$

$$\frac{d\delta(b)}{d\log b} = 2\delta(b) + u(b) f^{(2)}\big(T(b), \delta(b)\big)$$

$$\frac{du(b)}{d\log b} = \left[4-(d+z)\right]u(b) - u(b)^2 f^{(4)}\big(T(b), \delta(b)\big)$$

Sketch of the derivation:

Gaussian case:

$$S_G = \frac{1}{2}\sum_{\bar{q},\omega_n} G_0^{-1}(\bar{q},\omega_n)\varphi(\bar{q},\omega_n)\varphi(-\bar{q},-\omega_n)$$

$$f_G = -(\beta V)^{-1}\log Z_G = (2\beta V)^{-1}\sum_{\bar{q},\omega_n}\log\left[\delta + q^2 + |\,\omega_n\,|/q'\right] + const$$

$$\downarrow$$

$$f_G \propto \int d^d q \int d\varepsilon \coth\left(\varepsilon/2T\right)\arctan\left(\frac{\varepsilon/q'}{\delta + q^2}\right)$$

Integrate out the (safe) modes $\Lambda/b \le q \le \Lambda$ and rescale the variables to recover a form of f_G as the initial one.

$$\int_0^{\Lambda} d^d q(\ldots) = \int_0^{\Lambda/b} d^d q(\ldots) + \int_{\Lambda/b}^{\Lambda} d^d q(\ldots)$$

$$f_G = f_G^{'} + f_\Lambda$$

$$\bar{q} \to \bar{q}/b$$
$$\delta \to \delta/b^2$$
$$\varepsilon \to \varepsilon/b^z$$
$$T \to T/b^z$$

where z is determined by the condition

$$(q/b)'\,b^{2-z} = q'$$

Scaling equations: $\frac{dT(b)}{d\log b} = zT(b)$

$$\frac{d\delta(b)}{d\log b} = 2\delta(b)$$

$z = 2$ (antiferromagnet)

$z = 3$ (ferromagnet)

Case with *u>0*

$$e^{-S_{eff}(\varphi_<)} = \int D\varphi_> e^{-S(\varphi_< + \varphi_>)} = \int D\varphi_> e^{-S_G(\varphi_<) - S_G(\varphi_>) - S_{\text{int}}(\varphi_> + \varphi_<)} = e^{-S_G(\varphi_<)} Z_> \left\langle e^{-S_{\text{int}}(\varphi_> + \varphi_<)} \right\rangle_{>,G}$$

where

$$Z_> = \int D\varphi_> e^{-S_G(\varphi_>)}$$

$$\langle A \rangle_{>,G} = Z_>^{-1} \int D\varphi_> A e^{-S_G(\varphi_>)}$$

Now expand in interaction:

$$\left\langle e^{-S_{\text{int}}(\varphi_> + \varphi_<)} \right\rangle_{>,G} = 1 - \langle S_{\text{int}} \rangle_{>,G} + \frac{1}{2} \langle S_{\text{int}}^2 \rangle_{>,G} - \ldots \approx e^{\left[-\langle S_{\text{int}} \rangle_{>,G} + \frac{1}{2} \left(\langle S_{\text{int}}^2 \rangle_{>,G} - \langle S_{\text{int}} \rangle_{>,G}^2 \right) \right]}$$

After doing the interaction and rescaling, one arrives at the flow equations:

$$\frac{dT(b)}{d\log b} = zT(b)$$

$$\frac{d\delta(b)}{d\log b} = 2\delta(b) + u(b) f^{(2)}(T(b), \delta(b))$$

$$\frac{du(b)}{d\log b} = [4 - (d+z)] u(b) - u(b)^2 f^{(4)}(T(b), \delta(b))$$

Analysis of the flow equations (d>2)

$$\frac{dT(b)}{d\log b} = zT(b)$$

$$\frac{d\delta(b)}{d\log b} = 2\delta(b) + u(b) f^{(2)}(T(b),\delta(b))$$

$$\frac{du(b)}{d\log b} = [4-(d+z)]u(b) - u(b)^2 f^{(4)}(T(b),\delta(b))$$

- unstable Gaussian fixed point at T=u=δ=0
- upper critical dimension for the QPT d_u=4-z
- T(b) increases under scaling and for T>1 (upper cutoff) crossover to classical behaviour v(b)=u(b)T(b)

$\delta(b) \sim 1$ - scaling stops

- if this occurs with T(b) small – quantum regime

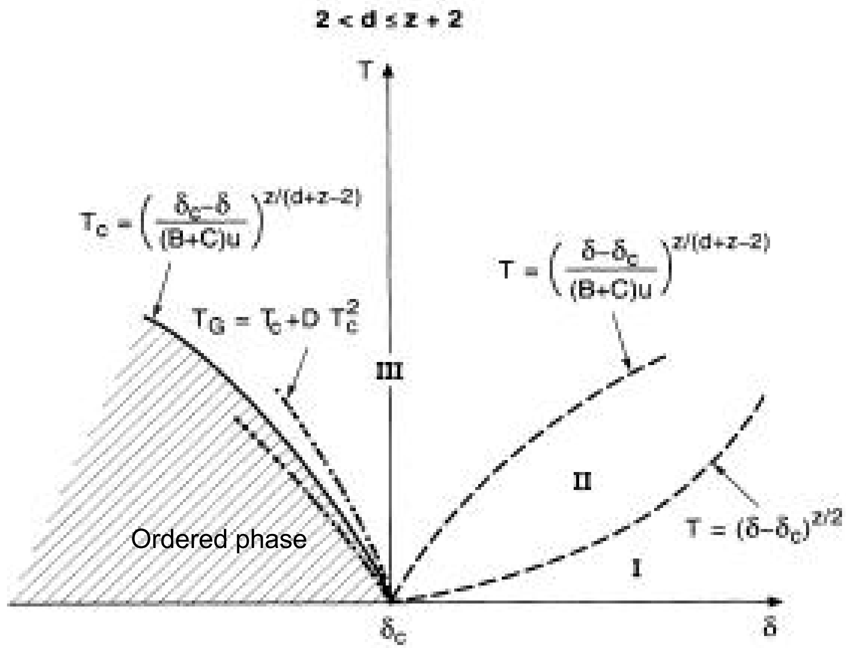
$$T << (\delta - \delta_c)^{z/2}$$

- otherwise: divide the flow into quantum (T(b)<1) and classical part (T(b)>1)
  - if δ(b)<1 with v(b)~1 – non-Gaussian regime ⟶ Ginzburg criterion

$$T_G \sim (\delta - \delta_c)^{z/(d+z-2)}$$ (additional logs in d=2)

  - from the point of view of ξ(δ,T), one identifies two more subregimes

Phase diagram (disordered phase, d>2)



(Millis, 1993)

I – disordered quantum regime
II – perturbative classical regime
III – classical Gaussian (quantum critical) regime

Nonlocal vertices and power counting

Antiferromagnet, d=2

$$S_H = \frac{1}{2}\int d\omega d^2 q \chi^{-1}(\omega, q)\varphi^2{}_{\omega,q} + \sum_{n=2}^{\infty}\int (d\omega d^2 q)^{2n-1} b_{2n}(\varphi_{\omega,q})^{2n}$$

$$[\omega] = z$$

$$[\varphi^2_{\omega,q}] = -4 - z$$

$$[b_{2n}] = 2 - (n-1)z$$

A claim: correct form of the n-th term in the effective action:

$$\sim g_{2n}\int (d\omega d^2 q)^{2n-1}\frac{|\omega|}{q^{2(n-1)}}(\varphi_{\omega,q})^{2n}$$

(Ar. Abanov, A. Chubukov, 2004)

(claimed to be a universal contribution generated by low-energy fermions)

But this yields:

$$[g_{2n}] = (2 - z)n$$

… and therefore for *z*=2 all the vertices are marginal …

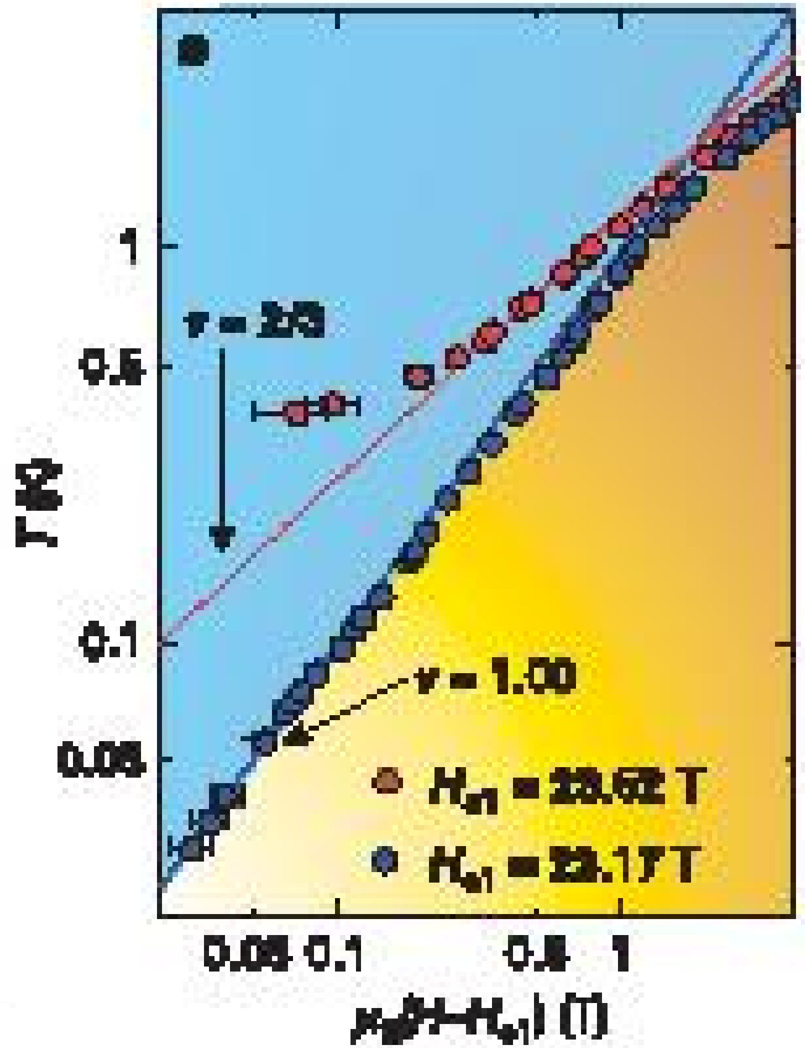
Remarks

- estimate of $T_c(\delta)$
- detecting the true T_c requires analysis in the phase with broken symmetry
- the starting point evades problems encountered in a careful derivation of the action
- a number of cases (e.g. with nesting property) not covered

Further remarks

- in ordered phase many special cases arise because:
  - symmetry of order parameter is important
  - order may affect fermionic spectrum

However…



…the H-M theory seems to work
In a number of cases, also in d=2…

(S. E. Sebastian et.. al. 2006)

QUANTUM PHASE TRANSITIONS IN ITINERANT FERMION SYSTEMS

PART II

Pawel Jakubczyk
MPI Stuttgart

Our contribution so far …

- No fermions
- No singular interactions

But …

- Extension to phases with broken symmetry
- Capturing non-gaussian fluctuations
- Covering also first order transitions and quantum tricritical scenario

However …

- No Goldstone modes (discrete symmetry breaking)
- Influence of gaps in the fermionic spectrum disregarded

Functional RG framework and the truncation

1PI scheme:

$$\partial_\Lambda \Gamma^\Lambda[\varphi] = \frac{1}{2} Tr \frac{\partial_\Lambda R^\Lambda}{\Gamma^{(2)}[\varphi] + R^\Lambda}$$

$\varphi = const$ $\rightarrow$ $\partial_\Lambda U = \ldots$

$\frac{\delta^2}{\delta\varphi^2}$ $\rightarrow$ $\partial_\Lambda \Gamma^{(2)}(\vec{p}, \omega_n) = \ldots$

Parametrization of $\Gamma^{(2)}(p, \omega_n)$

$$\Gamma^{(2)}(\vec{p}, \omega_n) = Z_p \vec{p}^{\,2} + Z_\omega \frac{|\omega_n|}{|\vec{p}|^{z-2}} + R^\Lambda(\vec{p})$$

Choice of cutoff function

$$R^\Lambda(p) = Z_p(\Lambda^2 - p^2)\theta(\Lambda^2 - p^2)$$

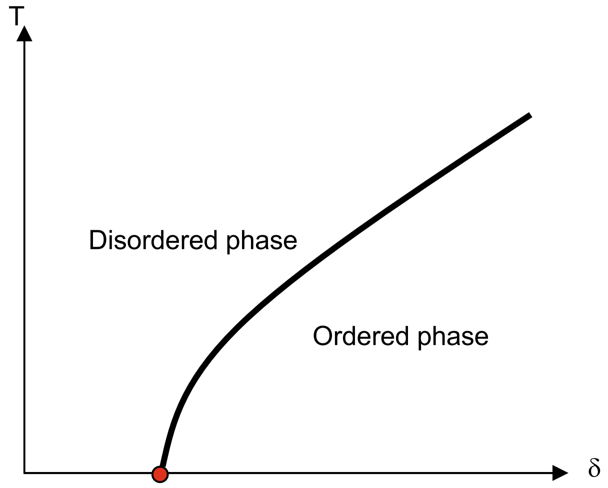
Effective potential:

$$U[\varphi] = \frac{u}{4!}\int_0^\beta d\tau \int d^d r \left(\varphi^2 - \varphi_0{}^2\right)^2 = \int_0^\beta d\tau \int d^d r \left[u\frac{\varphi'^4}{4!} + \sqrt{3\delta u}\frac{\varphi'^3}{3!} + \delta\frac{\varphi'^2}{2!} \right]$$

$$\begin{cases} \varphi = \varphi_0 + \varphi' \\ \delta = \dfrac{u\varphi_0{}^2}{3} \end{cases}$$

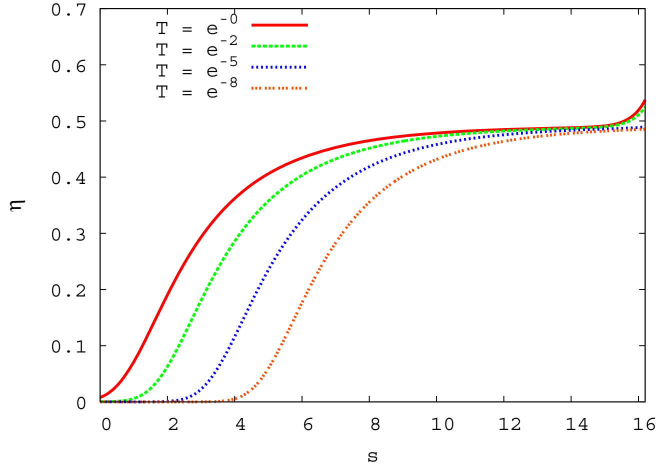
The procedure for computing T_C

- Fix *u, T*
- Choose δ_{UV}
- Run the flow
    - if $\varphi_0 \longrightarrow 0$ as the cutoff is removed, δ_{UV} corresponds to the disordered phase
    - otherwise δ_{UV} corresponds to the ordered phase



Transition and Ginzburg lines

d=2, z=3

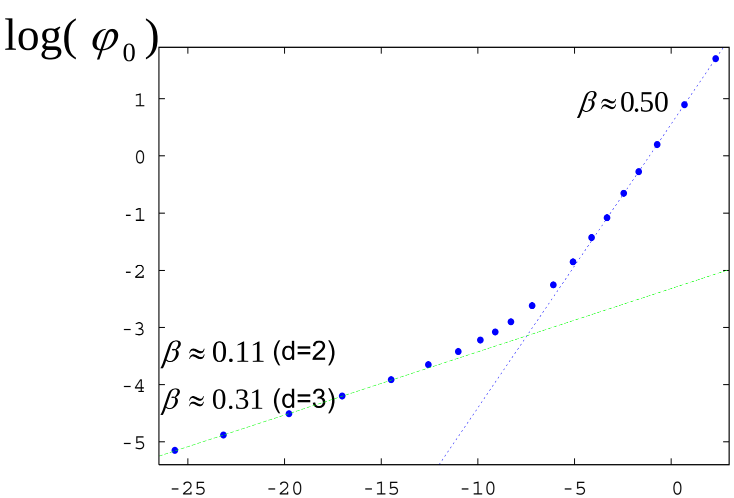


$$\Lambda_G \propto T_C^{1/(4-d)}$$

$\eta \approx 0.48$

$\Lambda = \exp(-s)$

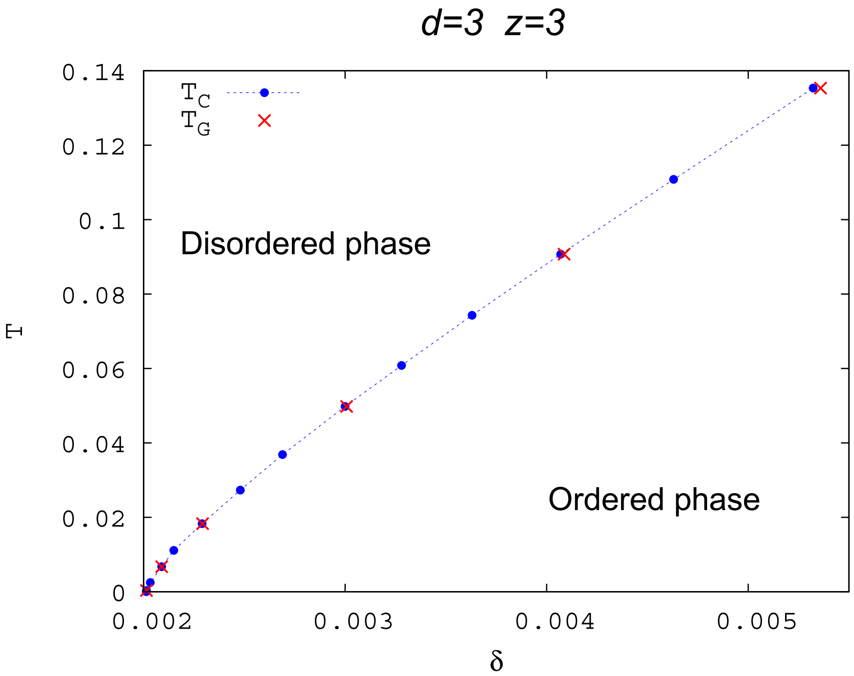
($\eta \approx 0.08$ for *d*=3)

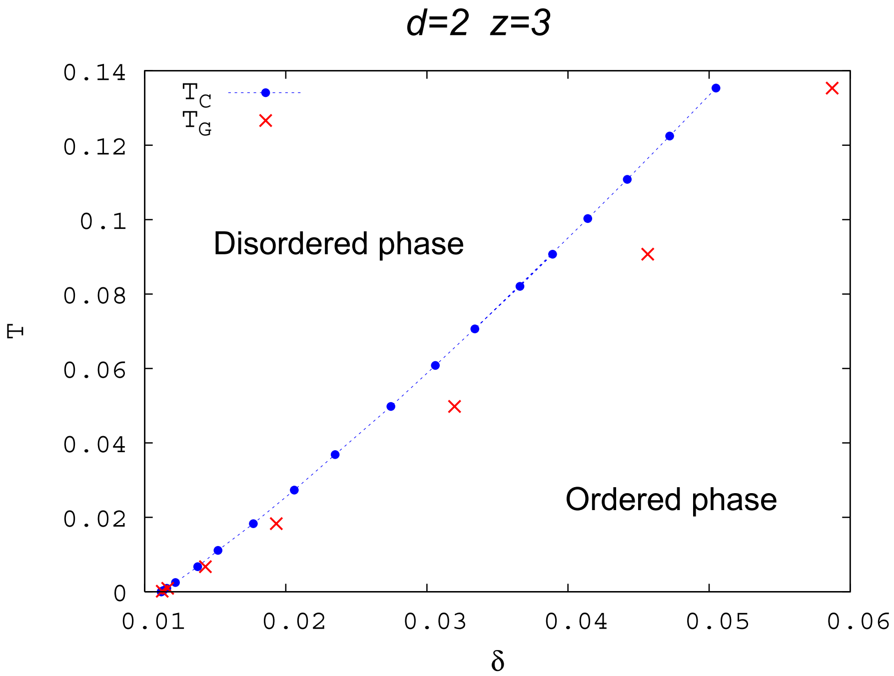


$$\varphi_0 \sim (\delta - \delta_C)^{\beta}$$

$\log(\delta - \delta_c(T))$

Phase diagrams (*z*=3)





$$T_C \propto (\delta - \delta_0)^{0.75}$$

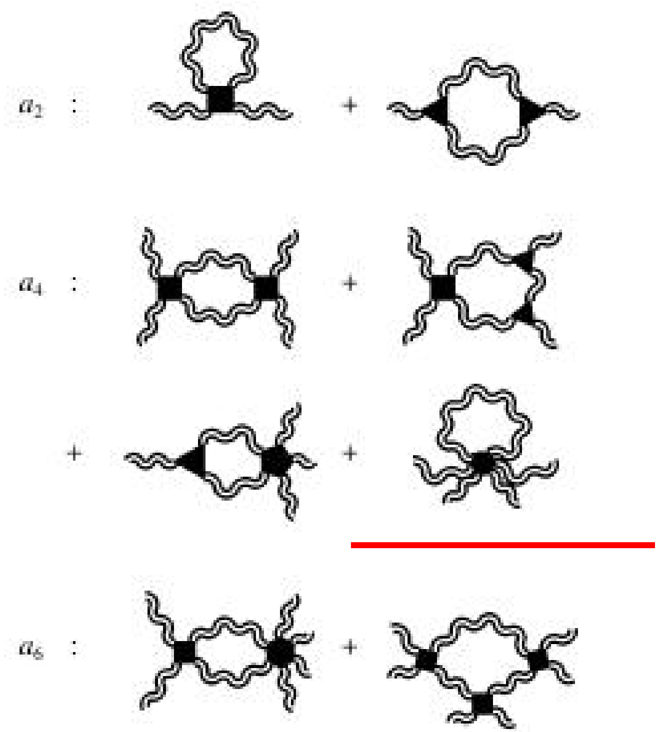
$$(\delta - \delta_0) \propto T_C \log T_C$$

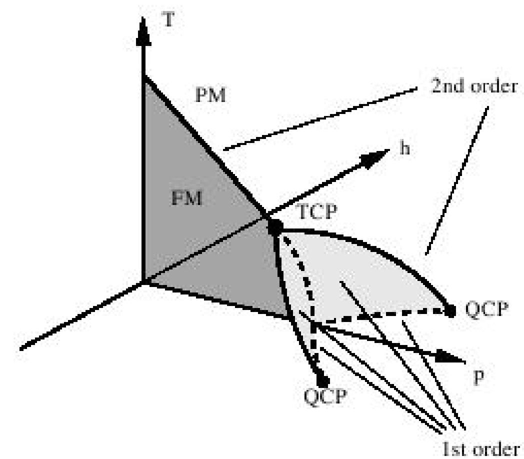
First order transitions (z=3)

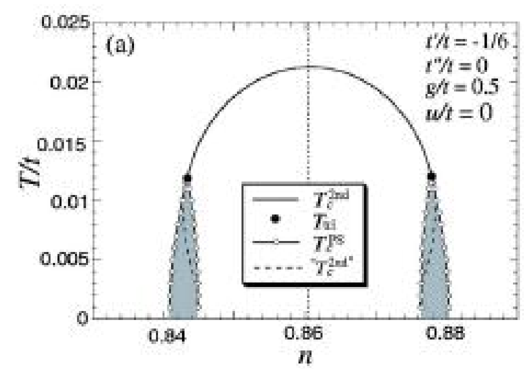
$$U[\varphi] = \int_0^\beta d\tau \int d^d x \left[a_6 \varphi^6 + a_4 \varphi^4 + a_2 \varphi^2 \right]$$

$$a_6 > 0$$
$$a_4 < 0$$

Can fluctuations influence the order of the transition?

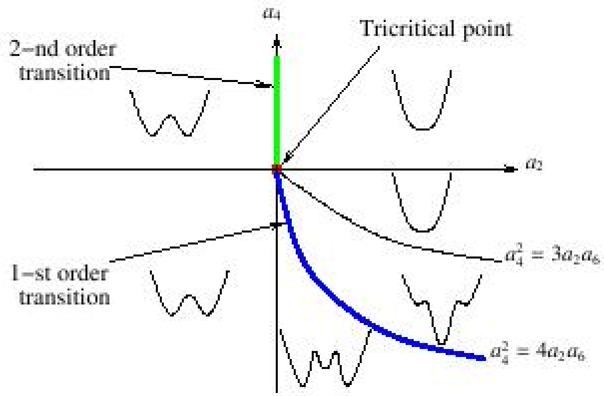


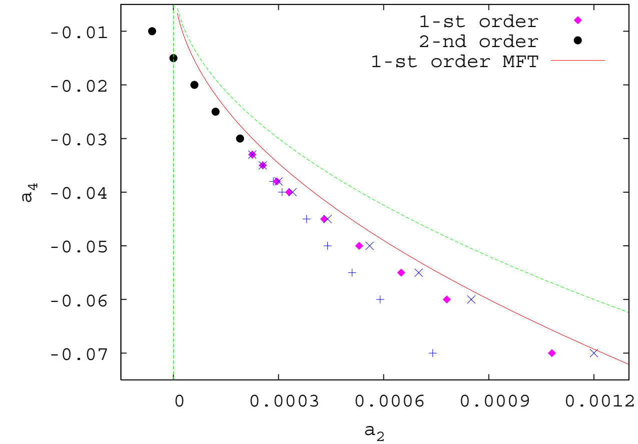


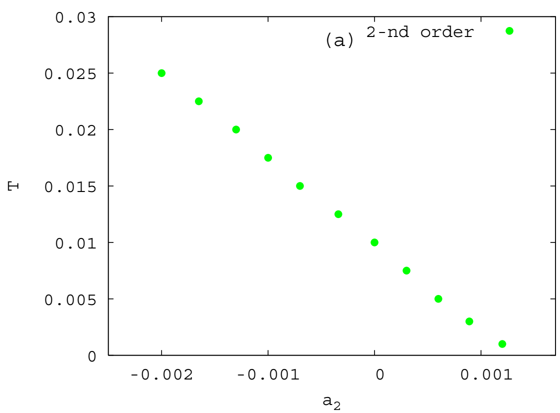


(H. Yamase et. al. 2005)

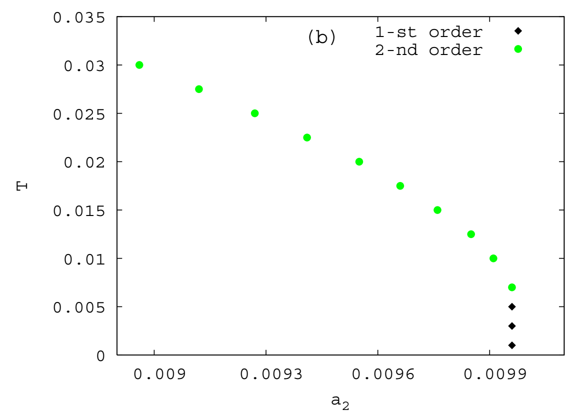
Phase diagrams:

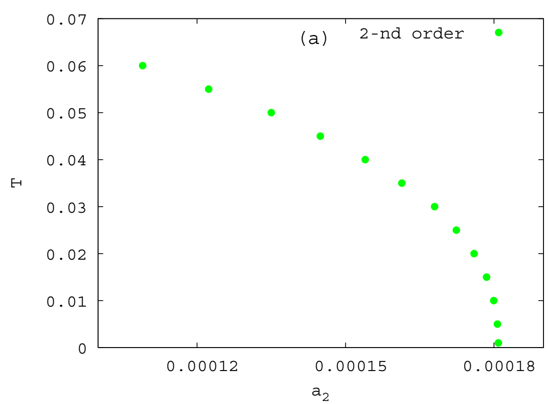




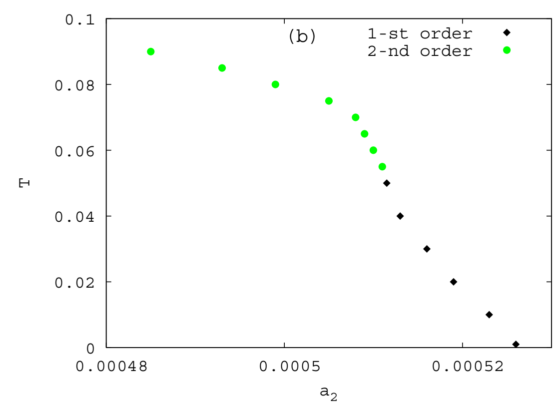


d=2



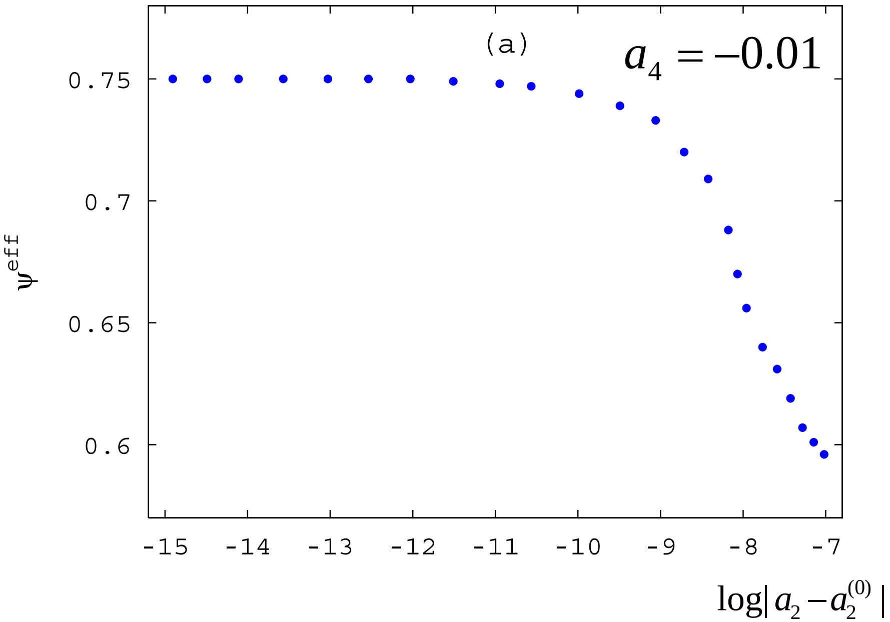


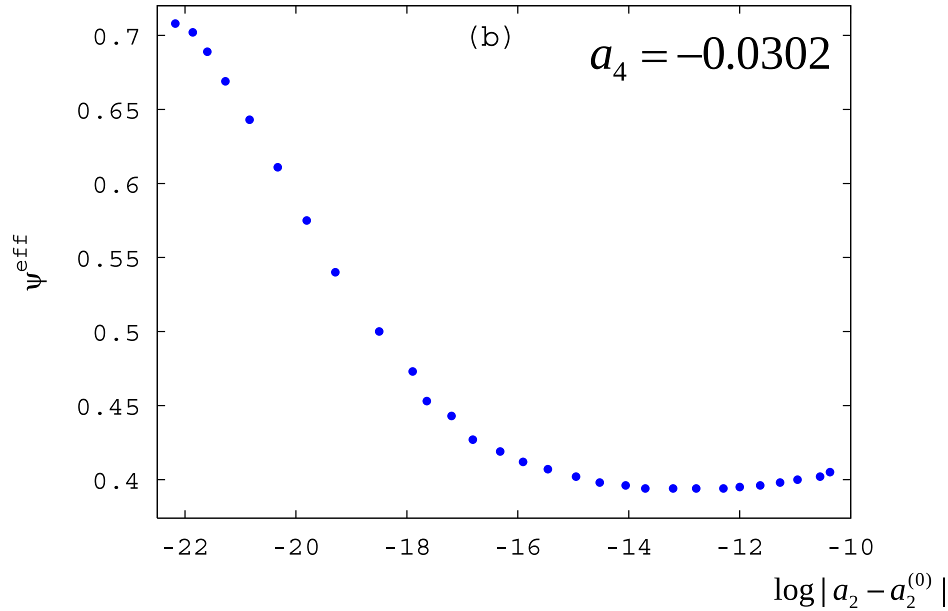
d=3



Crossover in the shift exponent

$a_4 \to a_4^{tri}(T=0)^+$





$$\Lambda^{tri} \sim (a_4 - a_4^{tri})/a_6$$

$$\psi^{HM} = 3/4 \longrightarrow \psi^{tri} = 3/8$$

Scaling analysis

$$f(a_2, T, h, a_n) = b^{-(d+z)} f(a_2 b^{1/\nu}, T b^z, h b^{y_h}, a_n b^{[a_n]})$$

$$\downarrow$$

$$\psi = \frac{z}{2 - [a_n]}$$

n=4: $\psi = \dfrac{z}{d + z - 2}$

n=6: $\psi = \dfrac{z}{2(d + z) - 4}$

d=z=3

$\psi^{HM} = 3/4$

$\psi^{tri} = 3/8$

d=3, z=2

$\psi^{HM} = 2/3$

$\psi^{tri} = 1/3$

No crossovers in ψ for d=2 (logs neglected)

Aims:

- identify the correct effective theories near specific QCPs

- when is the Hertz – Millis theory qualitatively correct?