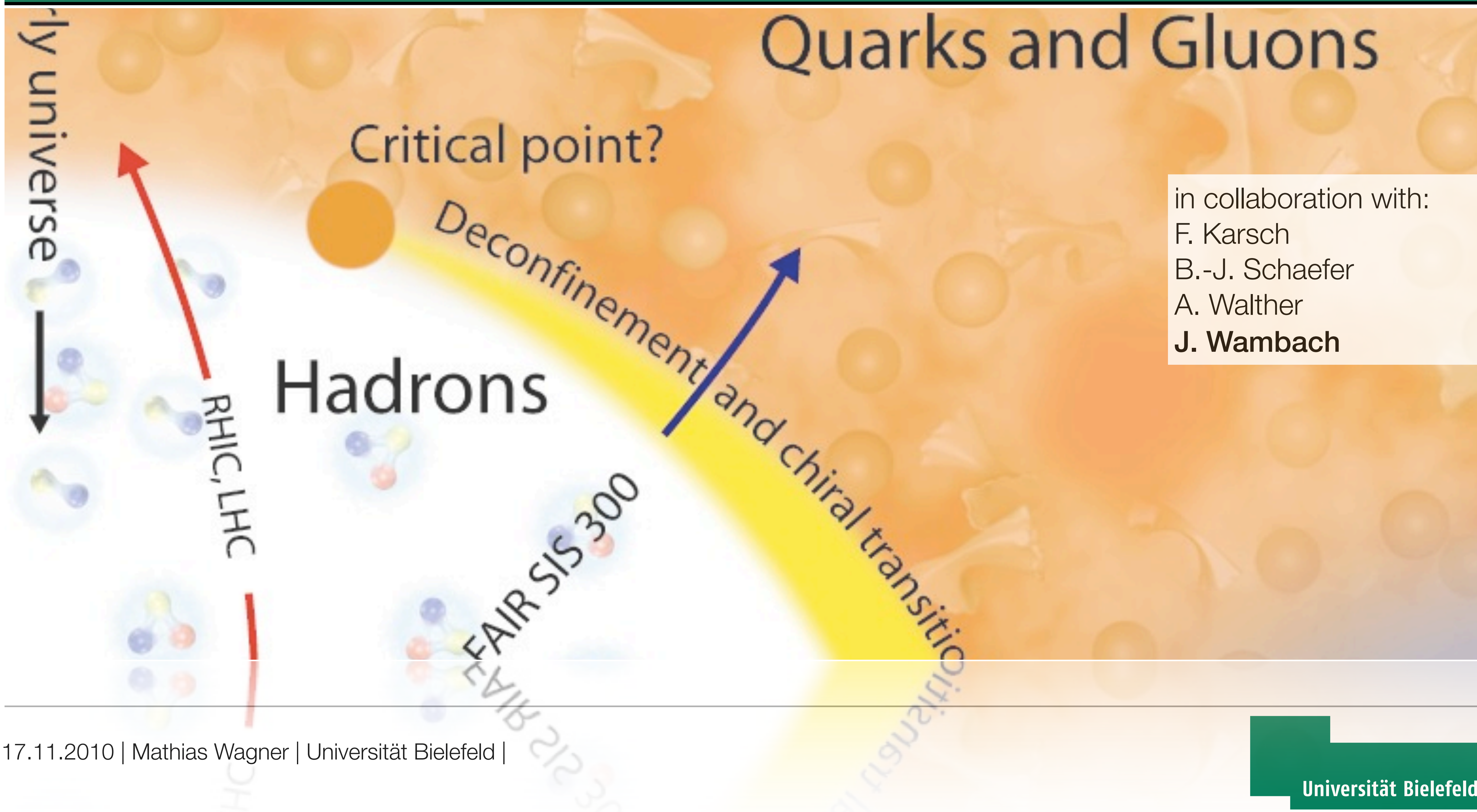
Towards finite density QCD with Taylor expansions



in collaboration with:
F. Karsch
B.-J. Schaefer
A. Walther
J. Wambach

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Outline

- Taylor expansion to finite density
- general aspects of the Taylor expansion
  - extracting the phase boundary
  - locating the critical point
- model analysis
  - including higher coefficients

Taylor expansion to finite density

- Taylor expansion

$$\frac{p(T,\mu)}{T^4} = \sum_{n=0}^{\infty} c_n(T) \left(\frac{\mu}{T}\right)^n \qquad c_n(T) = \frac{1}{n!} \frac{\partial^n \left(p(T,\mu)/T^4\right)}{\partial \left(\mu/T\right)^n}\bigg|_{\mu=0}$$

- coefficients calculated with standard (i.e. $\mu = 0$ methods)

- calculations by various lattice groups (e.g. Allton, C. Schmidt, Gavai & Gupta, deTar, Ejiri, ...)

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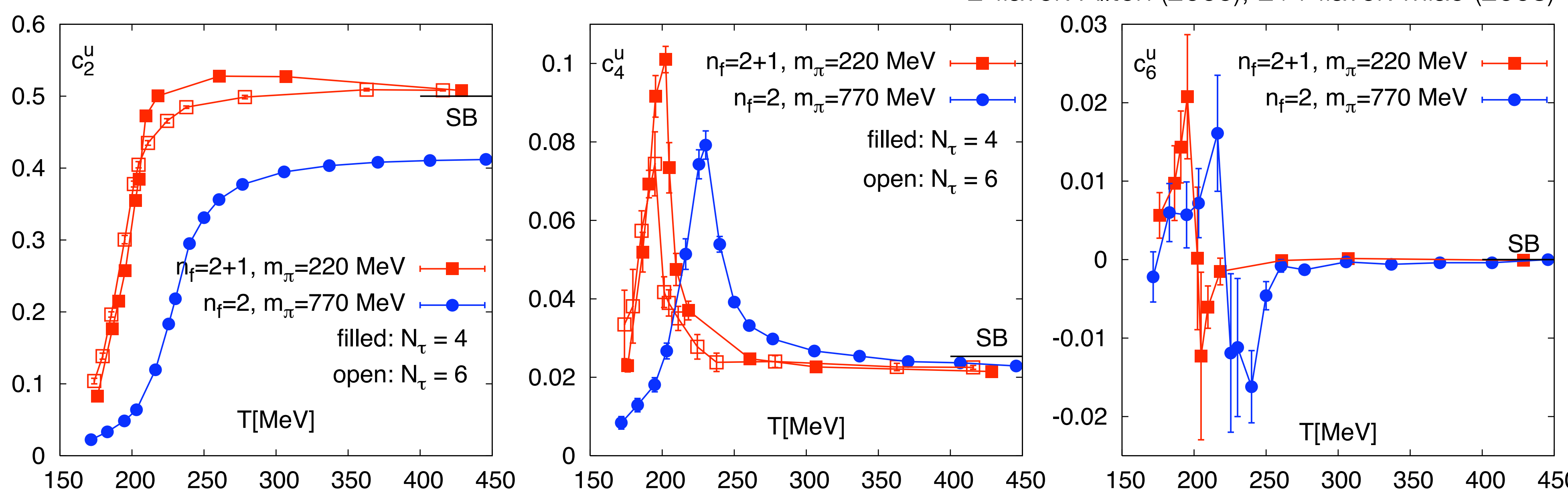
2-flavor: Allton (2005), 2+1 flavor: Miao (2008)



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Hopes

- works for small μ/T, i.e., $\mu/T < 1$
- only a few coefficients required for ‘convergence’
- calculate thermodynamic observables relevant for heavy-ion collisions
- might locate the critical endpoint
- troubles with phase transitions
  (divergences)

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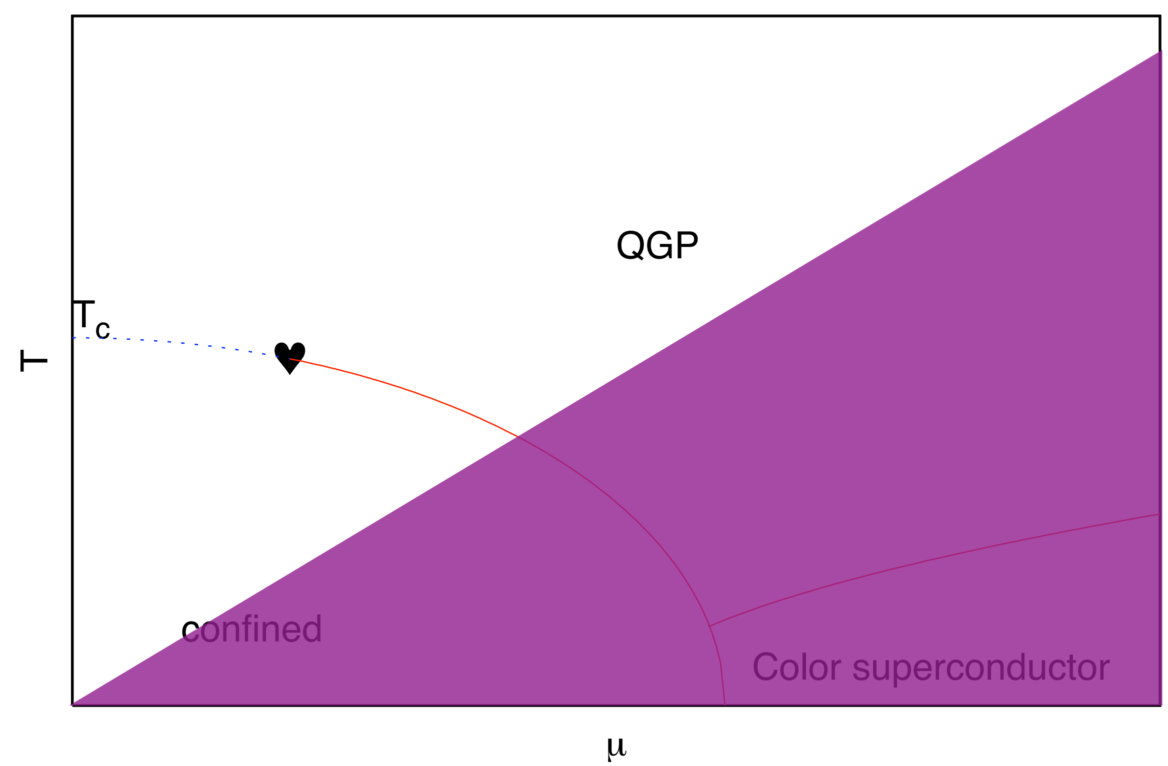
Philipsen (CPOD 2009)

The calculable region of the phase diagram



- 2001-present: sign problem not solved, circumvented by approximate methods: reweigthing, Taylor expansion, imaginary chem. pot., need $\mu/T \lesssim 1 \quad (\mu = \mu_B/3)$

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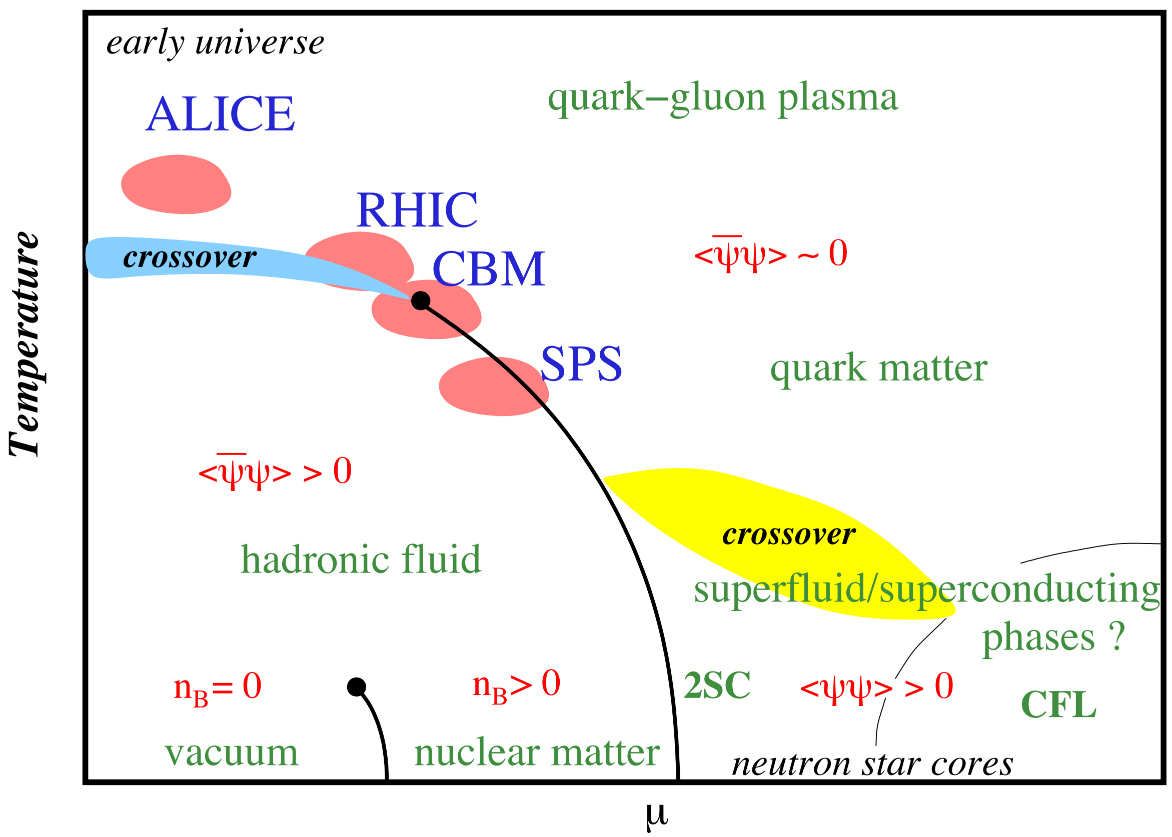


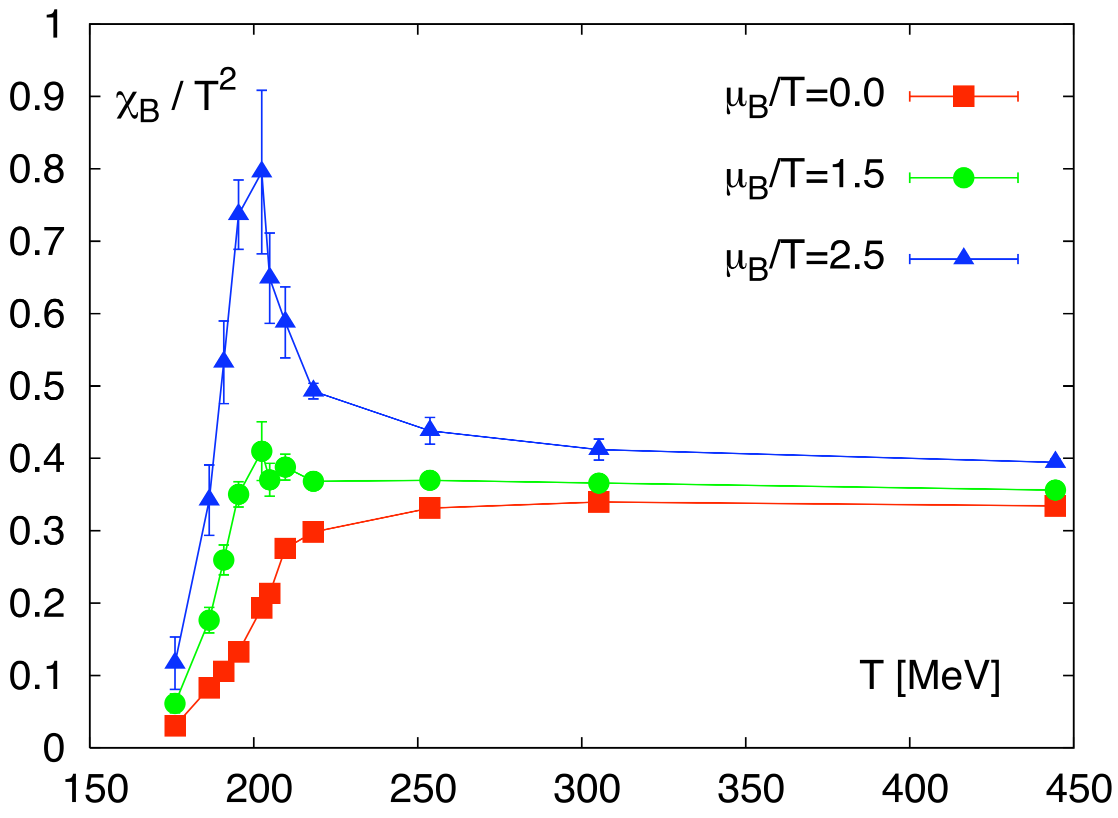
Signals of the critical endpoint ?

- quark number susceptibility

$$\frac{\chi_q(T,\mu)}{T^2} = -\frac{\partial^2\Omega(T,\mu)}{\partial\mu^2}$$

$$= \sum_{n=2,4,\ldots} n(n-1)c_n(T)\left(\frac{\mu}{T}\right)^{n-2}$$

C. Schmidt (2008)



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- convergence radius

$$r = \lim_{n\to\infty} r_{2n} = \lim_{n\to\infty}\left|\frac{c_{2n}}{c_{2n+2}}\right|^{1/2}$$

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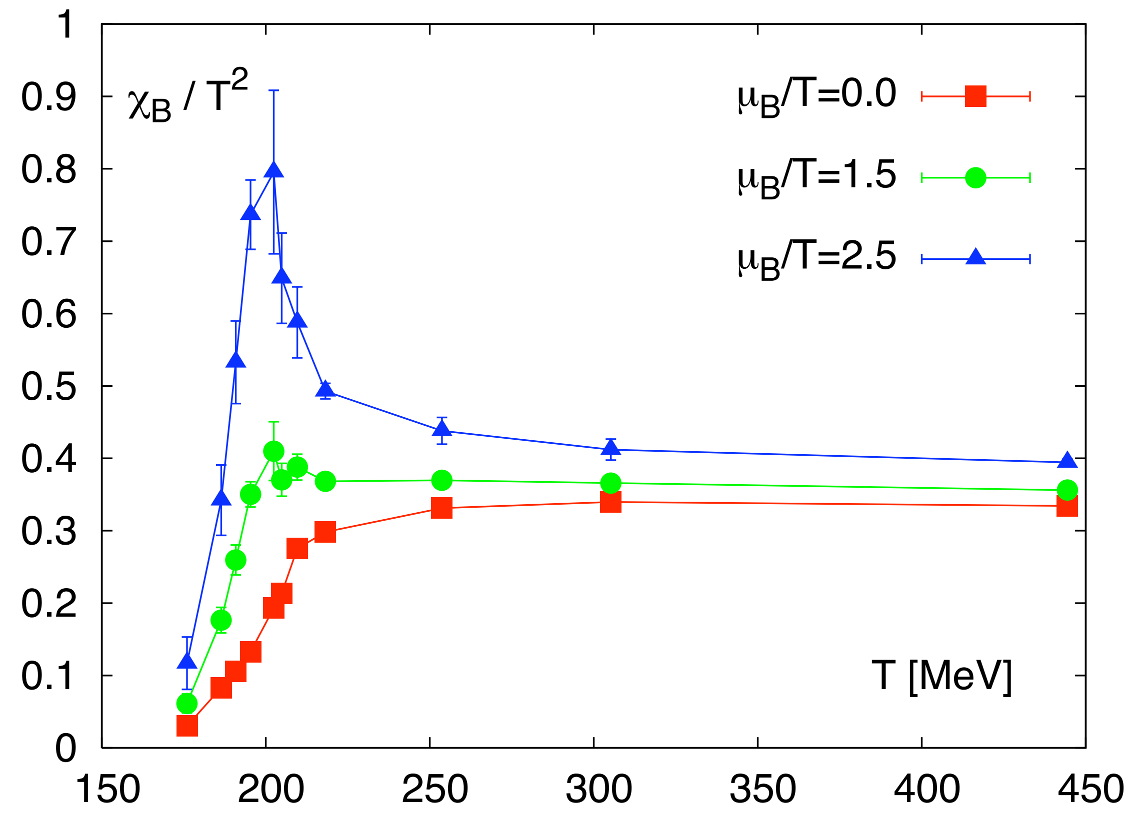

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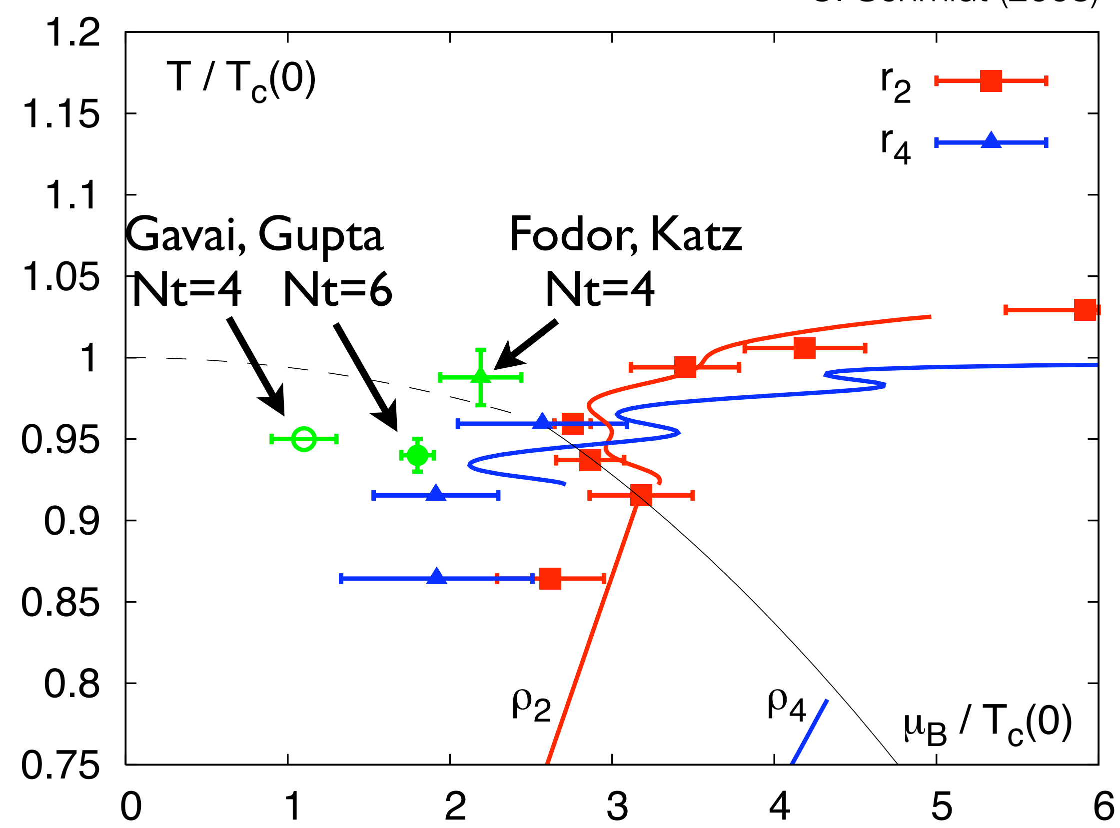

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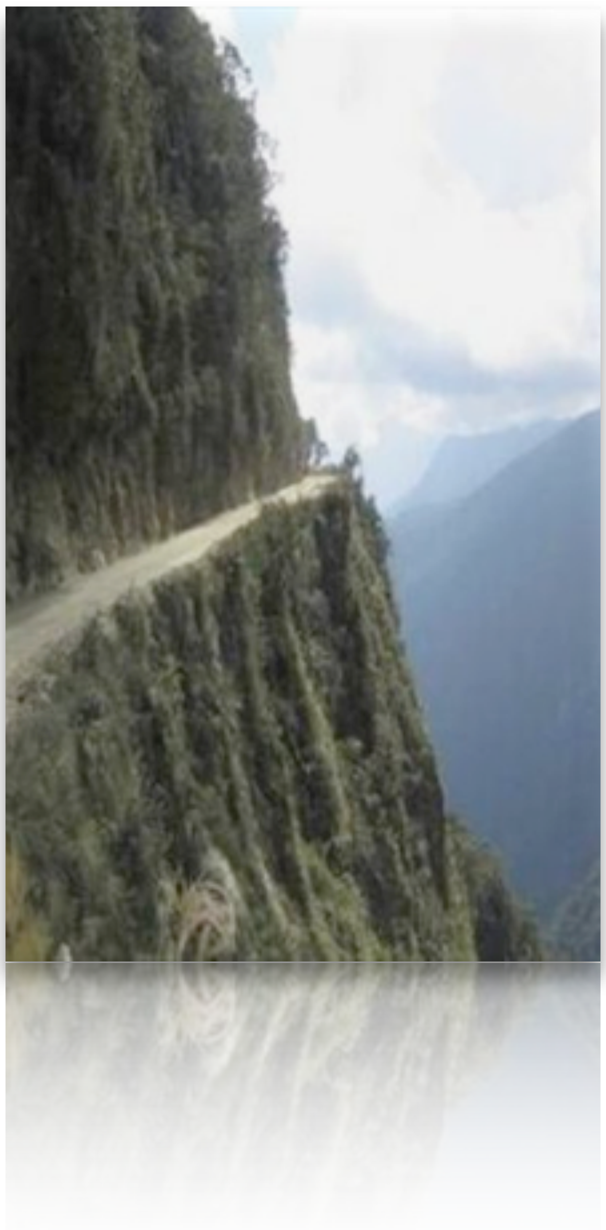
Can we trust the Taylor expansion ?



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- increasing errors for higher order coefficients
- convergence properties have obtained little attention

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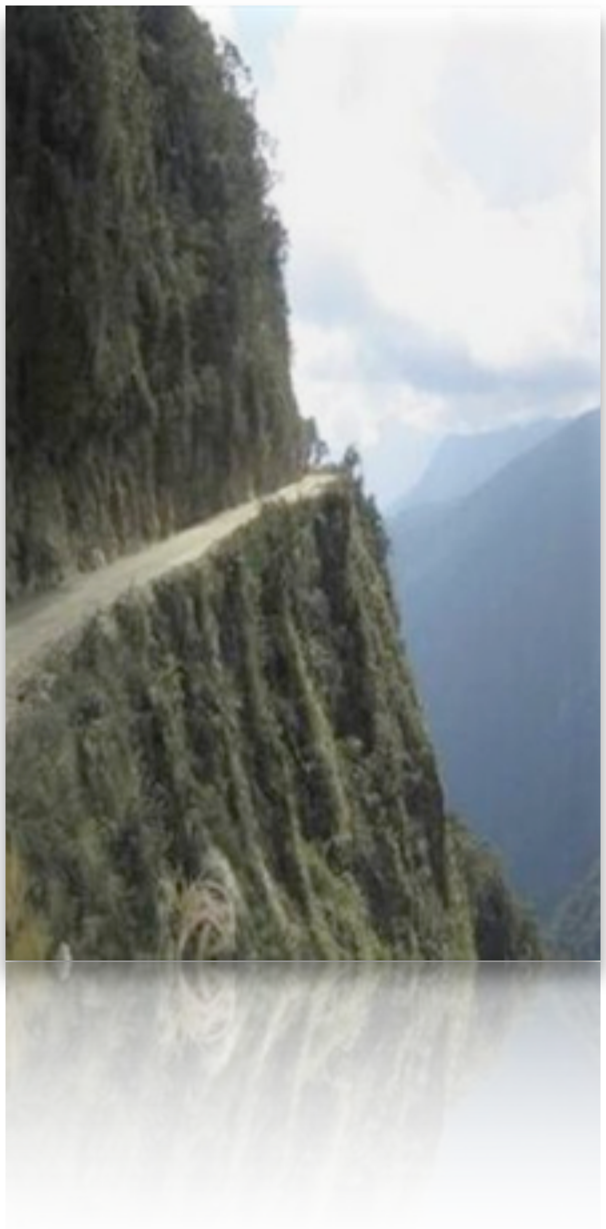

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- explore general aspects of Taylor expansion method
  - requires higher coefficients
  - comparison with ‘direct’ evaluation favorable

How to extract the phase boundary ?

F. Karsch, B-J. Schaefer, MW, J. Wambach, arXiv:1009.5211

- nearest singularity in the complex plane limits applicability of Taylor expansion
- convergence radius for pressure $r = \lim_{n\to\infty} r_{2n} = \lim_{n\to\infty} \left| \frac{c_{2n}}{c_{2n+2}} \right|^{1/2}$
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- only exact in the limit of infinite expansion
- different observables yield different estimates at finite order

$$r_{2n}^{\chi} = \left| \frac{c_{2n}^{\chi}}{c_{2n+2}^{\chi}} \right|^{1/2} = \left| \frac{(2n+2)(2n+1)}{(2n+3)(2n+4)} \right|^{1/2} r_{2n+2} \quad \Rightarrow \quad r_{2n}^{\chi} = r_{2n+2} \left(1 - \frac{1}{n} + \mathcal{O}(n^{-2}) \right)$$

- need apparent convergence to asymptotic value
- expected deviation from asymptotic value (near to the CEP)

$$r_{2n+2} \simeq r(1 + A/n) \qquad\qquad r_{2n}^{\chi} \simeq r(1 + (A-1)/n)$$

Beyond Taylor: Padé approximation

- Taylor: $t(x) = \sum_{i=0}^{N} t_{(i)} x^i$

- Padé: $[L/M] \equiv R_{L,M}(x) = \frac{p(x)}{q(x)} = \frac{p_0 + p_1 x + \cdots + p_L x^L}{1 + q_1 x + \cdots + q_M x^M}$

- require: $\left.\frac{\partial^i R_{L,M}(x)}{\partial x^i}\right|_{x=0} = \left.\frac{\partial^i t(x)}{\partial x^i}\right|_{x=0} \quad \text{for } i \leq N$

- i.e. uses same derivative information as Taylor expansion

- pole in$[N/2]$ at $x = \pm\sqrt{c_N / c_{N+2}}$, i.e. at r_N

- pole also used as estimate for phase boundary for general Padé series

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$$[L/M] = \frac{\begin{vmatrix} t_{(L-M+1)} & t_{(L-M+2)} & \cdots & t_{(L+1)} \\ t_{(L-M+2)} & t_{(L-M+3)} & \cdots & t_{(L+2)} \\ \vdots & \vdots & \ddots & \vdots \\ t_{(L)} & t_{(L+1)} & \cdots & t_{(L+M)} \\ \sum_{i=0}^{L-M} t_{(i)} x^{M+i} & \sum_{i=0}^{L-M+1} t_{(i)} x^{M+i-1} & \cdots & \sum_{i=0}^{L} t_{(i)} x^i \end{vmatrix}}{\begin{vmatrix} t_{(L-M+1)} & t_{(L-M+2)} & \cdots & t_{(L+1)} \\ t_{(L-M+2)} & t_{(L-M+3)} & \cdots & t_{(L+2)} \\ \vdots & \vdots & \ddots & \vdots \\ t_{(L)} & t_{(L+1)} & \cdots & t_{(L+M)} \\ x^M & x^{M-1} & \cdots & 1 \end{vmatrix}}$$

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Locating the critical endpoint

- convergence radius close to CEP

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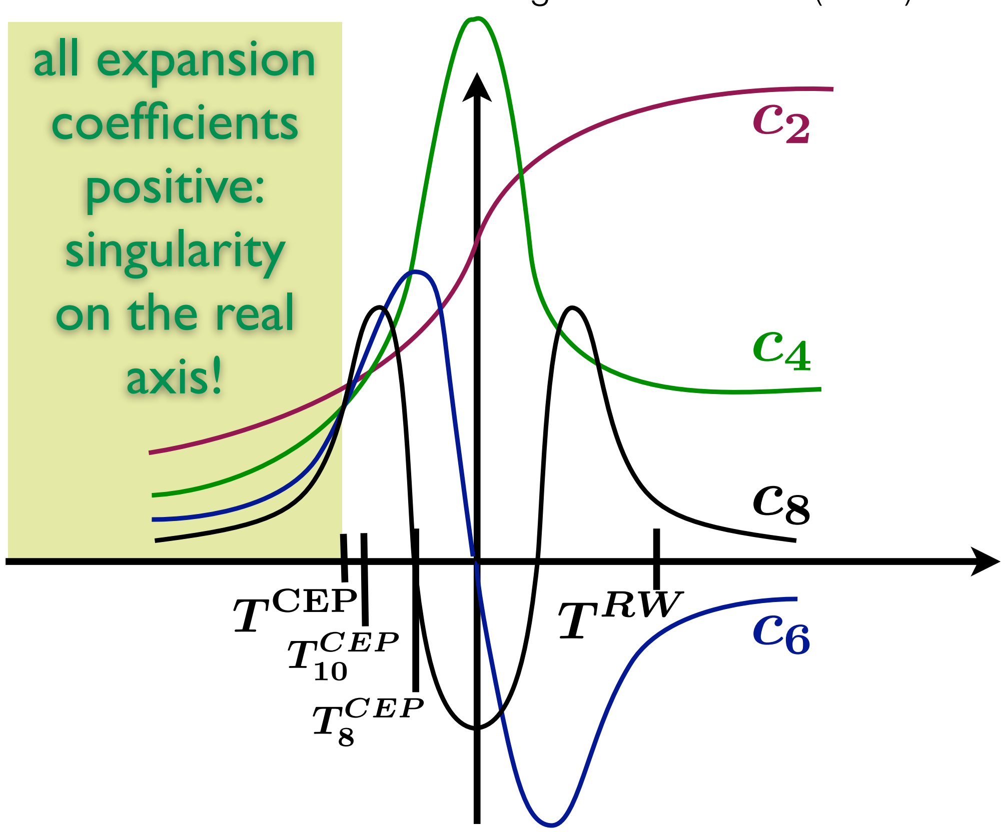
- need a way to determine T_c:
  sign of coefficients (Stephanov, Phys.Rev. D73 (2006) 094508)

- singularity at real chemical potential if all coefficients are positive

Figure: C. Schmidt (2009)



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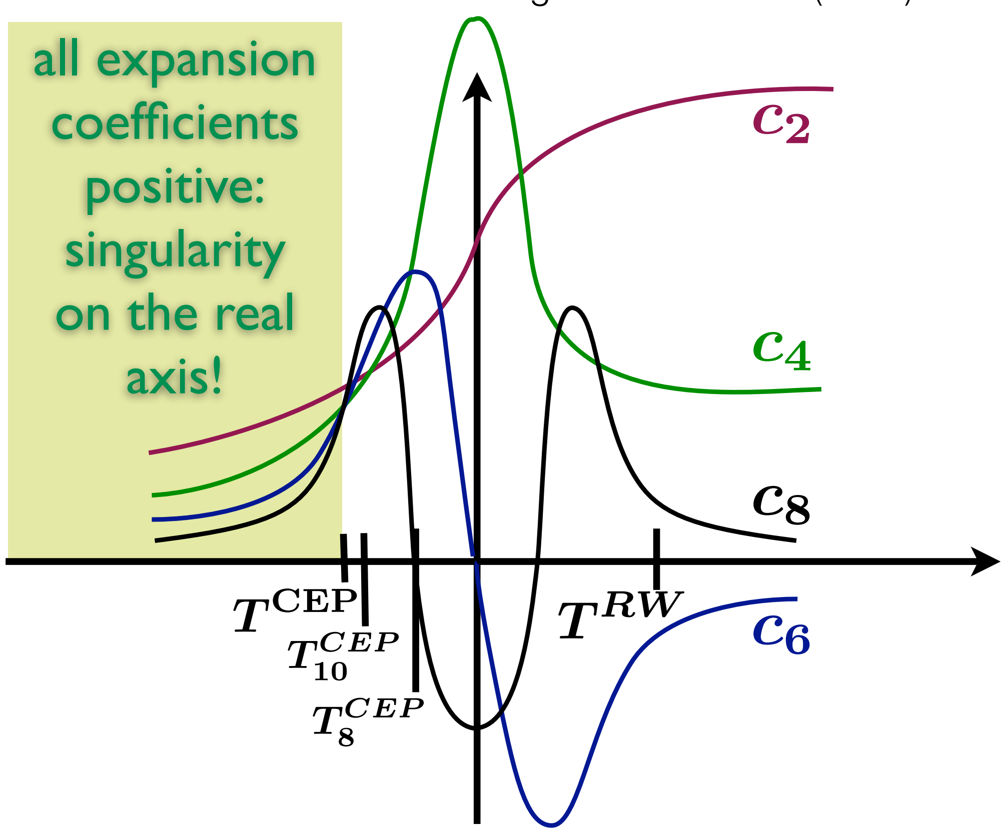
- at least n=8 required for non-trivial estimate

- extrapolation required: $T_c = \lim_{n\to\infty} T_{c,n}$

- asymptotic behavior unknown

Figure: C. Schmidt (2009)



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Polyakov-Quark-Meson (PQM) model

B-J. Schaefer, MW, J. Wambach, Phys. Rev. D 81, 074013

- relevant degrees of freedom: (2+1) quarks and mesons
  → PQM model

$$\mathcal{L}_{\mathrm{PQM}} = \bar{q}\left(i\not{D} - g\phi_5\right)q + \mathcal{L}_m - \mathcal{U}(\Phi, \bar{\Phi})$$

Polyakov loop variable

quarks / antiquarks

$$\mathcal{L}_m = \mathrm{Tr}\left(\partial_\mu \phi^\dagger \partial^\mu \phi\right) - m^2\,\mathrm{Tr}(\phi^\dagger \phi) - \lambda_1 \left[\mathrm{Tr}(\phi^\dagger \phi)\right]^2 - \lambda_2\,\mathrm{Tr}\left(\phi^\dagger \phi\right)^2 + c\left(\det(\phi) + \det(\phi^\dagger)\right) + \mathrm{Tr}\left[H(\phi + \phi^\dagger)\right]$$

mesonic fields

- here: logarithmic Polyakov loop potential (Roessner et al, Phys. Rev. D75, 034007)

$$\frac{\mathcal{U}_{\log}}{T^4} = -\frac{1}{2}a(T)\bar{\Phi}\Phi + b(T)\ln\left[1 - 6\bar{\Phi}\Phi + 4\left(\Phi^3 + \bar{\Phi}^3\right) - 3\left(\bar{\Phi}\Phi\right)^2\right]$$

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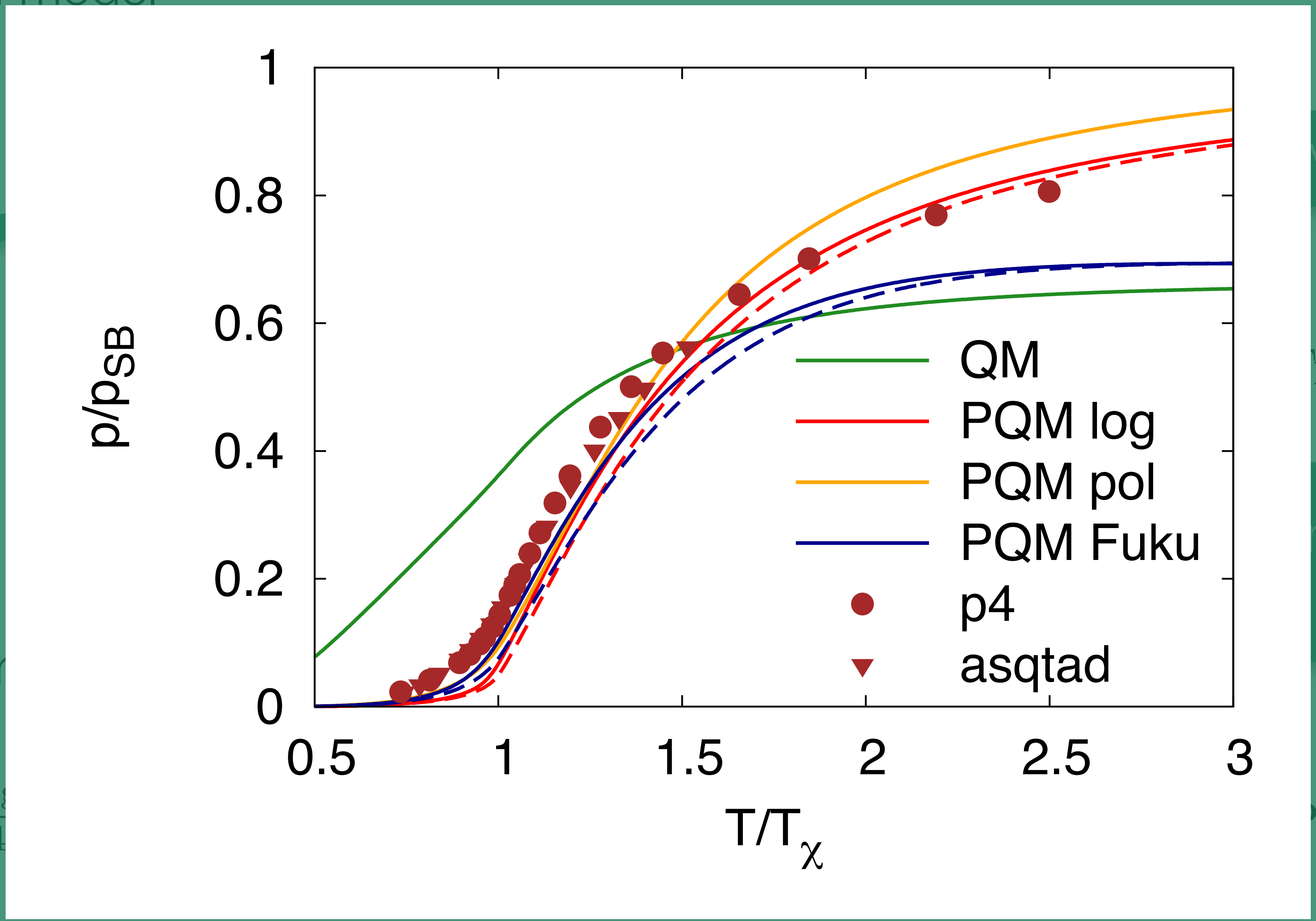

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Explicit and implicit μ-dependence

- mean-field approximation
- thermodynamic potential $\Omega = U\left(\sigma_x, \sigma_y\right) + \Omega_{\bar{q}q}\left(\sigma_x, \sigma_y, \Phi, \bar{\Phi}\right) + \mathcal{U}\left(\Phi, \bar{\Phi}\right)$
- quark contribution

$$\Omega_{\bar{q}q}(\sigma_x, \sigma_y, \Phi, \bar{\Phi}) = -2T \sum_{f=u,d,s} \int \frac{d^3p}{(2\pi)^3} \left\{ \ln\left[1 + 3(\Phi + \bar{\Phi} e^{-(E_{q,f}-\mu_f)/T}) e^{-(E_{q,f}-\mu_f)/T} + e^{-3(E_{q,f}-\mu_f)/T}\right] \right.$$
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  global minimum $\min(\mu, T) = \left(\sigma_x = \langle\sigma_x\rangle, \sigma_y = \langle\sigma_y\rangle, \Phi = \langle\Phi\rangle, \bar{\Phi} = \langle\bar{\Phi}\rangle\right)$

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Why we need a novel technique

- numerical derivatives / divided differences
  - error prone $$\frac{d^2\Omega}{d\mu^2} = \frac{1}{\Delta\mu^2}\left[\Omega(\mu-\Delta\mu) - 2\Omega(\mu) + \Omega(\mu+\Delta\mu)\right] + \mathcal{O}(\Delta\mu^2)$$
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  - algebra systems can help $$\frac{d^2\Omega}{d\mu^2} = \frac{\partial^2\sigma}{\partial\mu^2}\frac{\partial\Omega}{\partial\sigma} + \left(\frac{\partial\sigma}{\partial\mu}\right)^2\frac{\partial^2\Omega}{\partial\sigma^2} + 2\frac{\partial\sigma}{\partial\mu}\frac{\partial\Omega^2}{\partial\sigma\partial\mu} + \frac{\partial^2\Omega}{\partial\mu^2}$$
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Algorithmic Differentiation

MW, A. Walther, B.-J. Schaefer, Comp. Phys. Commun., 181, pp. 756

- idea: 'differentiate' the algorithm using the chain rule
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  - arbitrary orders without further coding
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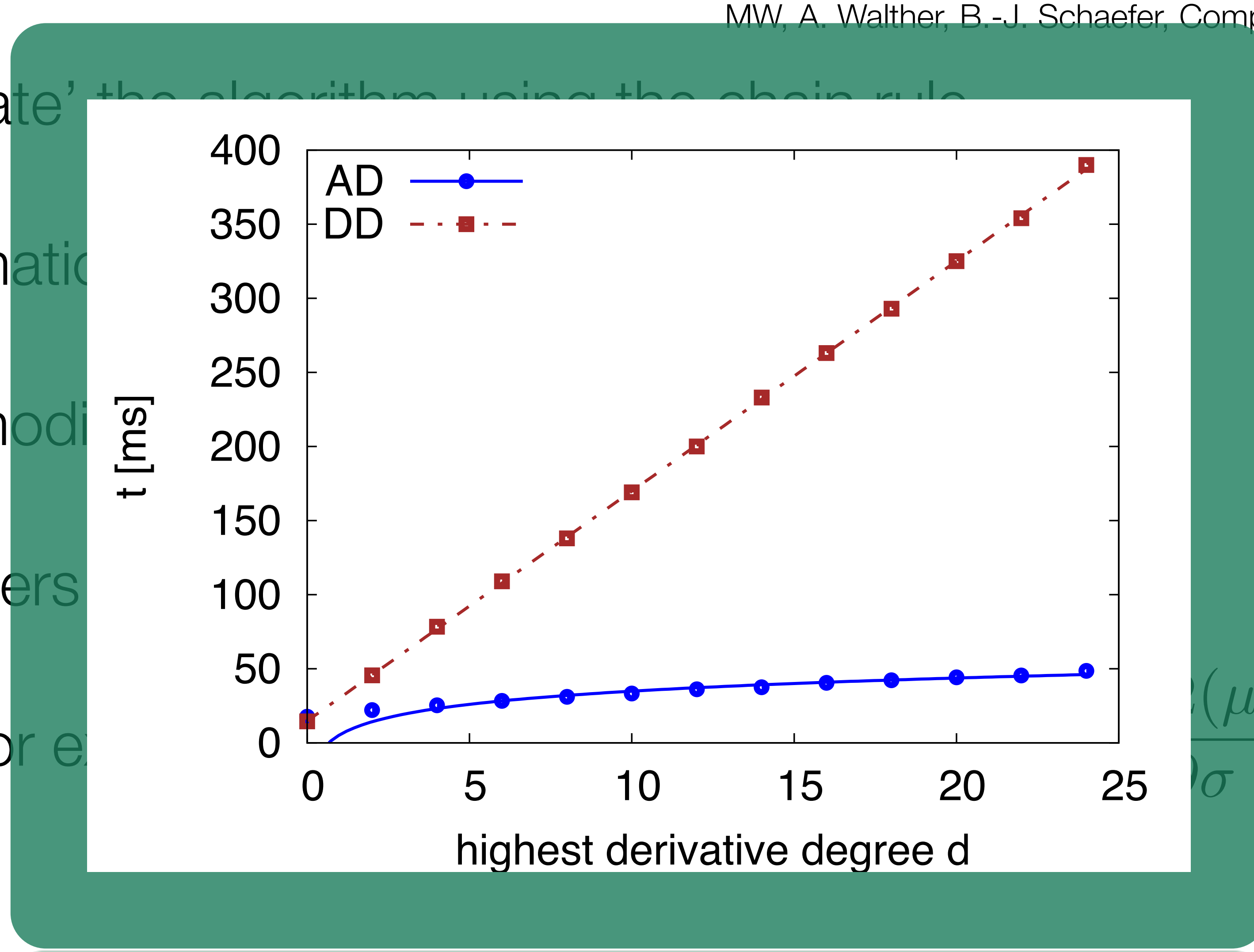

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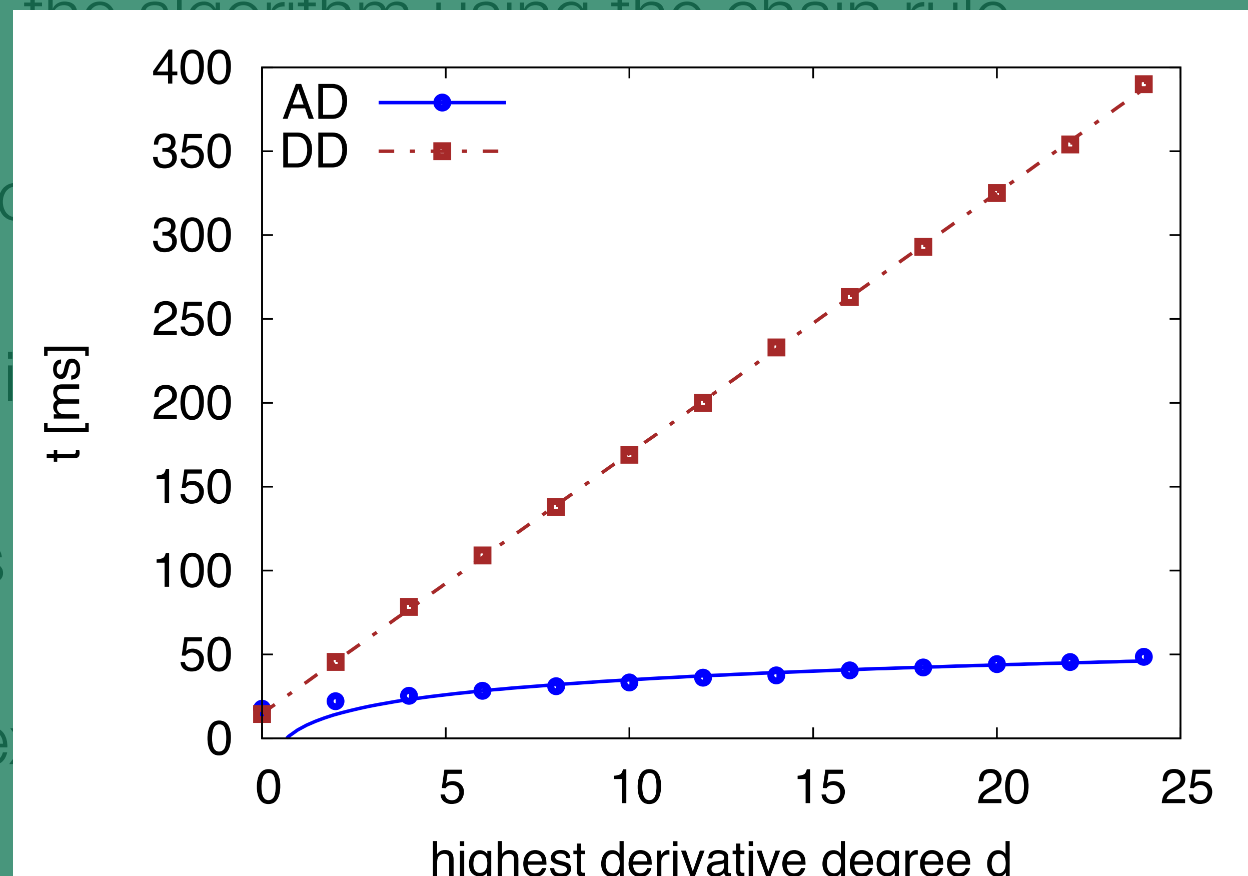

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Algorithmic Differentiation is a general technique !

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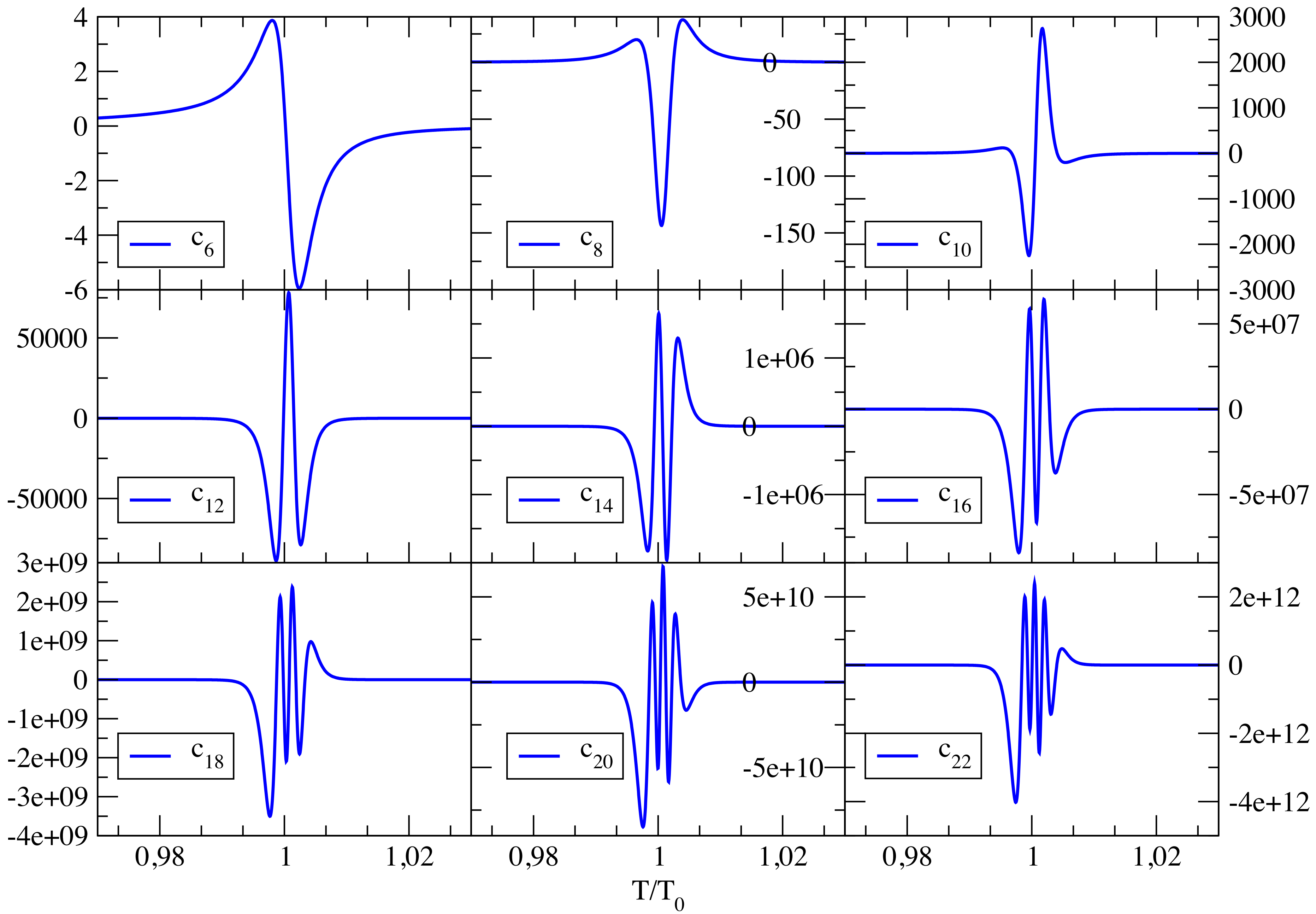
Higher order coefficients available

B.-J. Schaefer, MW, J. Wambach, PoS CPOD2009, 017



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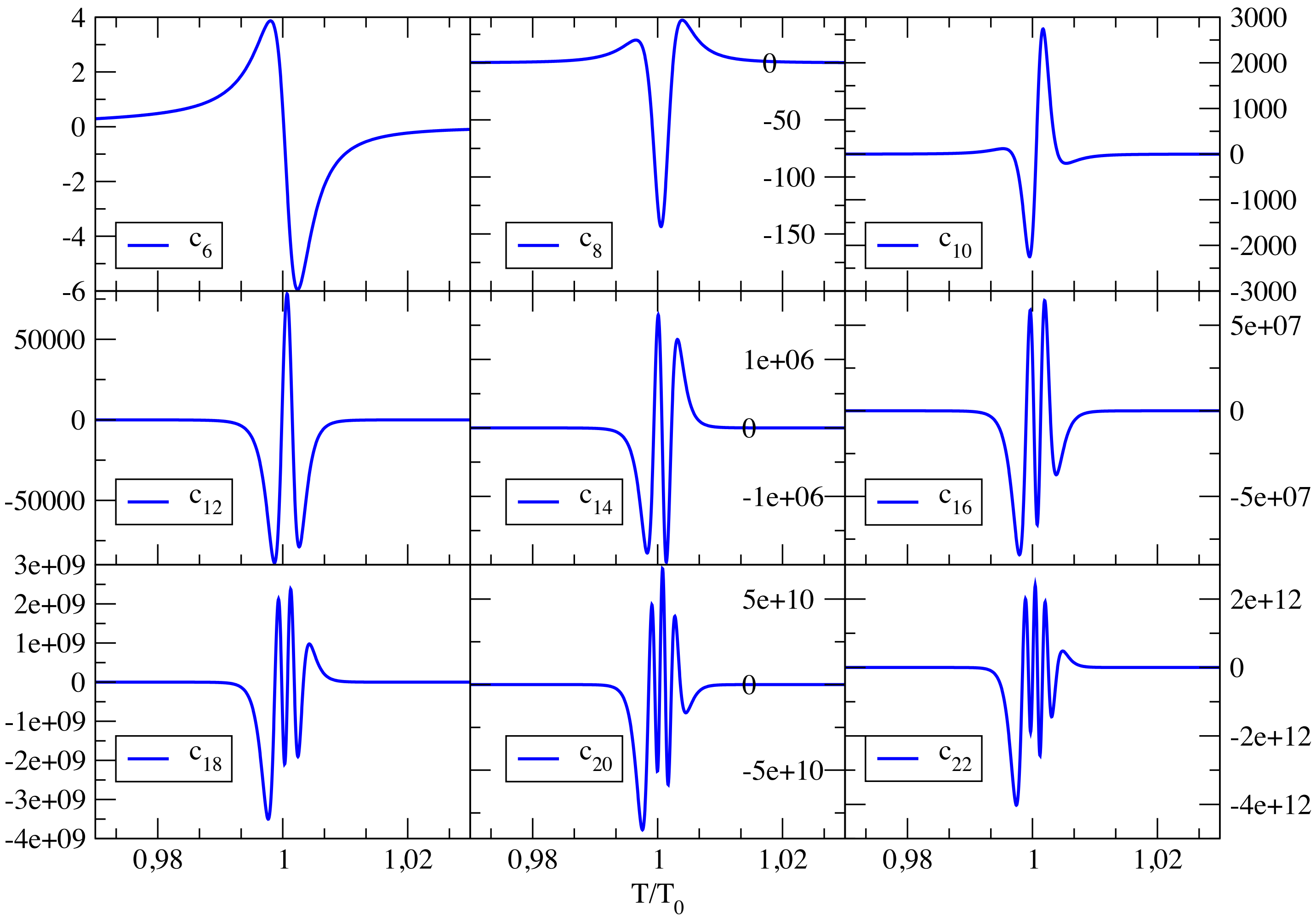

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- not negligible for $\mu/T < 1$
- small outside transition region
- no ‘numerical noise’
- singular contribution depends linear on T and quadratically on μ

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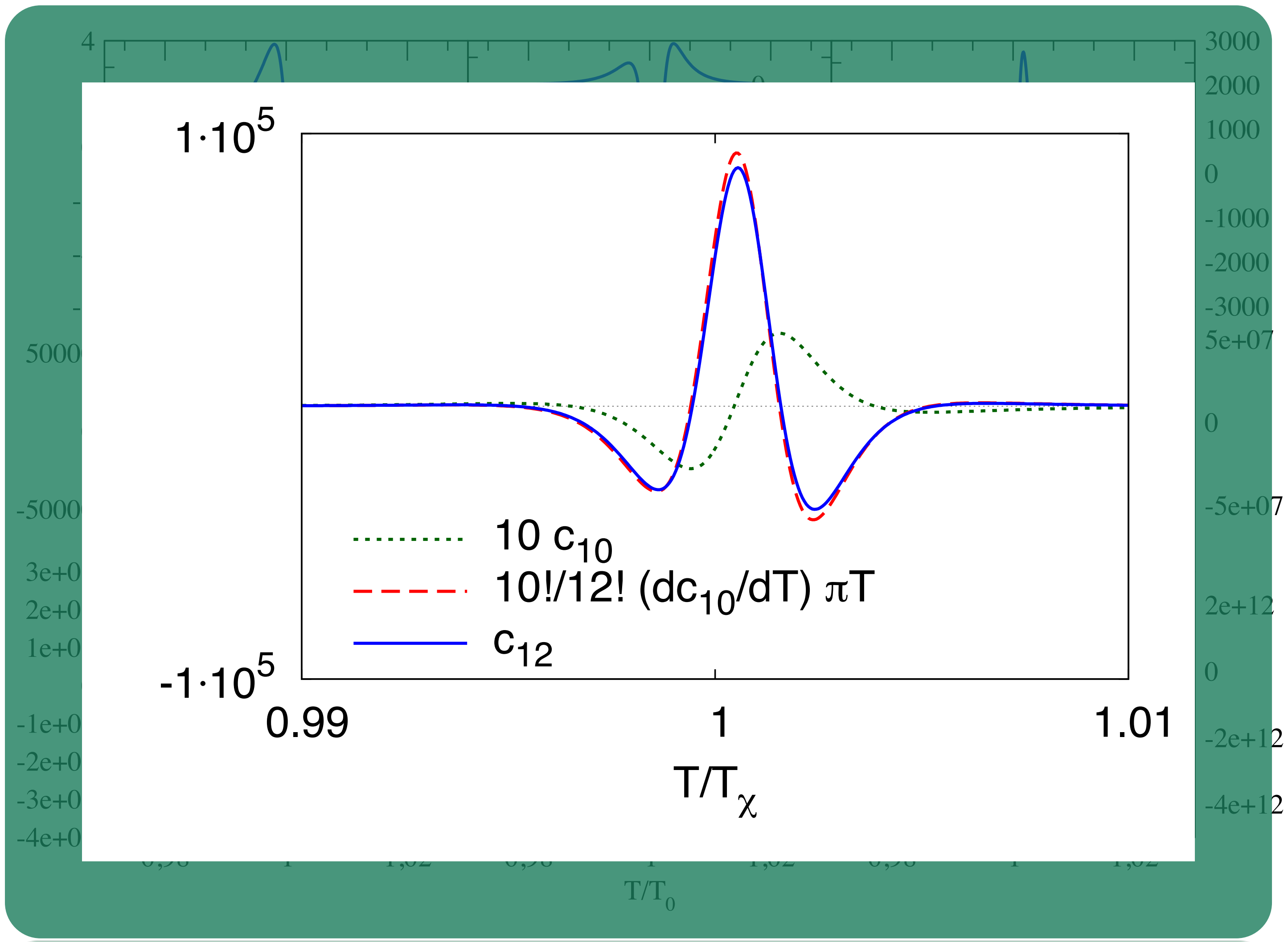

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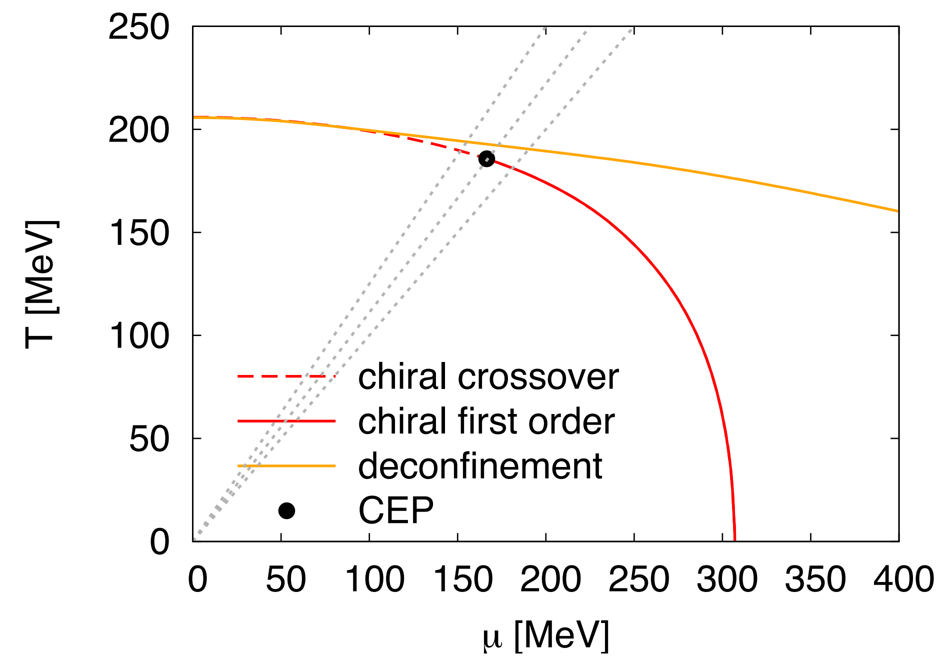
Thermodynamics near the CEP

- quark number susceptibility
  - diverges at CEP
- lower orders also in PNJL (Ratti et al. Phys. Lett. B649, 57-60)
- breakdown of Taylor expansion or signal ?



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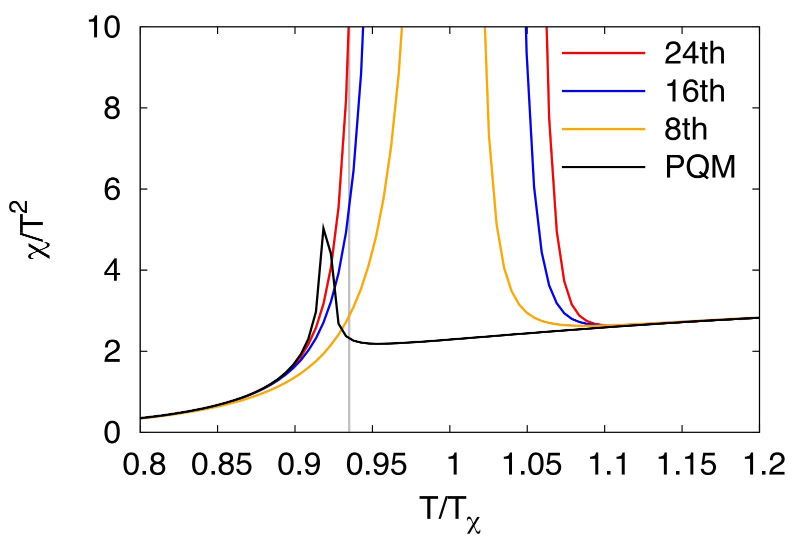

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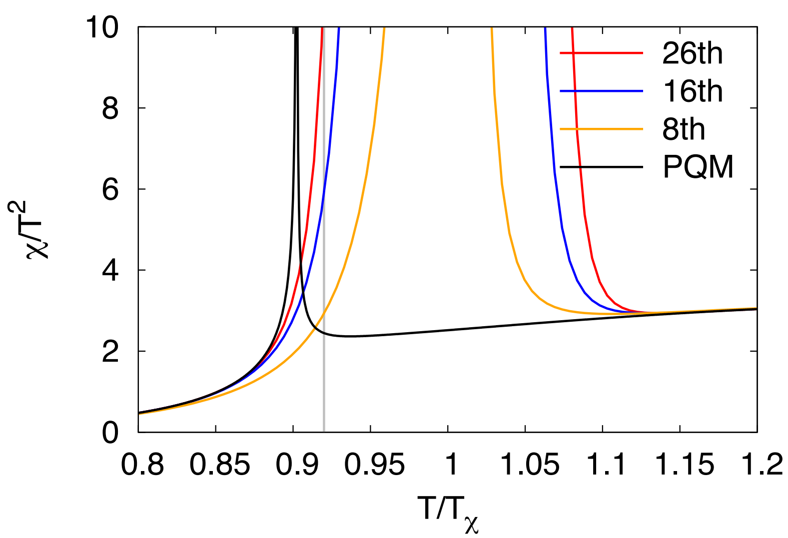

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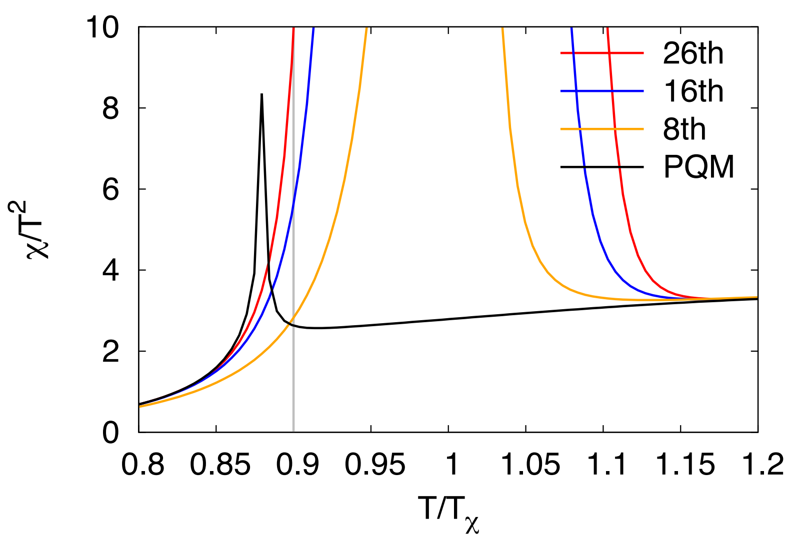
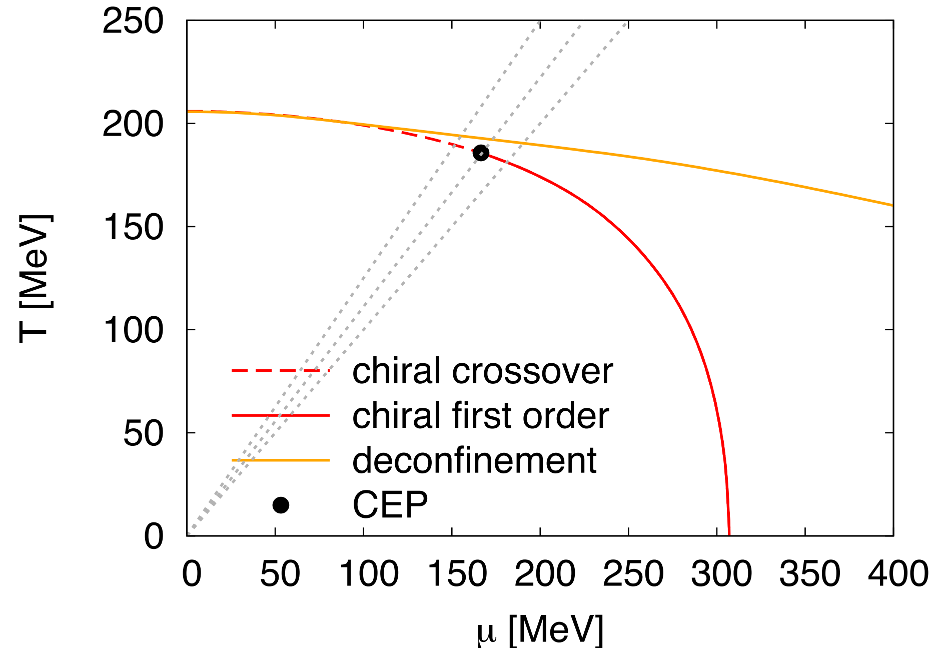
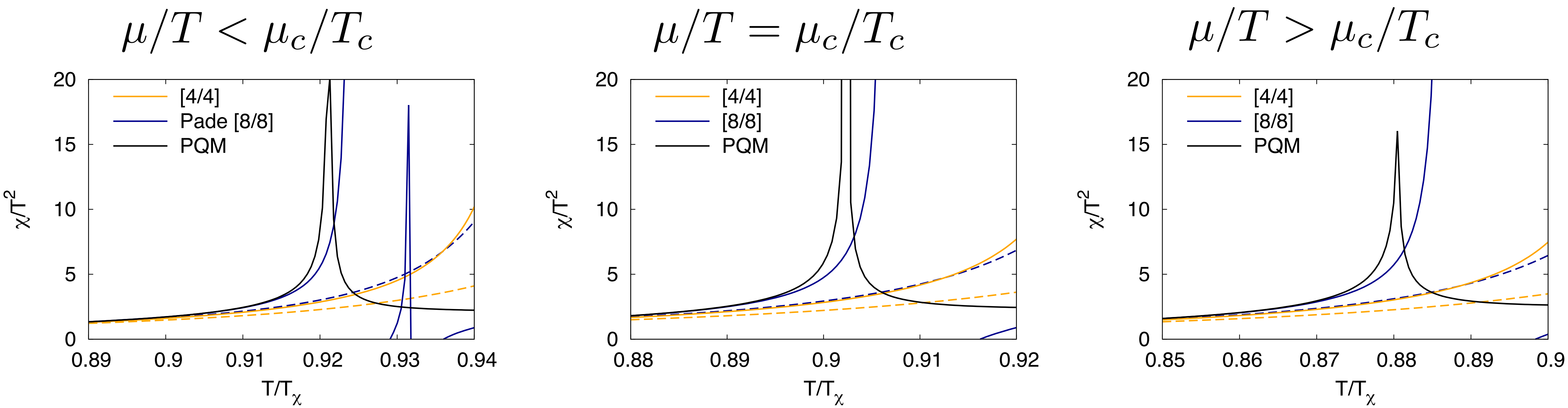


Padé-improved thermodynamics

- $[L/M] \equiv R_{L,M}(x) = \frac{p(x)}{q(x)} = \frac{p_0 + p_1 x + \cdots + p_L x^L}{1 + q_1 x + \cdots + q_M x^M}$
- rarely used for μ-extrapolations
  (M. P. Lombardo PoS LAT2005, 168)
- more suitable for description of singularities, i.e. divergent susceptibility at the CEP



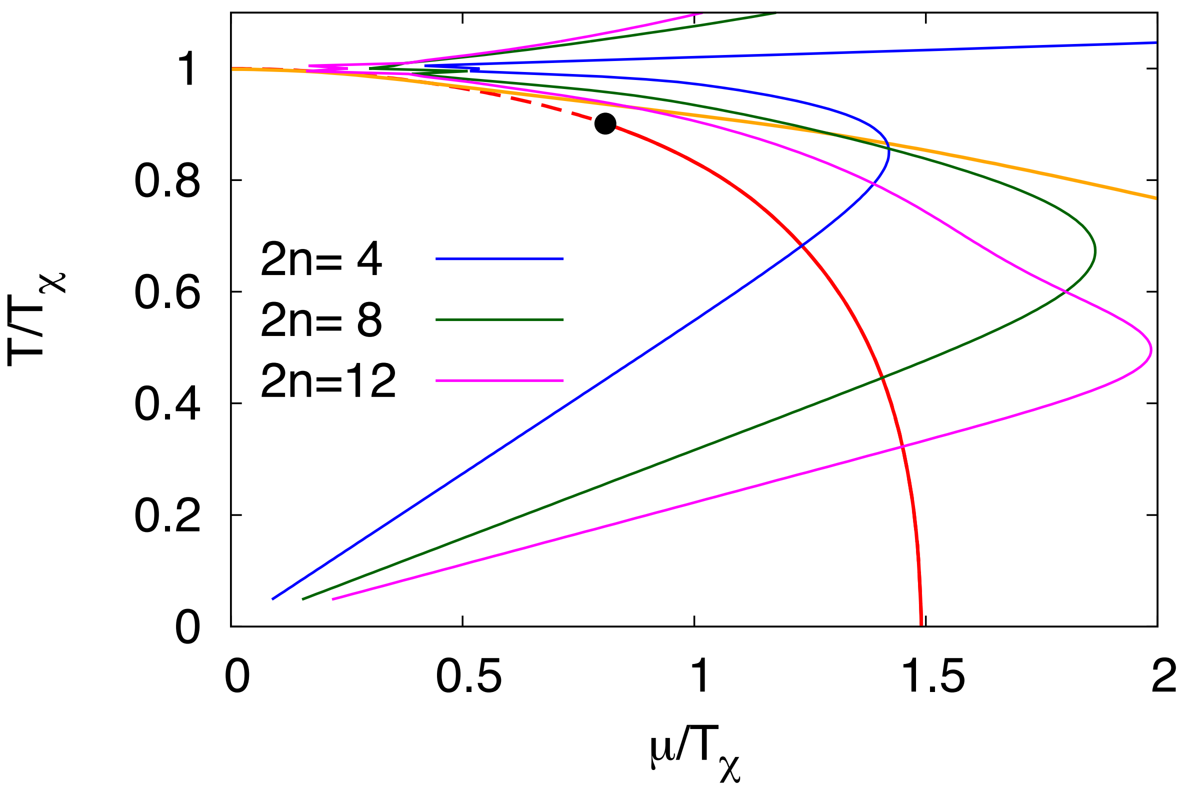


solid: Padé-approximation; dashed: Taylor expansion at corresponding order

Convergence radii and phase boundary

F. Karsch, B-J. Schaefer, MW, J. Wambach, arXiv:1009.5211

$$r = \lim_{n\to\infty} r_{2n} = \lim_{n\to\infty} \left| \frac{c_{2n}}{c_{2n+2}} \right|^{1/2}$$



Red line: chiral crossover (dotted), 1st order (solid)
Yellow line: deconfinement crossover
Black dot: chiral critical end point

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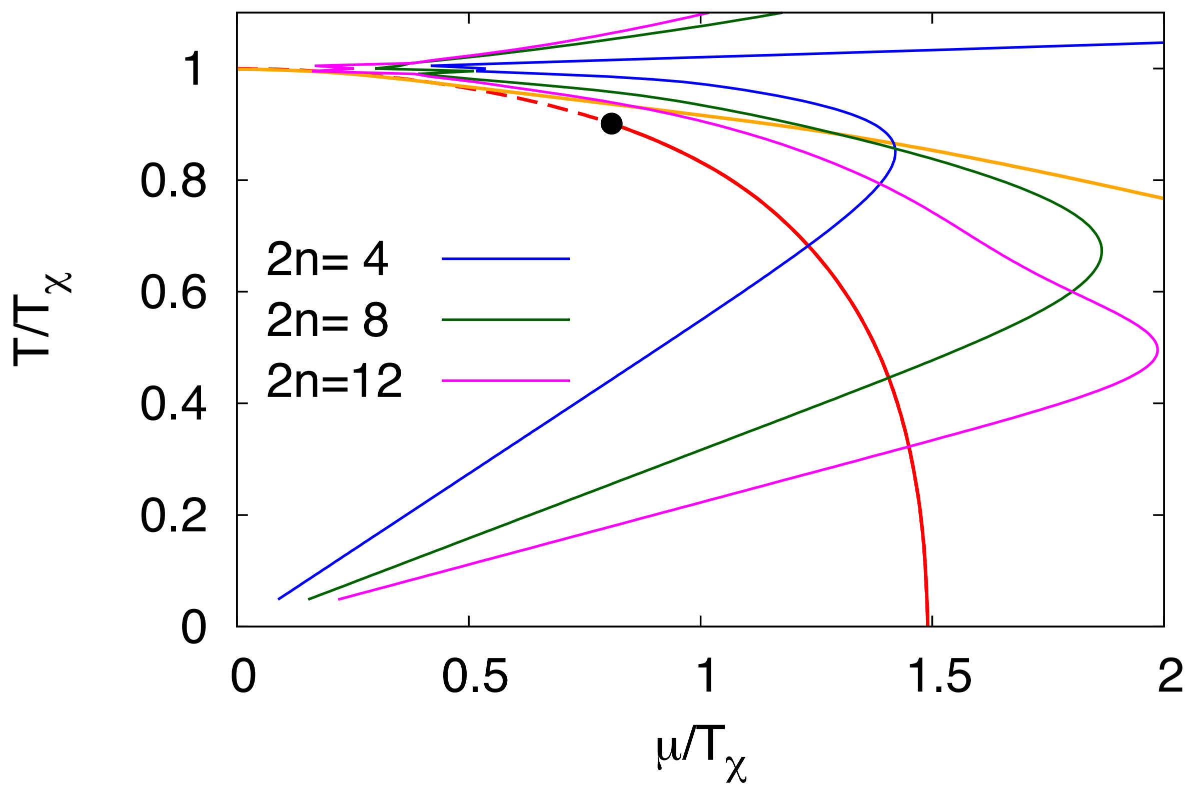

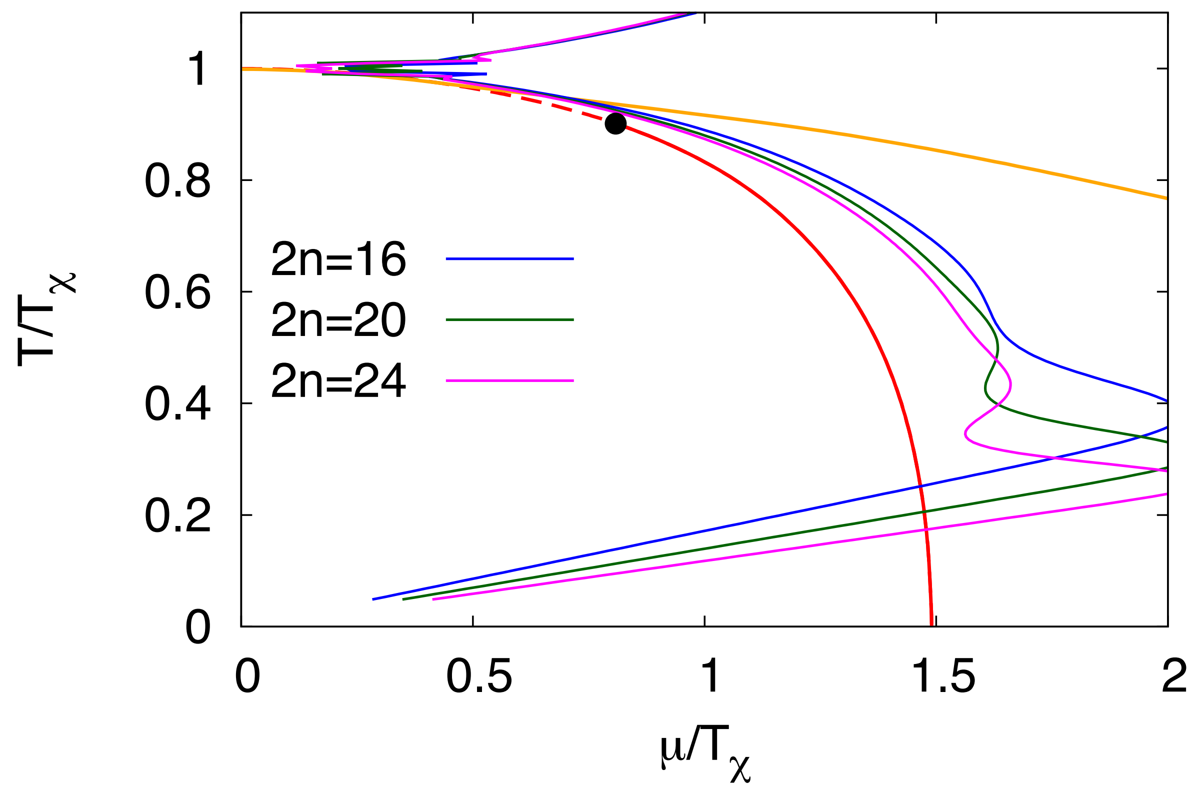

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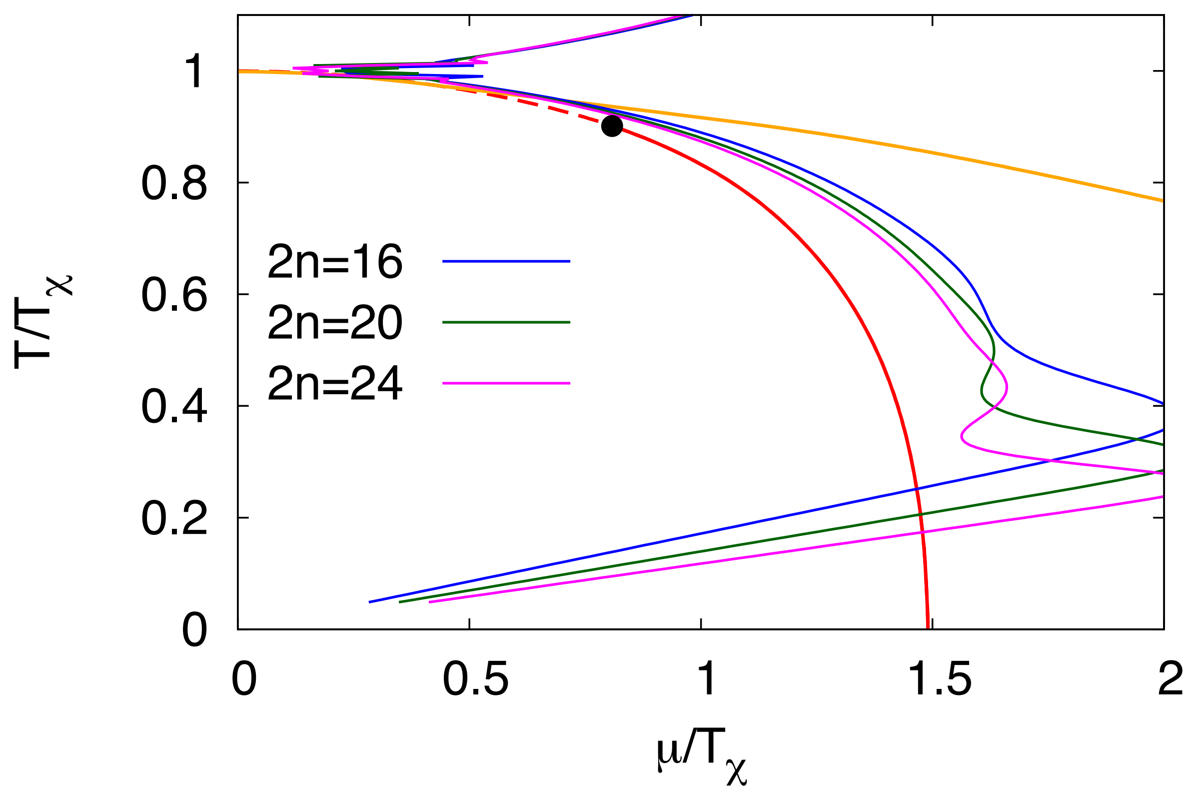

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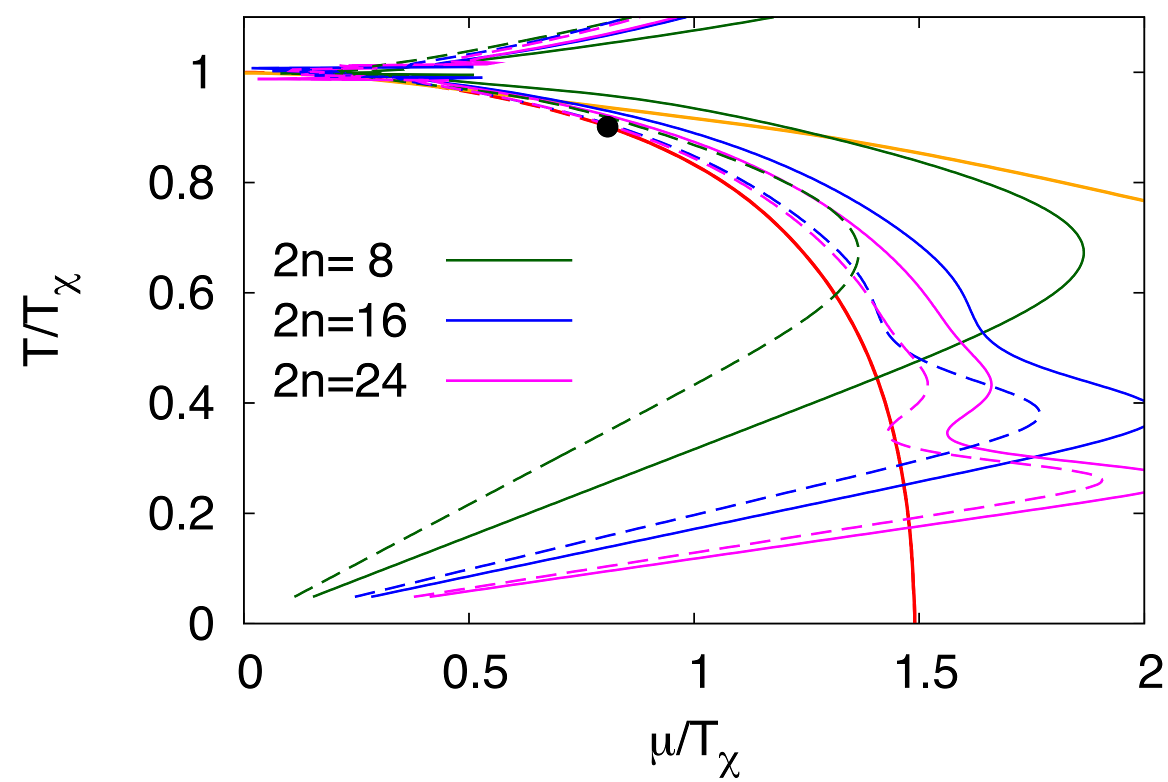
- quark number susceptibility

$$r_{2n}^{\chi} = \left| \frac{c_{2n}^{\chi}}{c_{2n+2}^{\chi}} \right|^{1/2} = \left| \frac{(2n+2)(2n+1)}{(2n+3)(2n+4)} \right|^{1/2} r_{2n+2}$$



solid lines: convergence radius estimate for the pressure at finite n
dashed lines: estimate for the quark number susceptibility

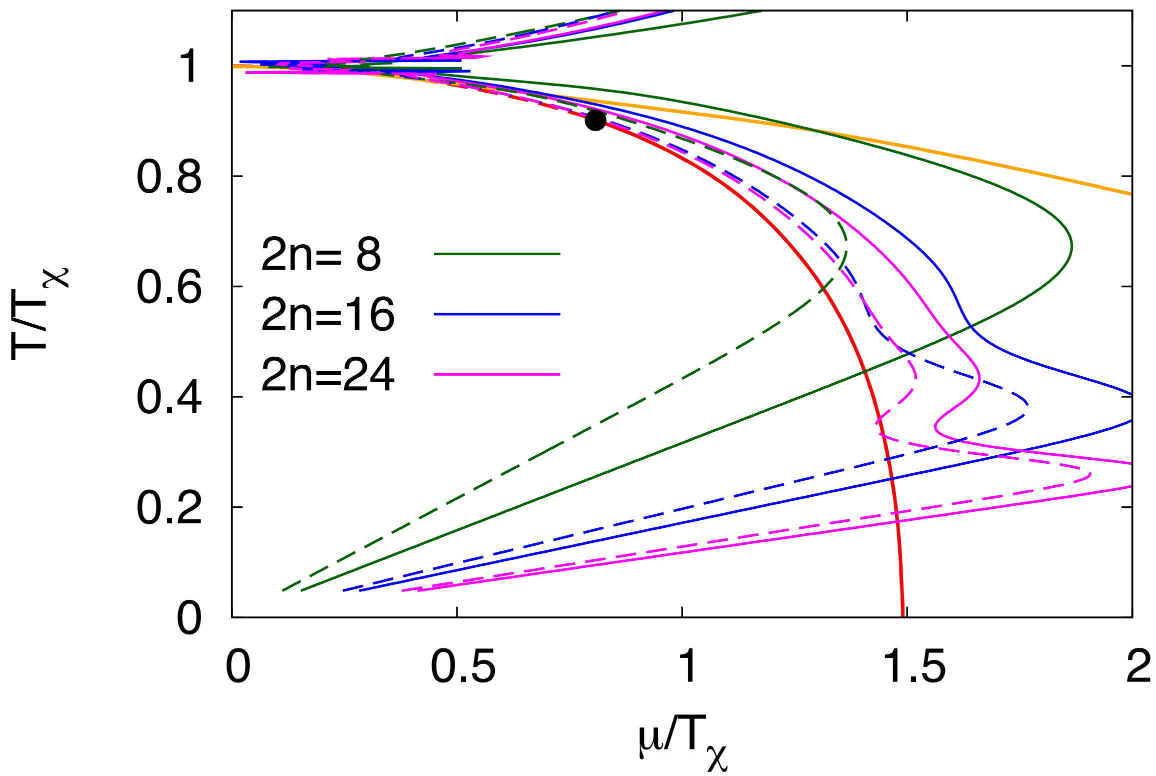
Convergence radii and phase boundary

F. Karsch, B-J. Schaefer, MW, J. Wambach, arXiv:1009.5211

- only finite number of coefficients
- apparent convergence
- nice reproduction at large T
- at lower temperatures:
  1st order transition
  →conceptual problem
- expansion works also for $\mu/T > 1$
- better estimate with susceptibility

- quark number susceptibility

$$r^{\chi}_{2n} = \left| \frac{c^{\chi}_{2n}}{c^{\chi}_{2n+2}} \right|^{1/2} = \left| \frac{(2n+2)(2n+1)}{(2n+3)(2n+4)} \right|^{1/2} r_{2n+2}$$



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Comparison of criteria for phase boundary

F. Karsch, B-J. Schaefer, MW, J. Wambach, arXiv:1009.5211

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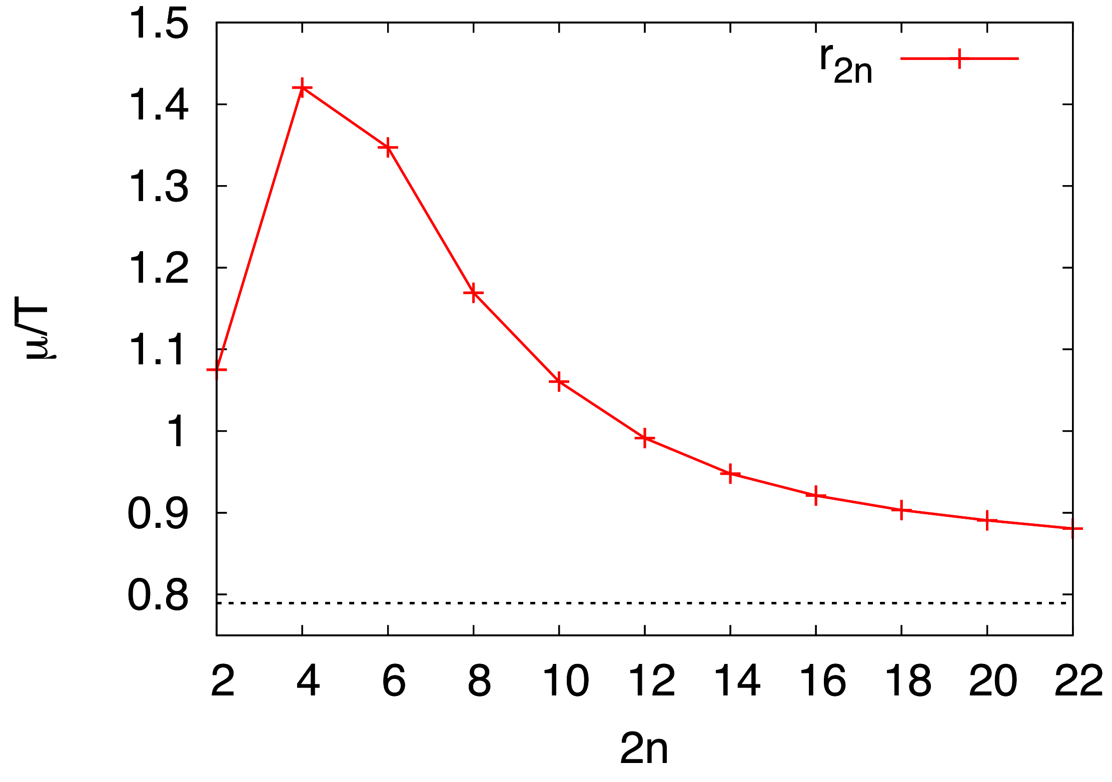
  - for pressure



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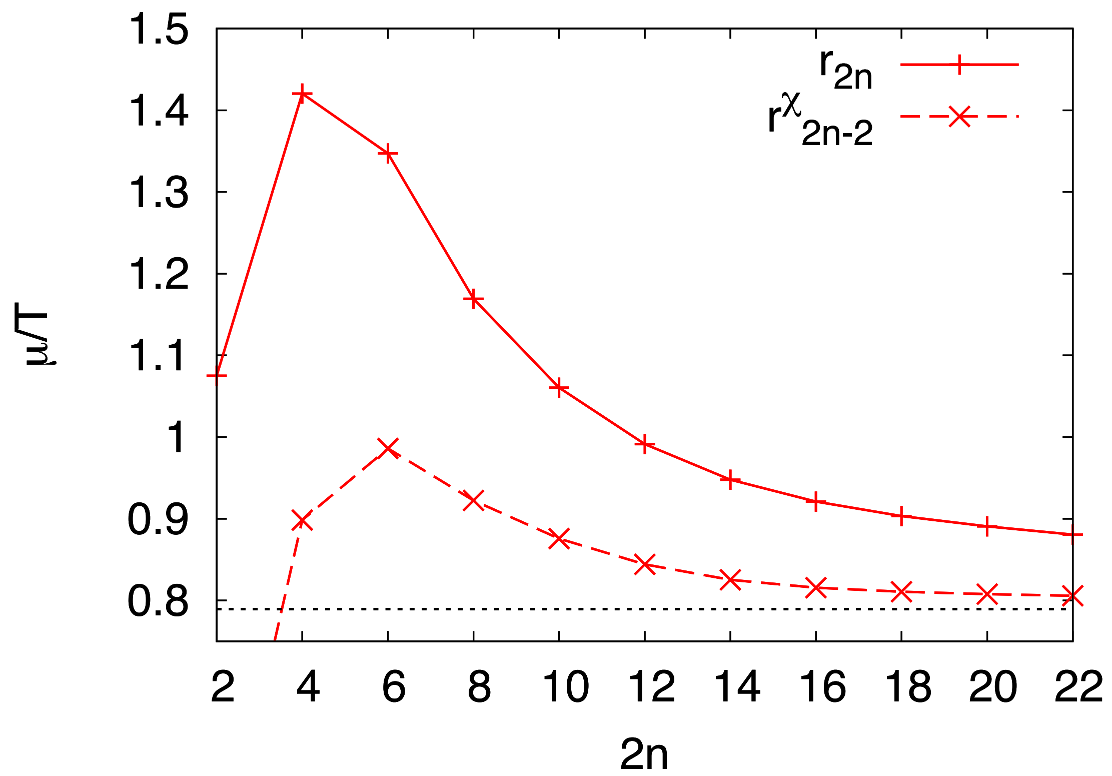

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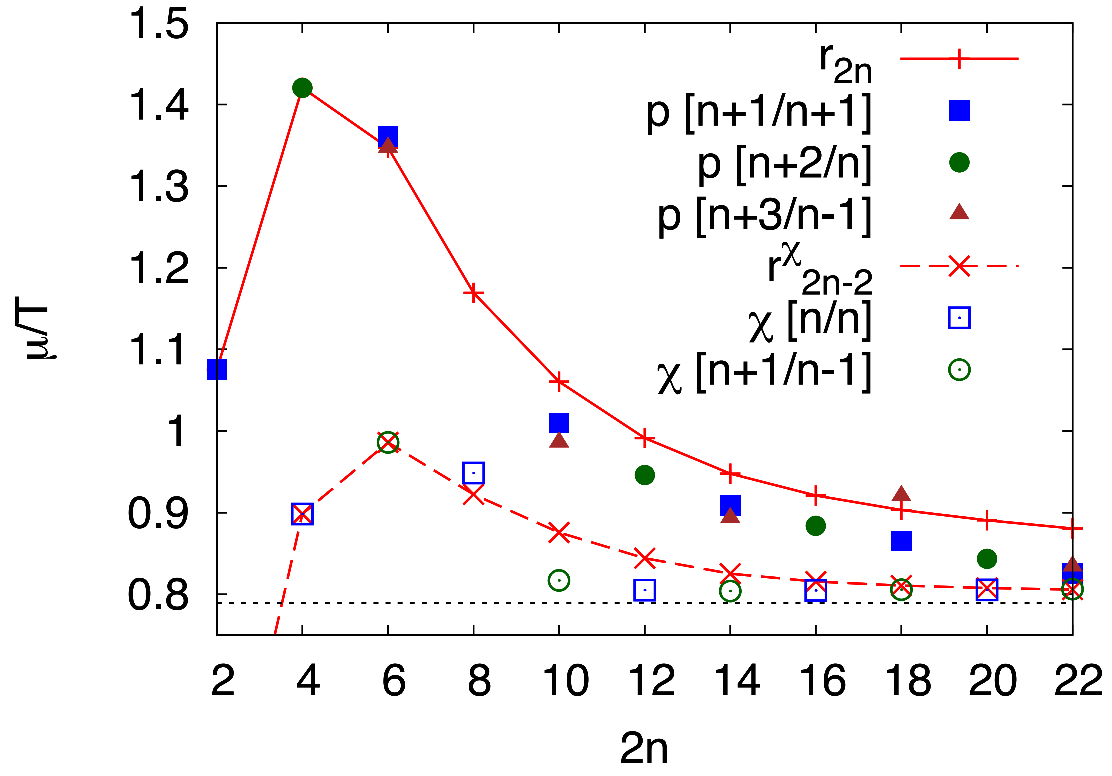
  - requires at least 3 coefficients
  - uses all coefficients as input
  - error propagation is more involved; under control with AD



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significant improvement for susceptibility and Padé approximation

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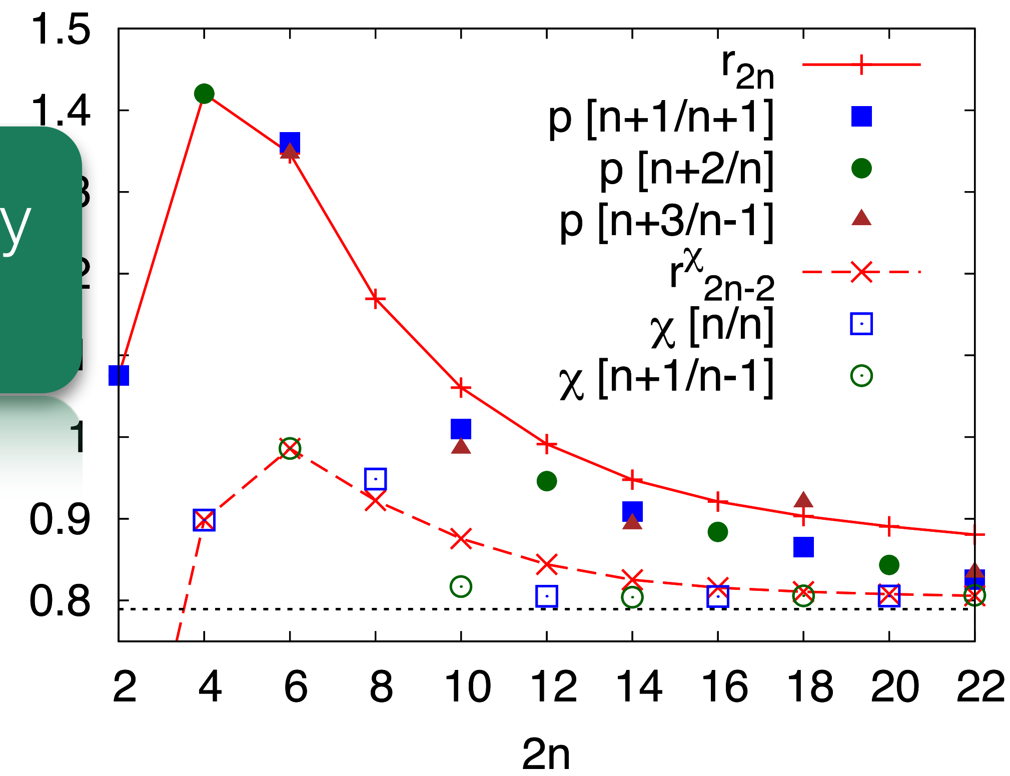

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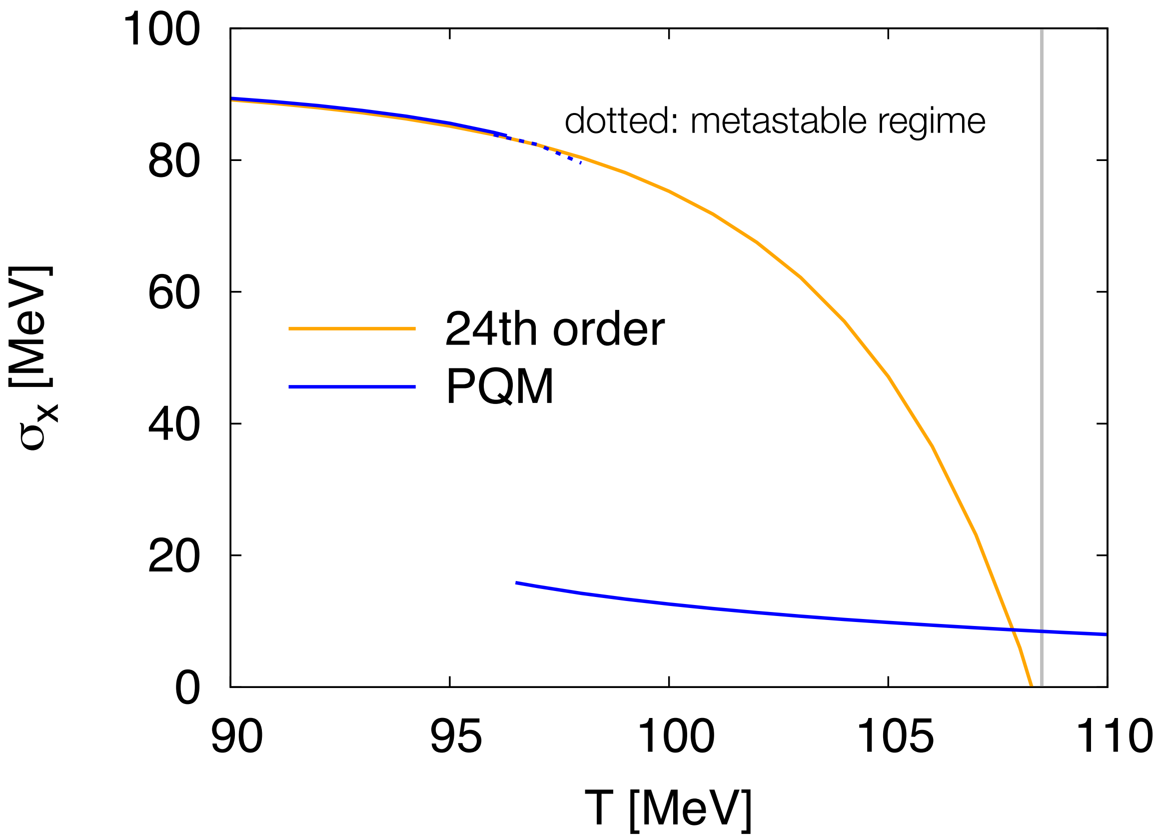
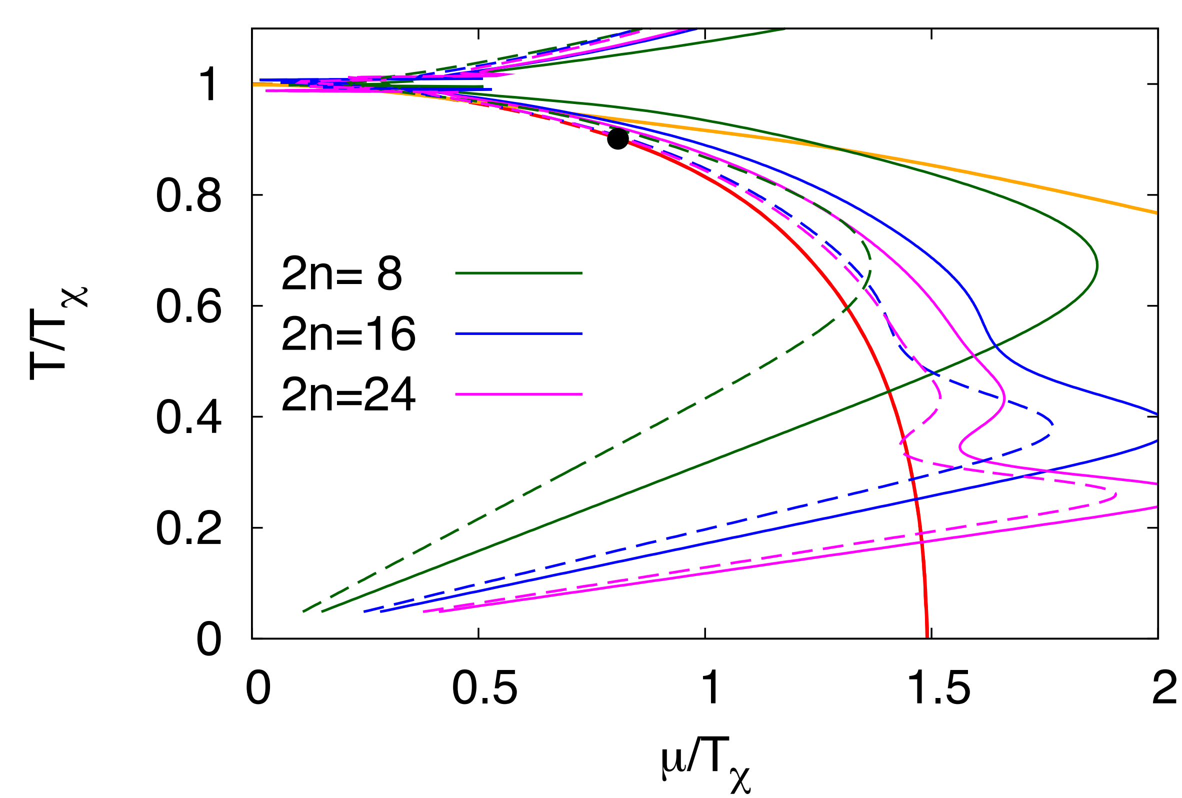
Closer look at first-order transition

- consider $\mu/T = 3$
- first order transition: new global minimum in grand potential
  - not captured by Taylor expansion





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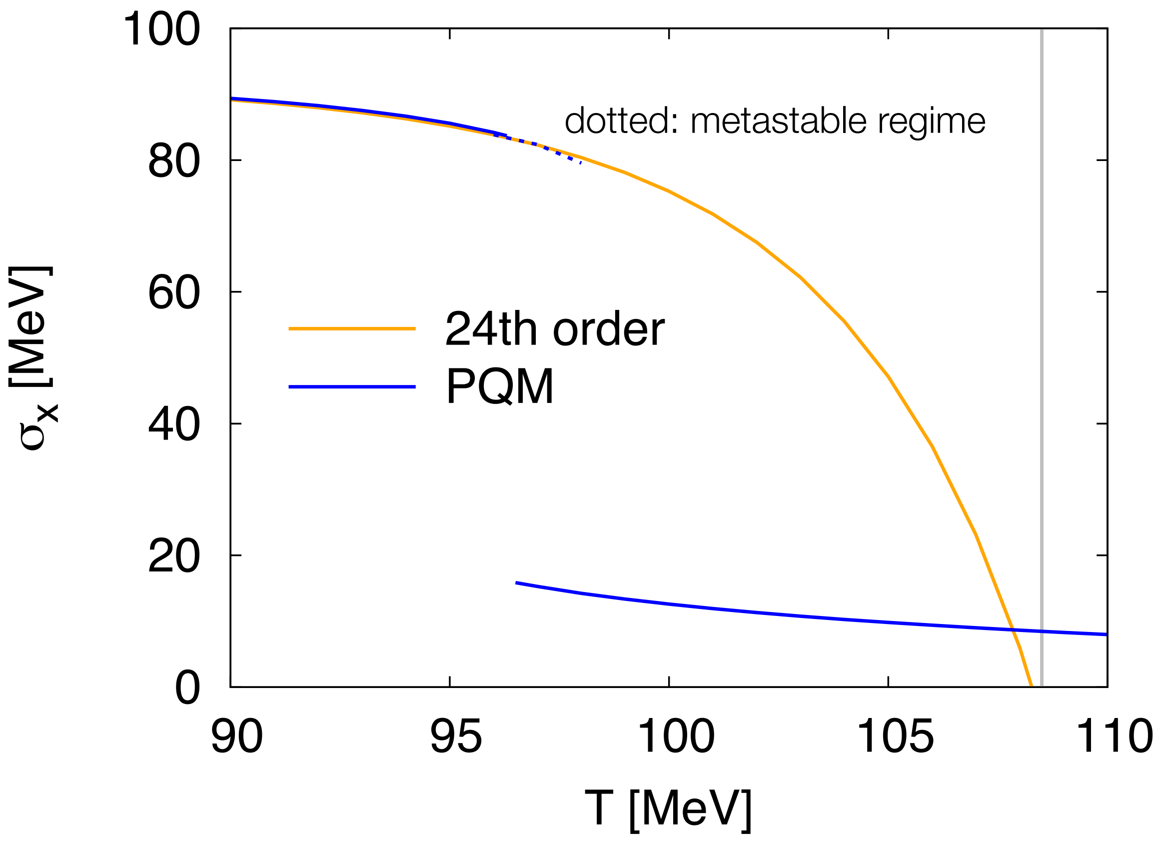
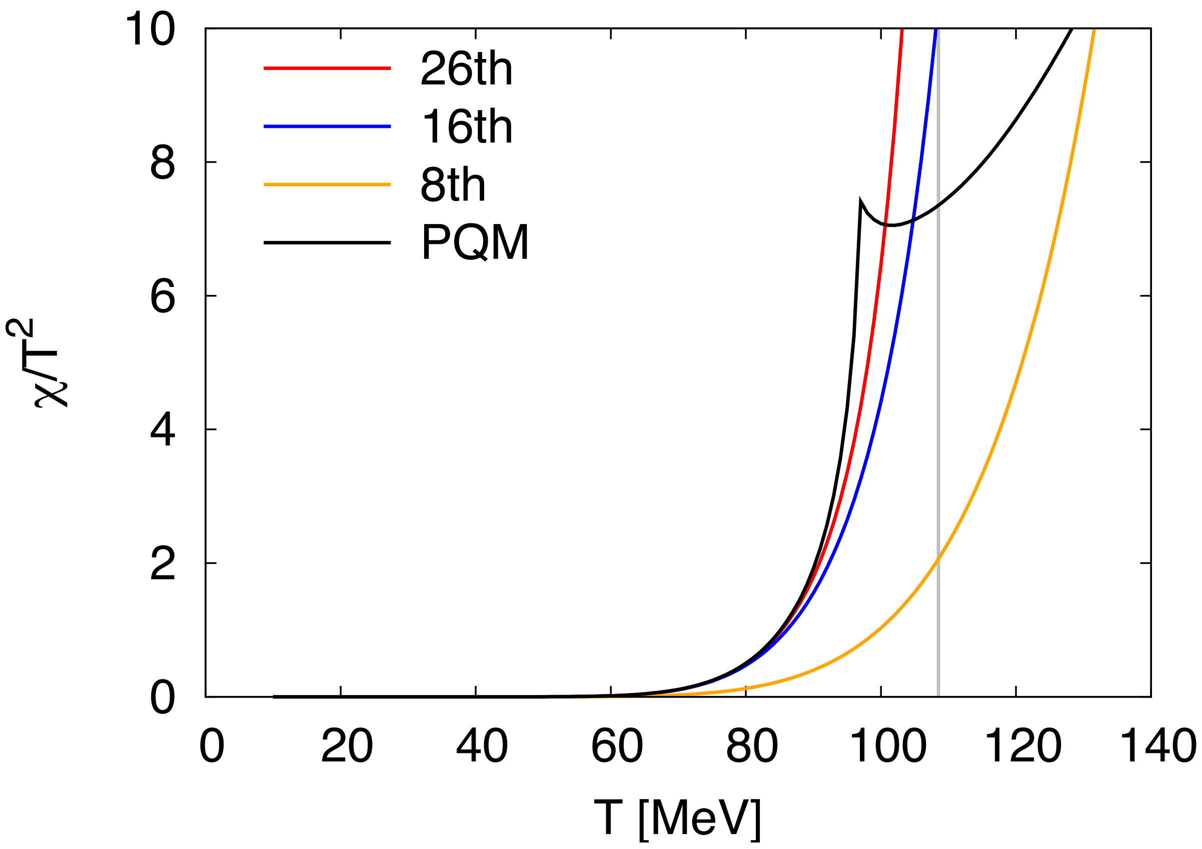
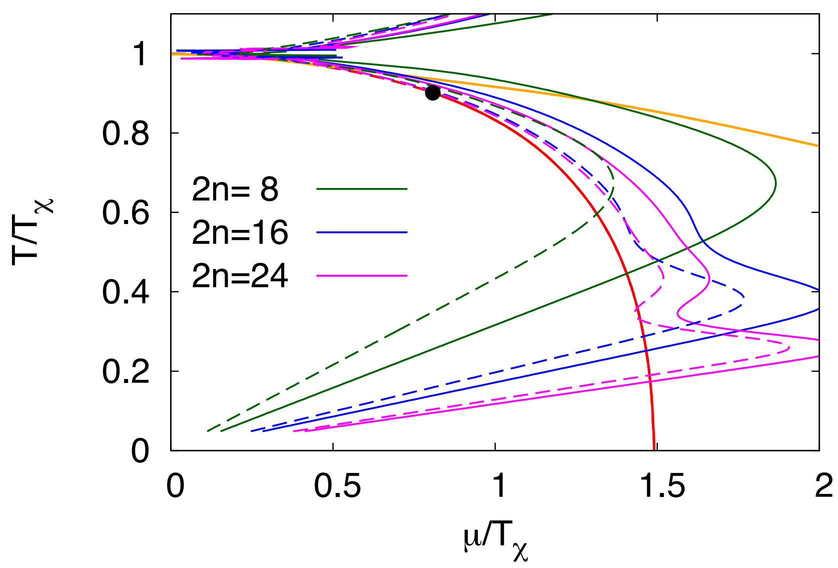




Locating the critical endpoint

- phase boundary already estimated
- still need determine T_c : sign of coefficients
- consider $T \sim T_{c,16}$, i.e. where c_{16} changes sign



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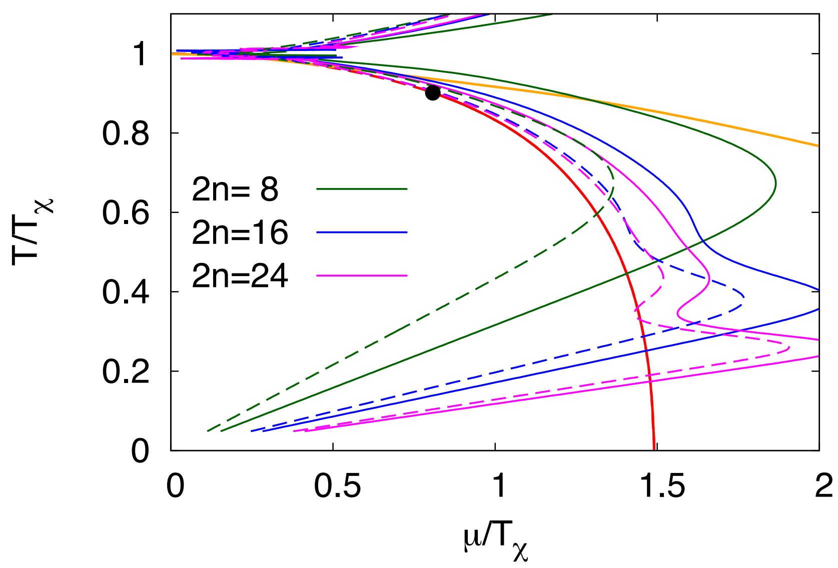
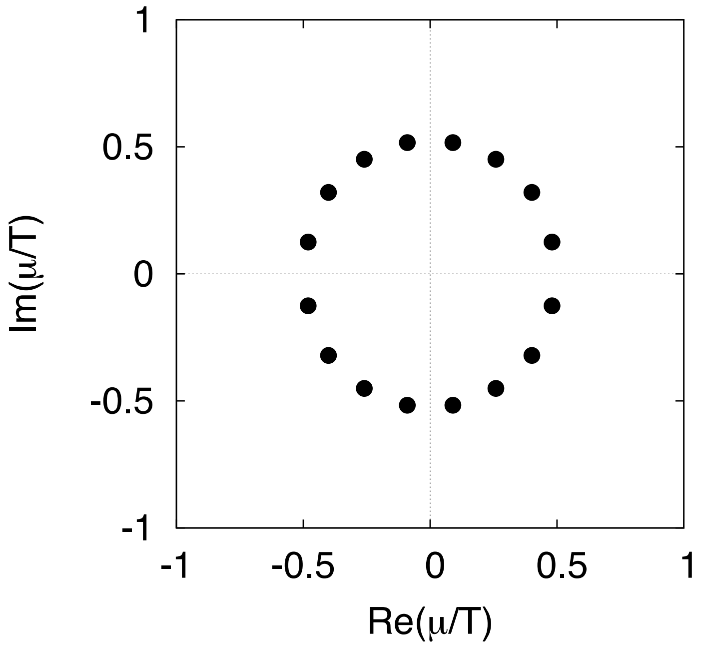


$c_{16} > 0$



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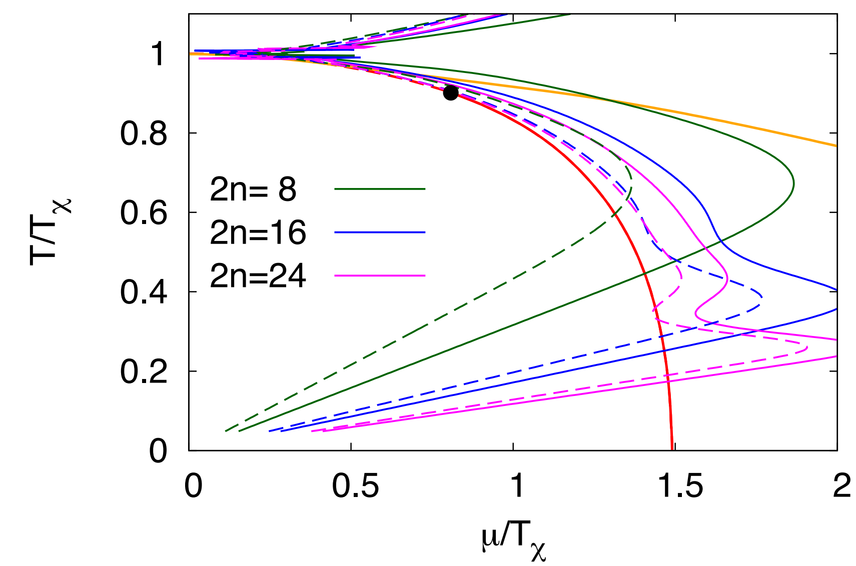

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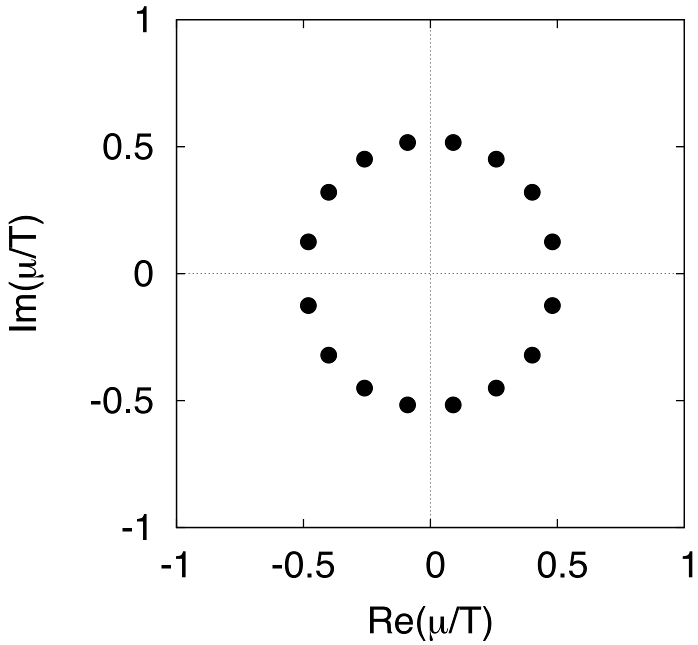

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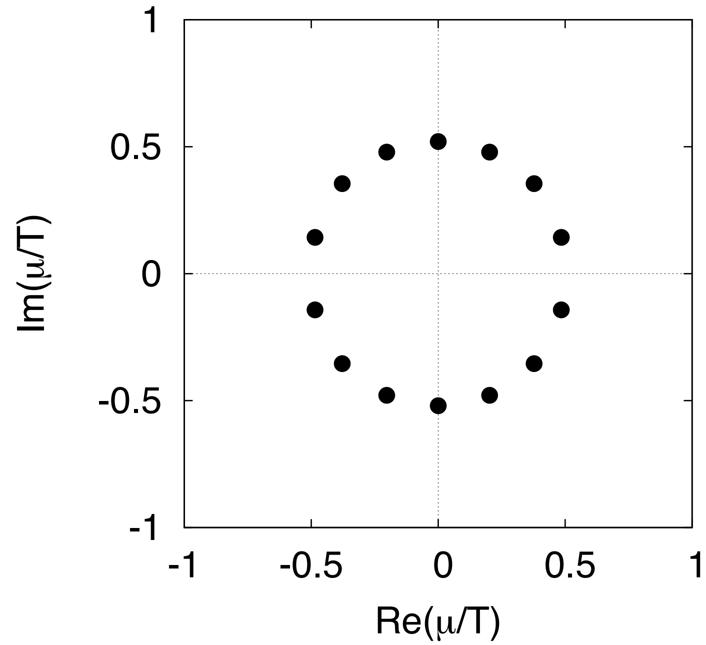

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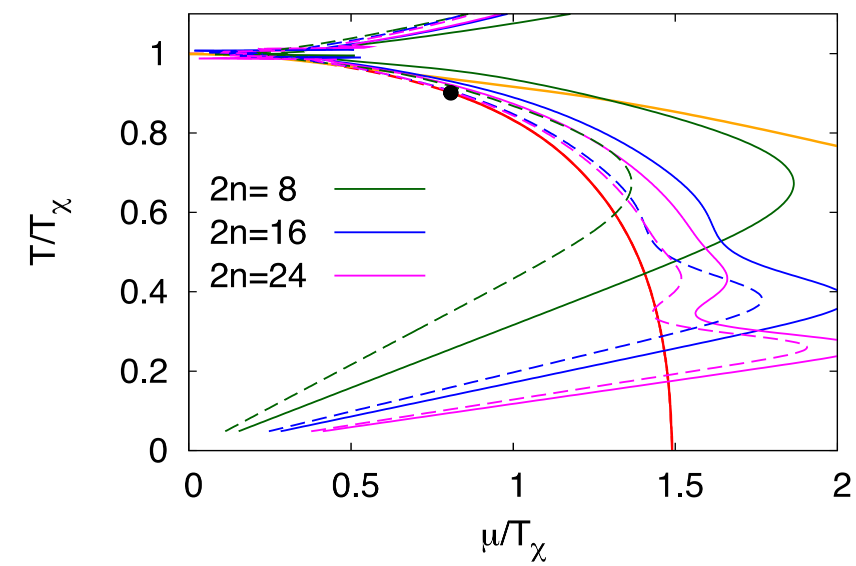

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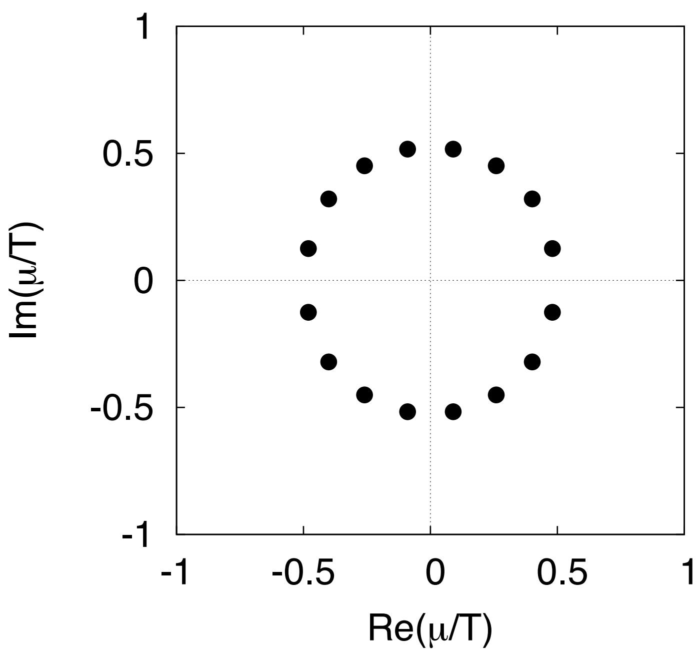

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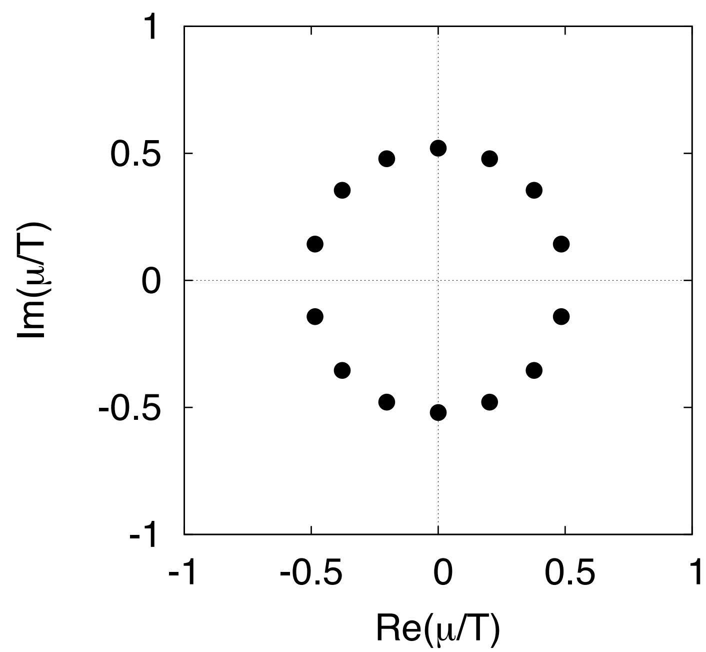

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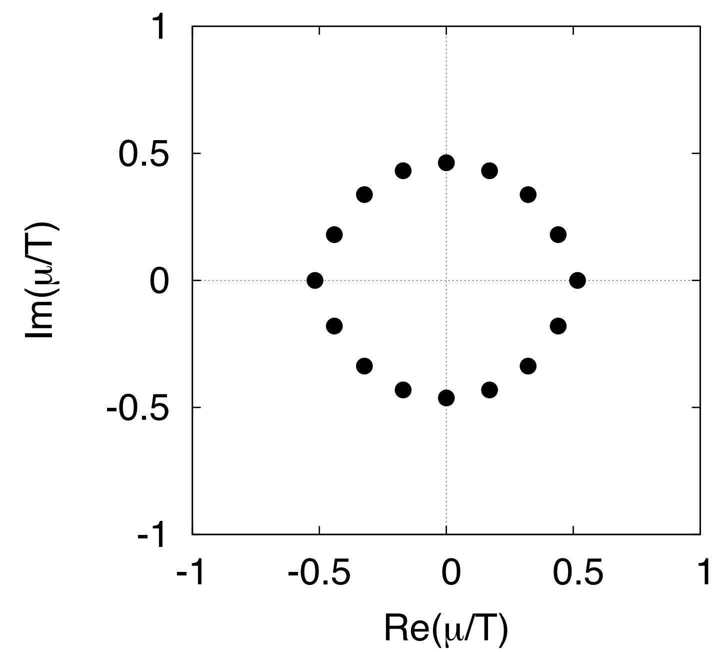

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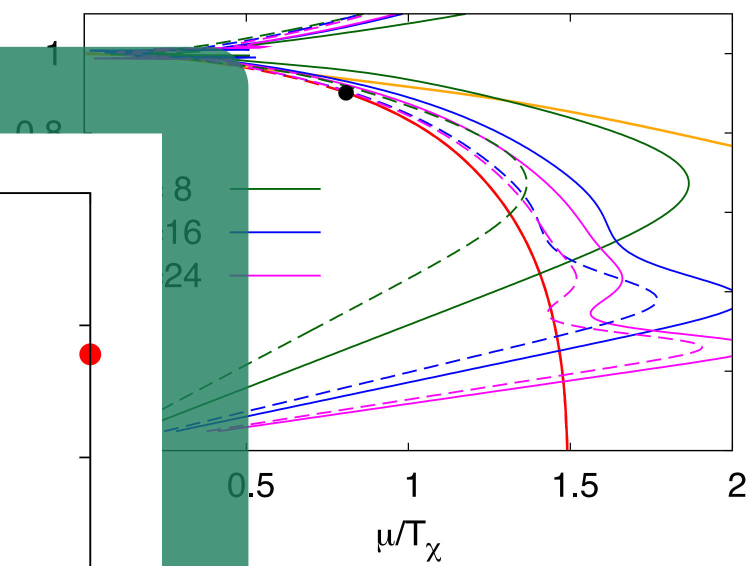

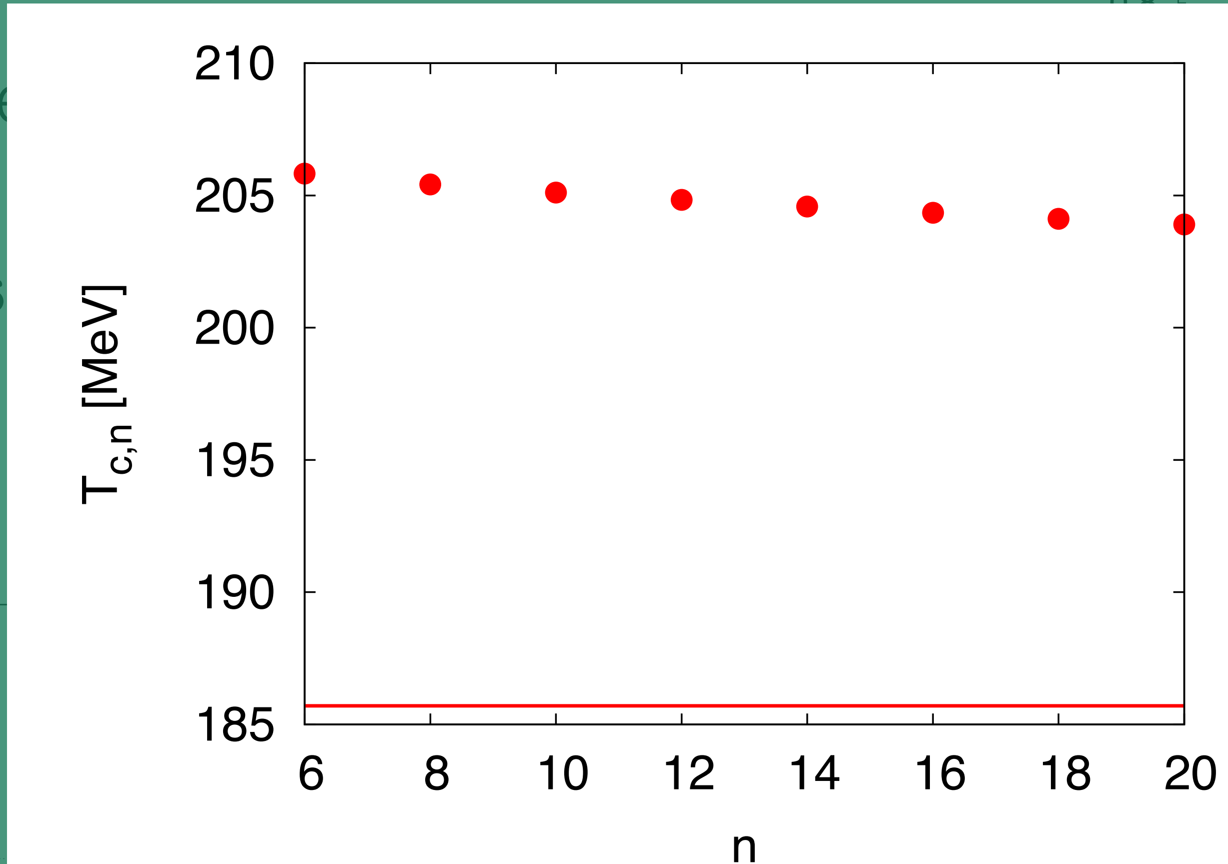

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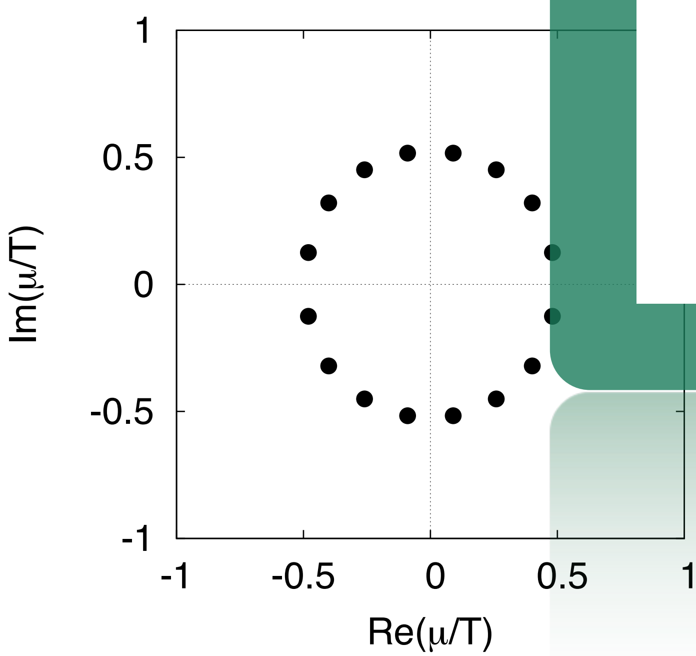

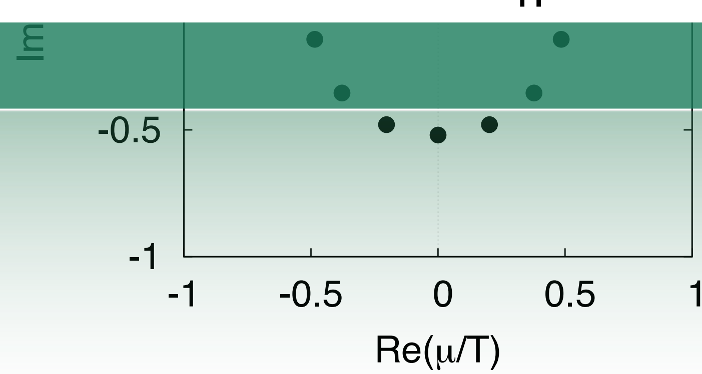

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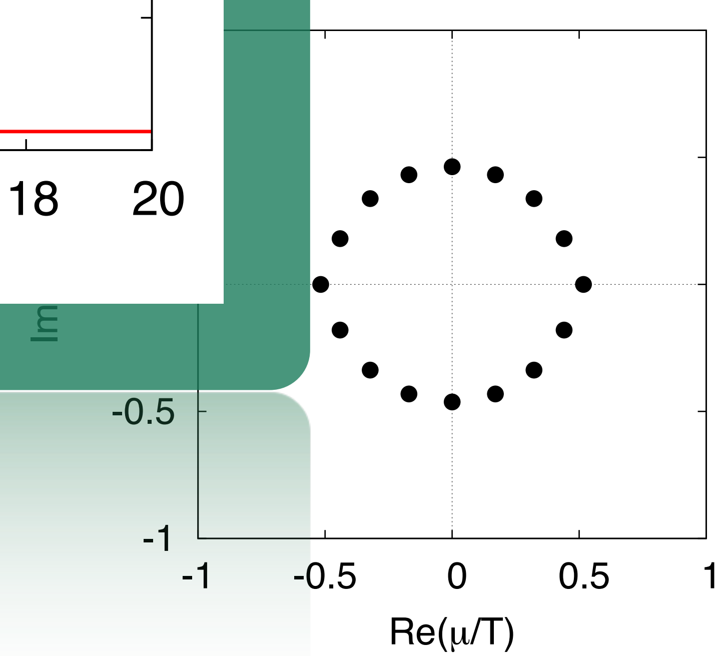

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  - from Taylor expansion
  - better estimate with susceptibility
  - higher coefficients are necessary (obtained with AD)
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    - exploit the Padé approximation
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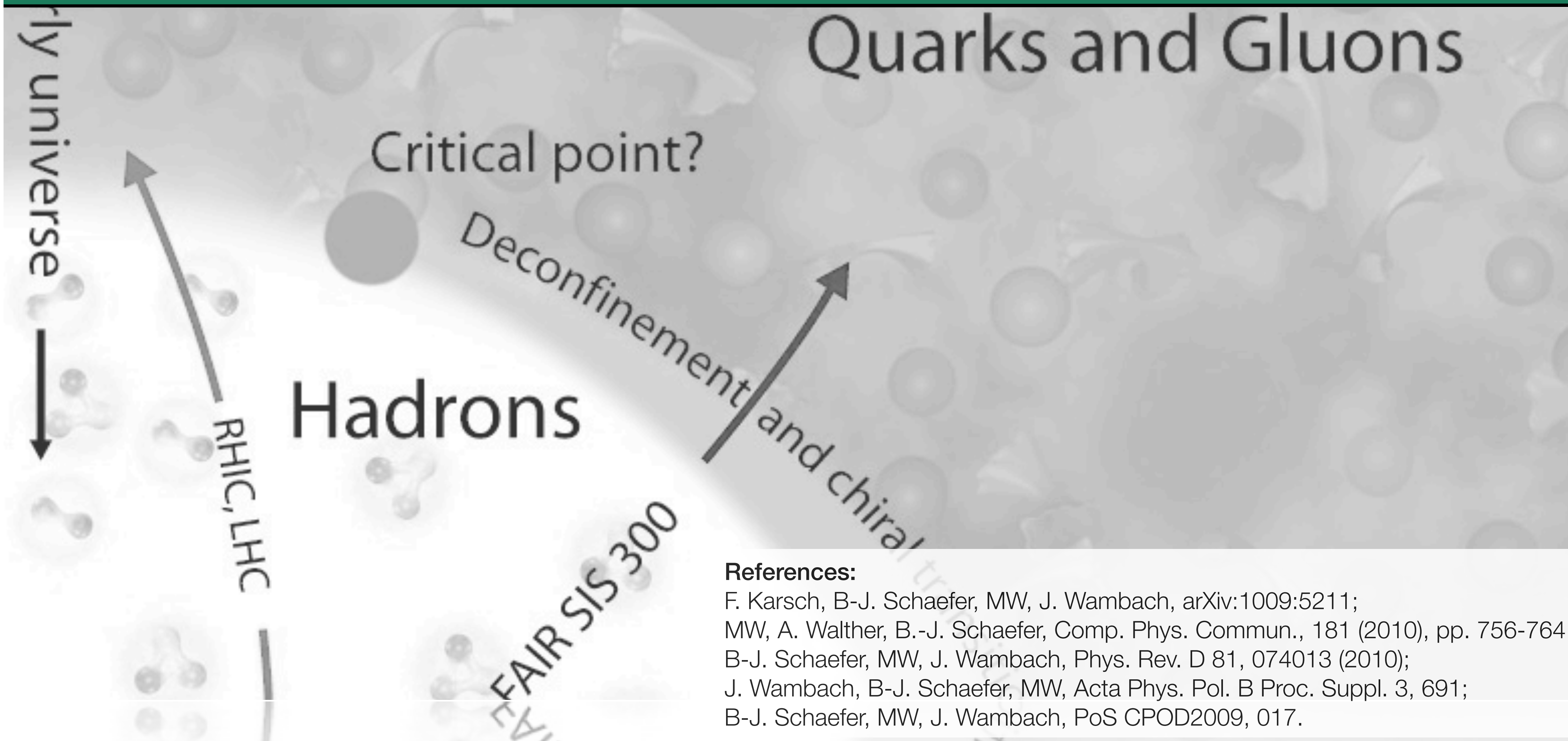
- functional studies:
    - μ-corrections in Polyakov loop potential (Schaefer et al., Phys.Rev. D76, 074023)
    - include fluctuations (RG) ? (e.g. Herbst et al., arXiv:1008.0081; Skokov et al., arXiv:1008.4570)

Towards finite density QCD with Taylor expansions



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