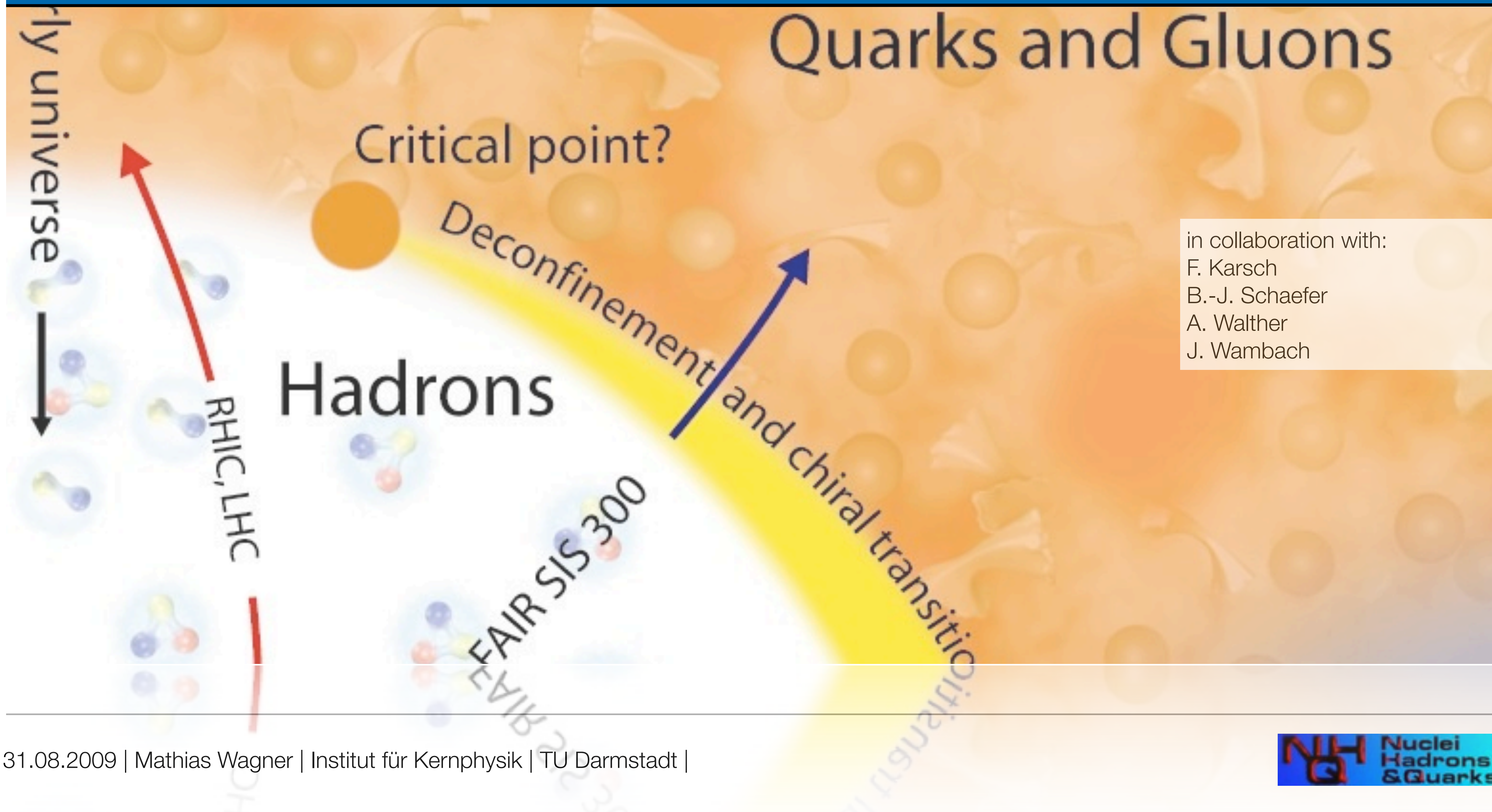
Can we locate the QCD critical endpoint with the Taylor expansion ?



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

Outline

- Taylor expansion
  - expectations & lattice results
- higher orders in the PQM model
- convergence
- locating the critical endpoint

Taylor expansion

- expand pressure around $\mu = 0$

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

- coefficients evaluated at $\mu = 0$, i.e. Monte Carlo techniques applicable
- easy access to quark number densities & susceptibilities

Hopes

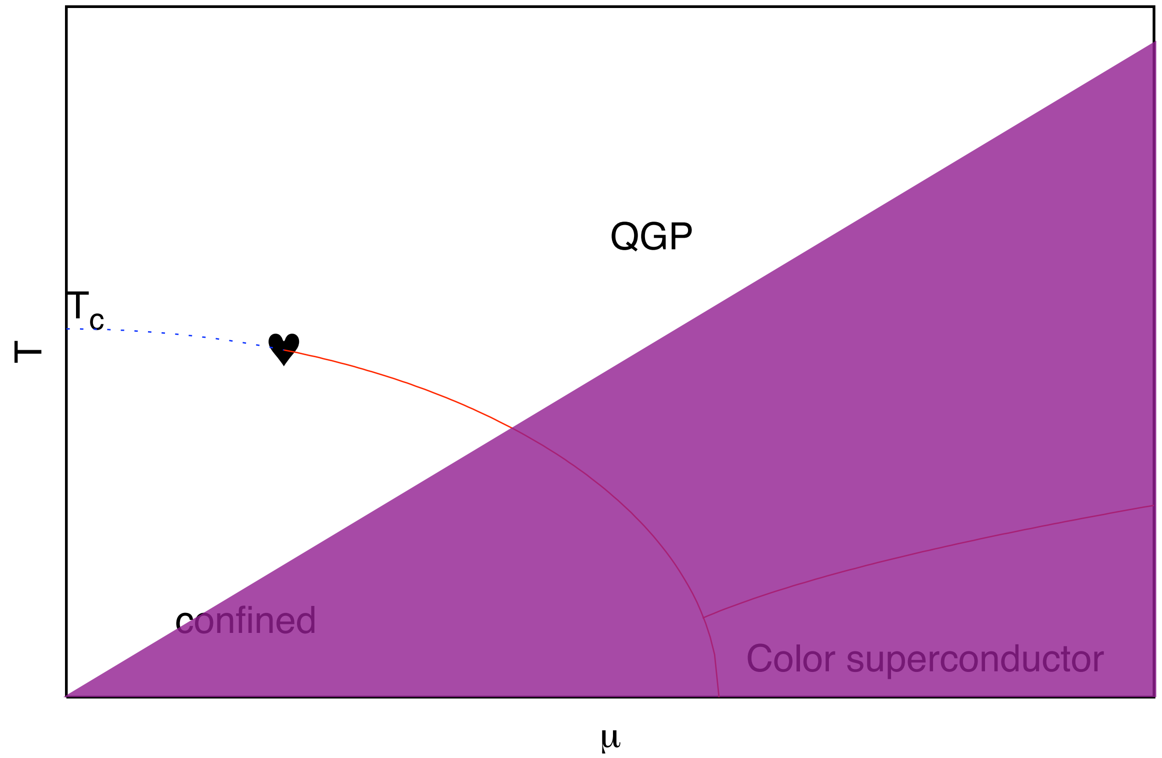
- works for small μ/T, i.e., $\mu/T < 1$
- only a few coefficients required for ‘convergence’

Hopes

- works fo
- only a fe

Philipsen (CPOD 2009)

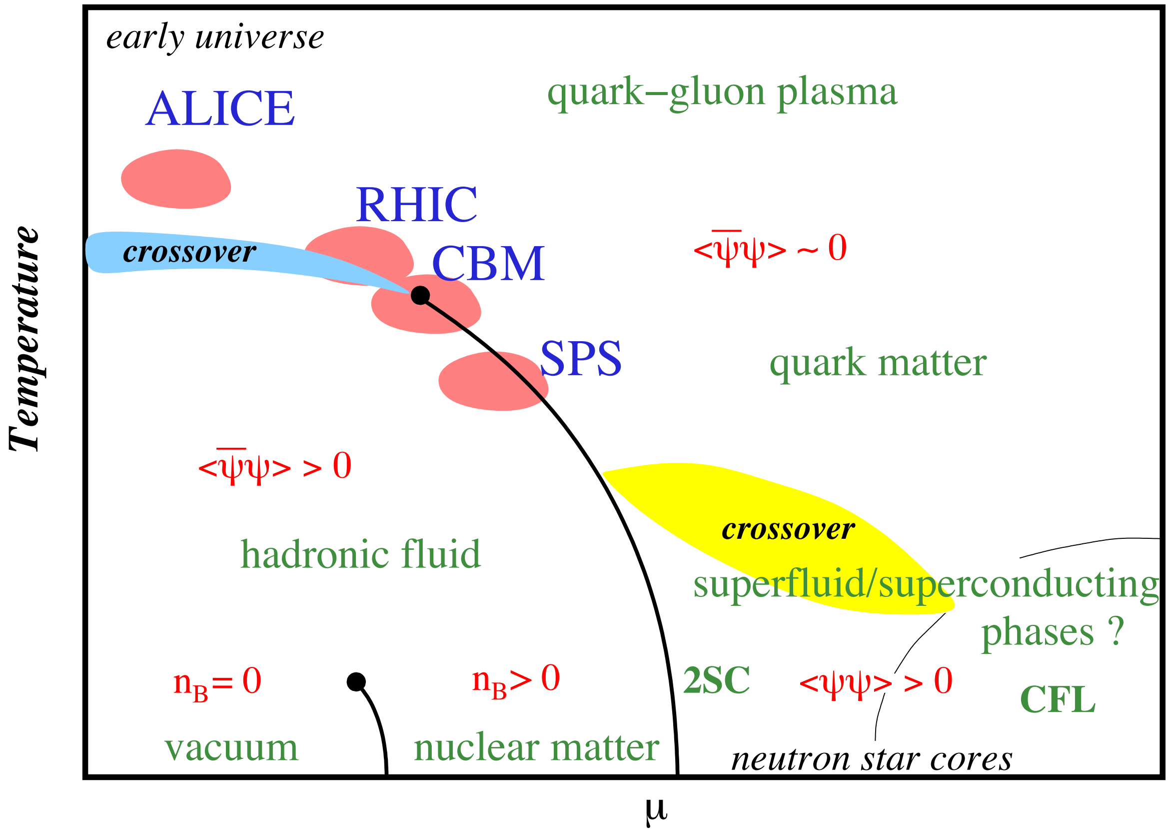
The calculable region of the phase diagram



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

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)



Convergence radius

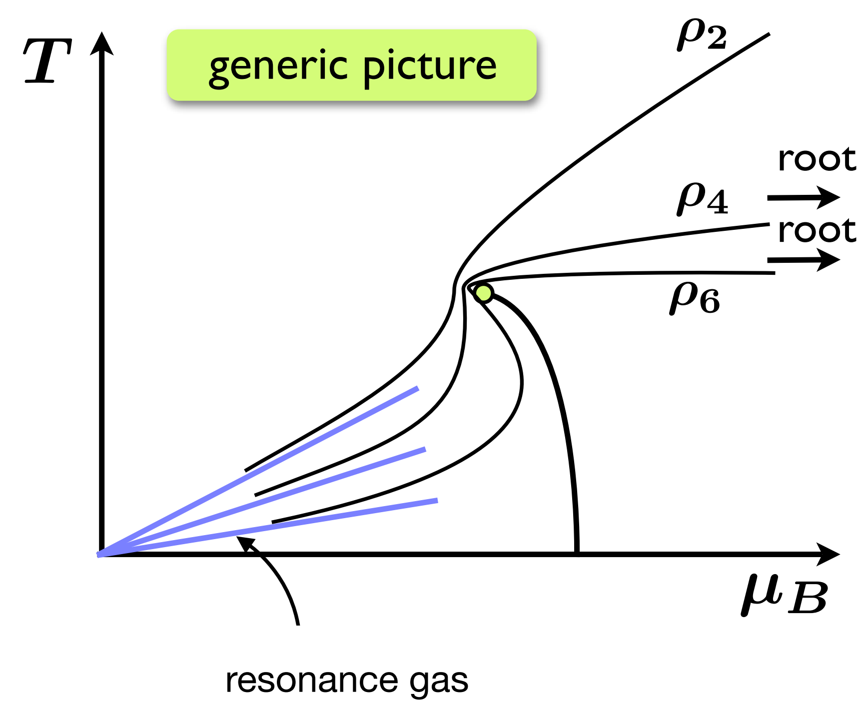
- defines where the expansion should work

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

- extrapolation to $n \to \infty$
- Stefan-Boltzmann limit:
  - $c_n \to 0$ for $n \geq 6$
- resonance gas: $r^{\mathrm{HRG}} \to \infty$

$$\left(r^{\mathrm{HRG}}_{(n)}\right)^2 = \left(\frac{c_n}{c_{n+2}}\right) = \frac{(n+2)(n+1)}{9}$$

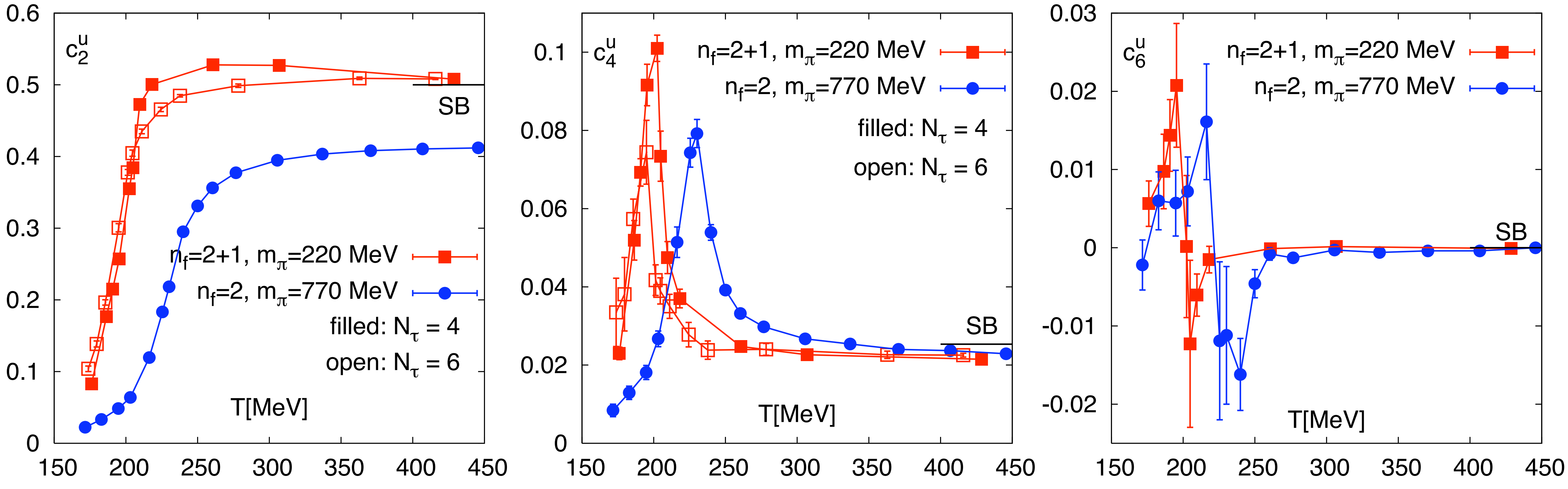
C. Schmidt (2008)



Results on the lattice

- coefficients are conceptually easy to simulate on the lattice

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



Signals of the critical endpoint ?

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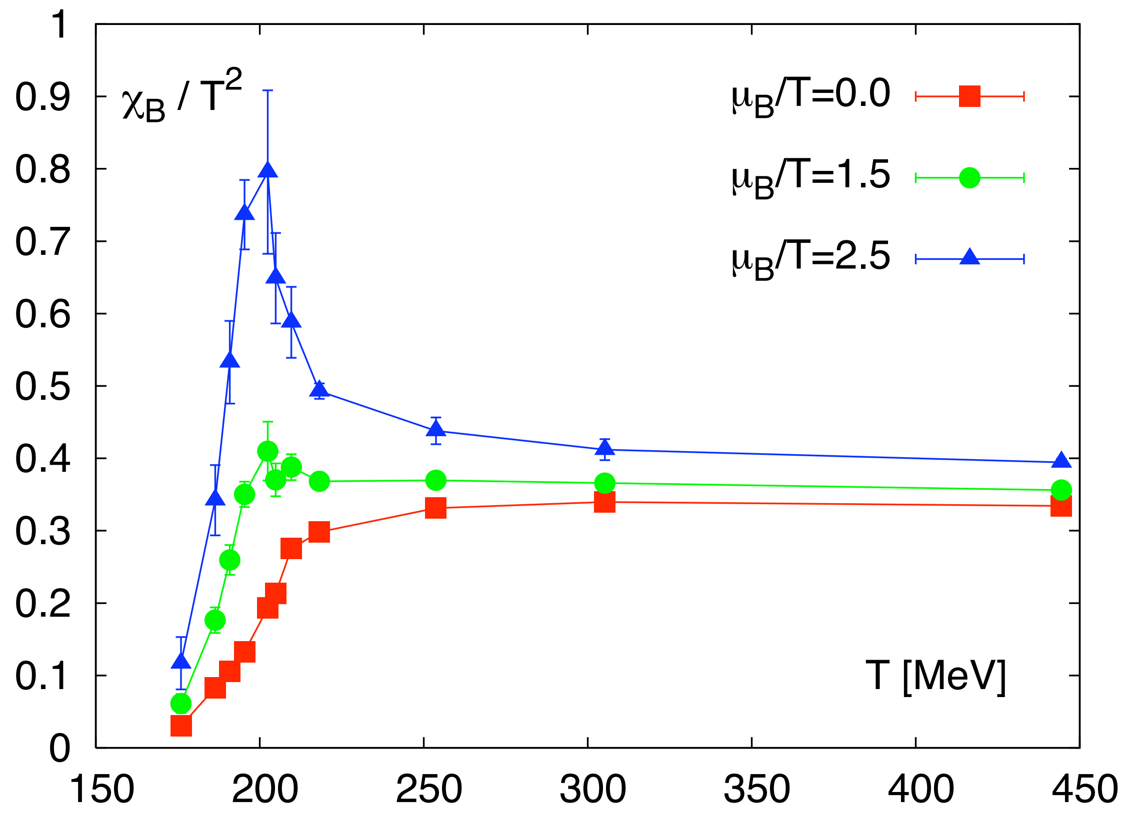
- quark number susceptibility

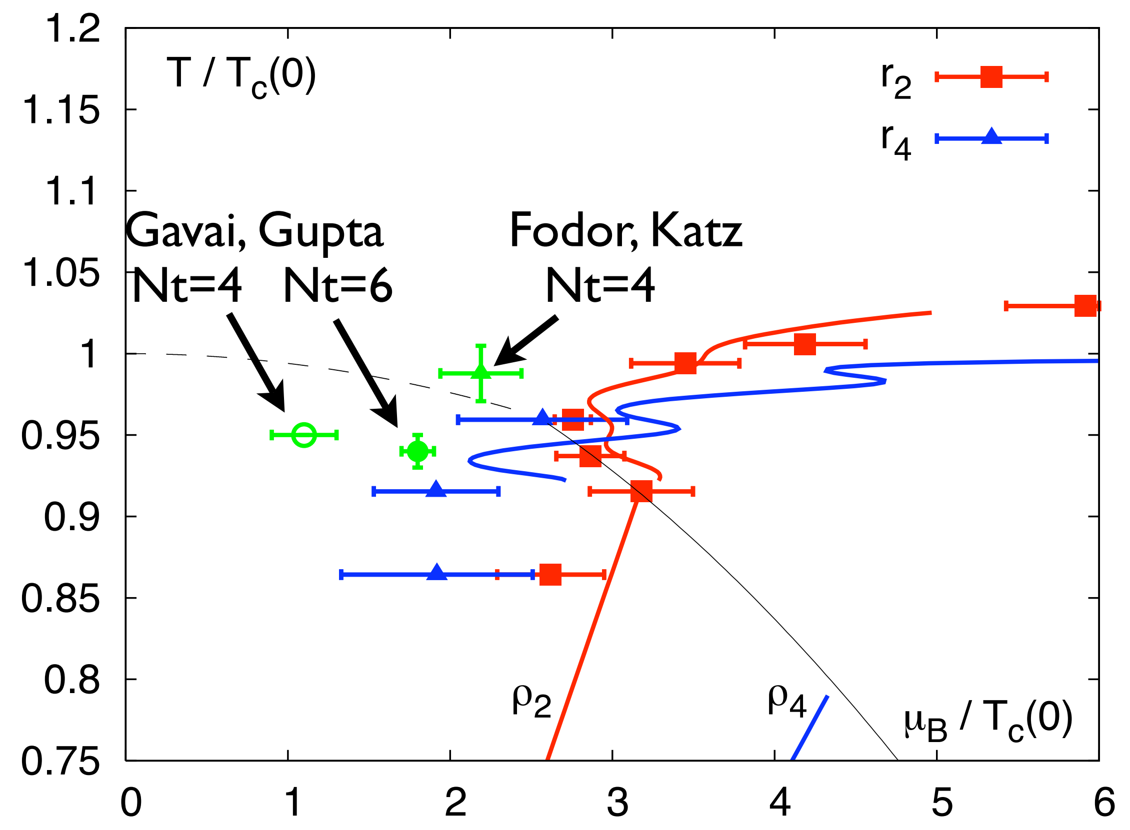
$$\frac{\chi_q(T,\mu)}{T^2} = -\frac{\partial^2 \Omega(T,\mu)}{\partial \mu^2}$$
$$= \sum_{n=2,4,\ldots} n(n-1)c_n(T)\left(\frac{\mu}{T}\right)^{n-2}$$

- convergence radius

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

C. Schmidt (2008)





Nuclei Hadrons & Quarks

Polyakov-Quark-Meson (PQM) model

B-J. Schaefer, MW, J. Wambach (in preparation)

- relevant degrees of freedom: quarks and mesons
  → PQM model

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

Polyakov loop variable

quarks / antiquarks

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

mesonic fields

- logarithmic Polyakov loop potential (Roessner 2006)

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

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

$$\Omega_{\bar{q}q}(\sigma_x, \sigma_y, \Phi, \bar{\Phi}) = -2T \sum_{f=u,d,s} \int \frac{d^3p}{(2\pi)^3} \Big\{ \ln \Big[1 + 3(\Phi + \bar{\Phi} e^{-(E_{q,f}-\mu_f)/T}) e^{-(E_{q,f}-\mu_f)/T} + e^{-3(E_{q,f}-\mu_f)/T} \Big]$$
$$+ \ln \Big[1 + 3(\bar{\Phi} + \Phi\, e^{-(E_{q,f}+\mu_f)/T}) e^{-(E_{q,f}+\mu_f)/T} + e^{-3(E_{q,f}+\mu_f)/T} \Big] \Big\}$$

explicit μ-dependence

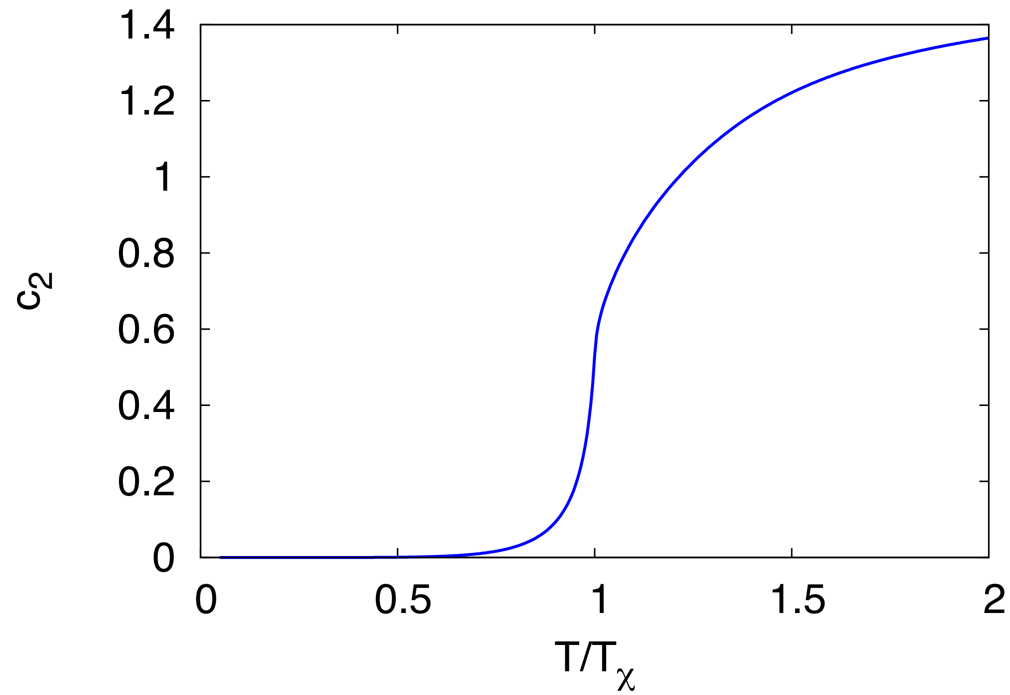
- equations of motion $\left.\frac{\partial \Omega}{\partial \sigma_x} = \frac{\partial \Omega}{\partial \sigma_y} = \frac{\partial \Omega}{\partial \Phi} = \frac{\partial \Omega}{\partial \bar{\Phi}}\right|_{\min} = 0$

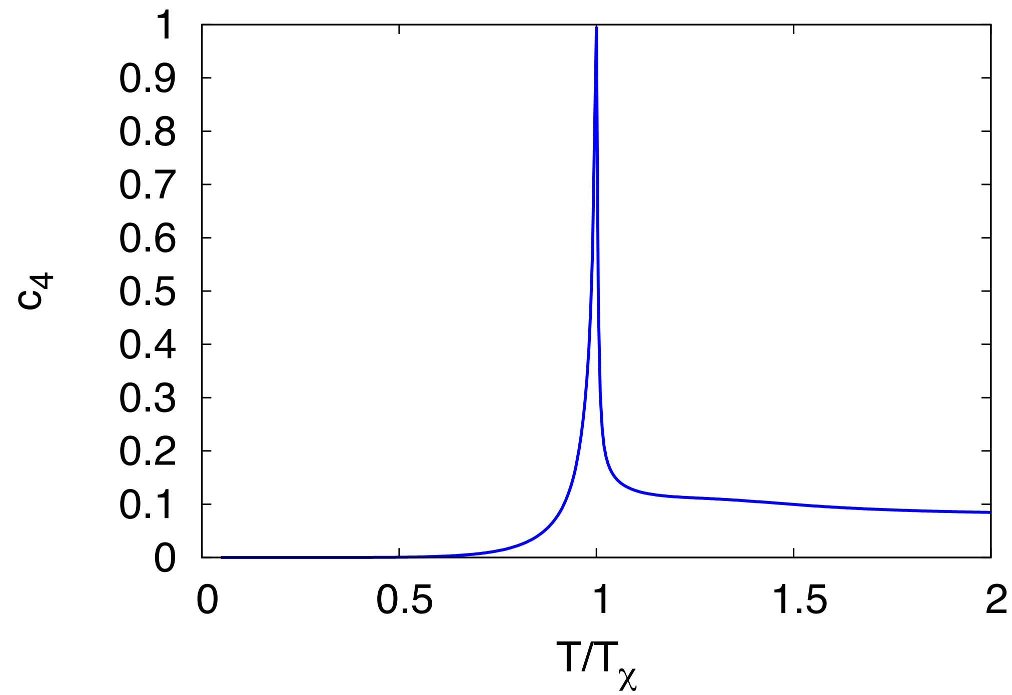
implicit μ-dependence

global minimum $\min(\mu, T) = \left(\sigma_x = \langle \sigma_x \rangle, \sigma_y = \langle \sigma_y \rangle, \Phi = \langle \Phi \rangle, \bar{\Phi} = \langle \bar{\Phi} \rangle\right)$

Coefficients in the PQM-model

- comparison of calculation at μ with extrapolation to μ possible





- higher orders ?

Why we need a novel technique

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(MW, A. Walther, B.-J. Schaefer, submitted to Comm. Phys. Commun. '09)

- numerical derivatives / divided differences
  - error prone $$\frac{d^2\Omega}{d\mu^2} = \frac{1}{\Delta\mu^2}\left[\Omega(\mu-\Delta\mu) - 2\Omega(\mu) + \Omega(\mu+\Delta\mu)\right] + \mathcal{O}(\Delta\mu^2)$$
  - need at least (n+1) function evaluations for n-th derivative
- analytic derivatives
  - rapidly increasing number of terms $$\Omega\left(\mu, \sigma_x(\mu), \sigma_y(\mu), \Phi(\mu), \bar{\Phi}(\mu)\right)$$
  - algebra systems can help $$\frac{d^2\Omega}{d\mu^2} = \frac{\partial^2\sigma}{\partial\mu^2}\frac{\partial\Omega}{\partial\sigma} + \left(\frac{\partial\sigma}{\partial\mu}\right)^2 \frac{\partial^2\Omega}{\partial\sigma^2} + 2\frac{\partial\sigma}{\partial\mu}\frac{\partial\Omega^2}{\partial\sigma\partial\mu} + \frac{\partial^2\Omega}{\partial\mu^2}$$
  - still a lot of coding required
  - cannot help with implicit dependencies

Nuclei Hadrons & Quarks

Algorithmic differentiation

(MW, A. Walther, B.-J. Schaefer, submitted to Comm. Phys. Commun. '09)

- idea: 'differentiate' the algorithm using the chain rule
  - no approximations, i.e. machine precision
  - only slight modifications of the code necessary
  - arbitrary orders without further coding
  - inverse Taylor expansion to treat implicit derivatives $\frac{\partial \Omega(\mu)}{\partial \sigma} \Rightarrow \frac{\partial \sigma}{\partial \mu}$
- performance
  - AD: 1 evaluation of grand potential and equations of motion
  - DD: (n+1) evaluations of grand potential (including minimization)

Algorithmic differentiation

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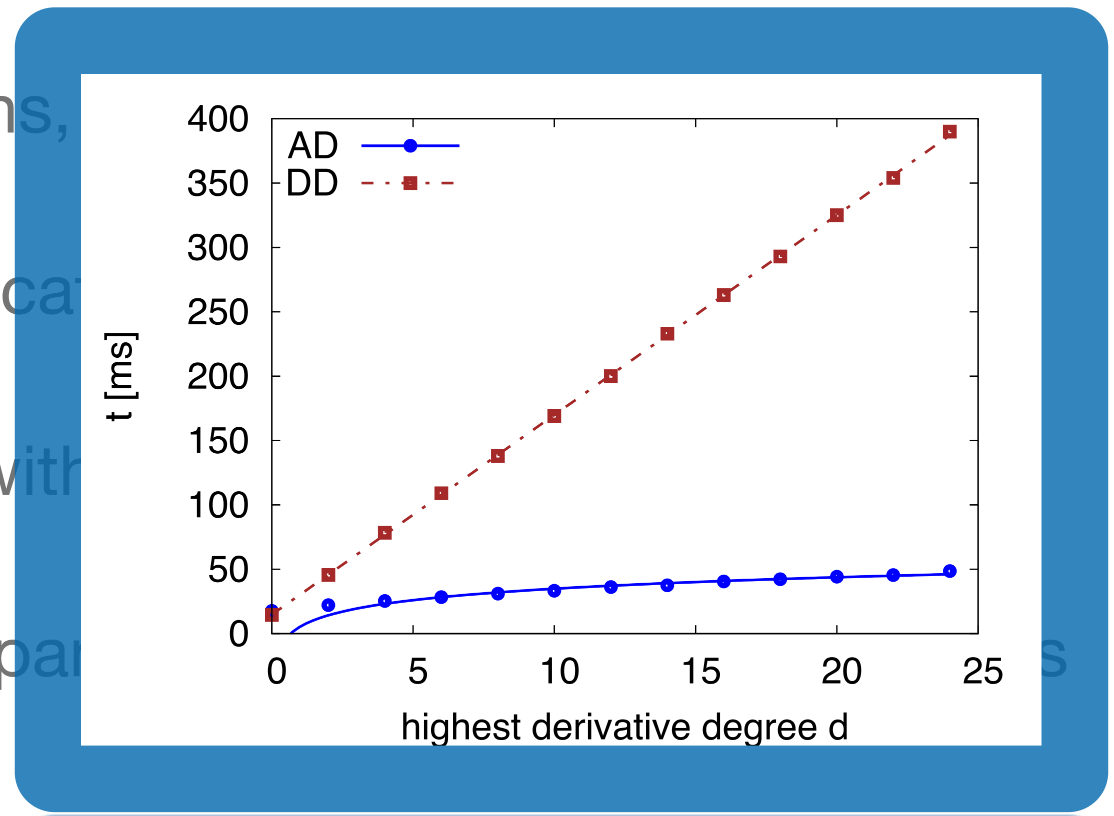
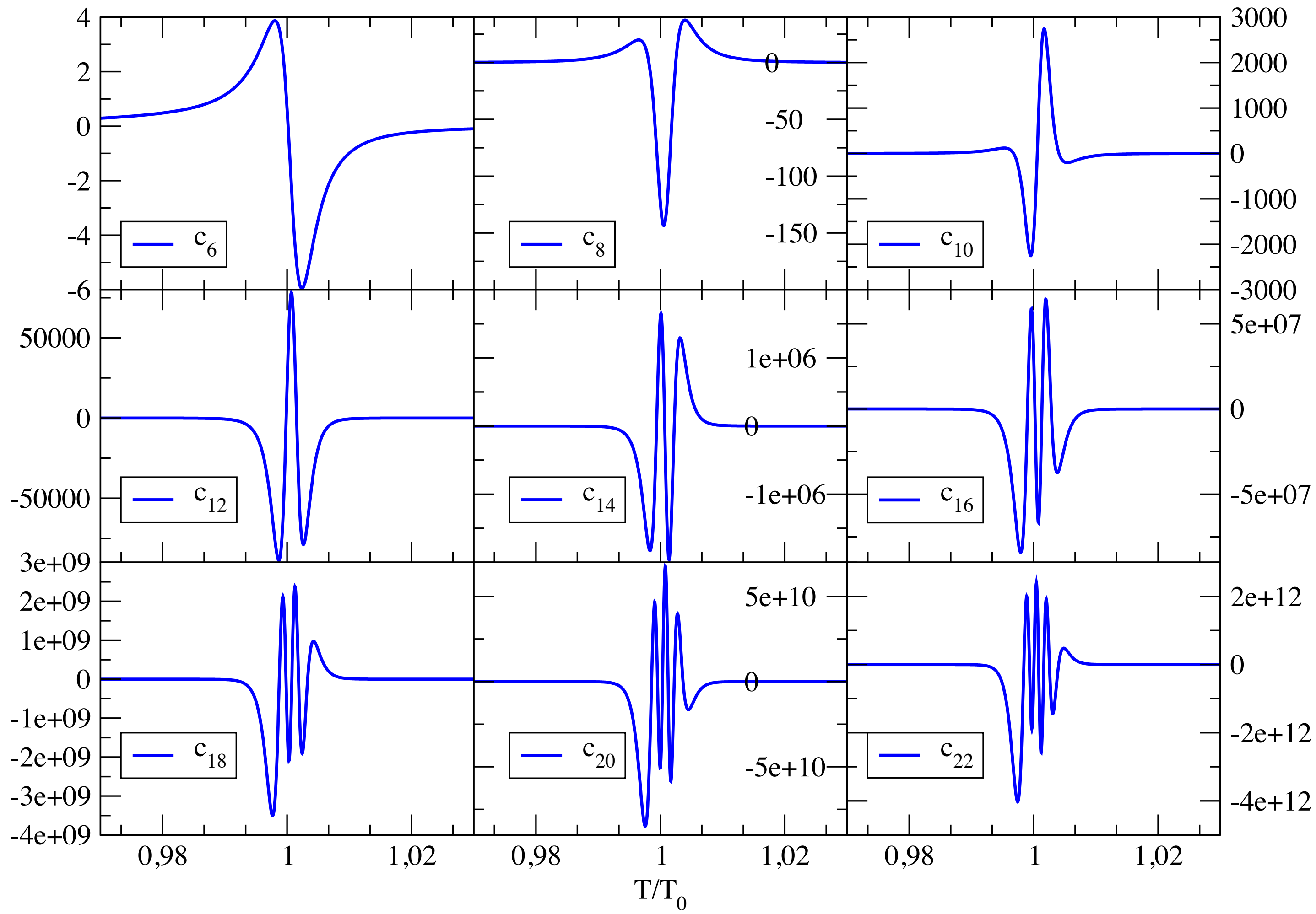


$$\frac{\partial\Omega(\mu)}{\partial\sigma} \Rightarrow \frac{\partial\sigma}{\partial\mu}$$

- performance
  - AD: 1 evaluation of grand potential and equations of motion
  - DD: (n+1) evaluations of grand potential (including minimization)

Higher orders



F. Karsch, B-J. Schaefer, MW, J. Wambach (in preparation)

- higher coefficients are oscillating near transition
- increasing amplitude
- not negligible for $\mu/T < 1$
- small outside transition region
- 22nd (!) order
- no ‘numerical noise’

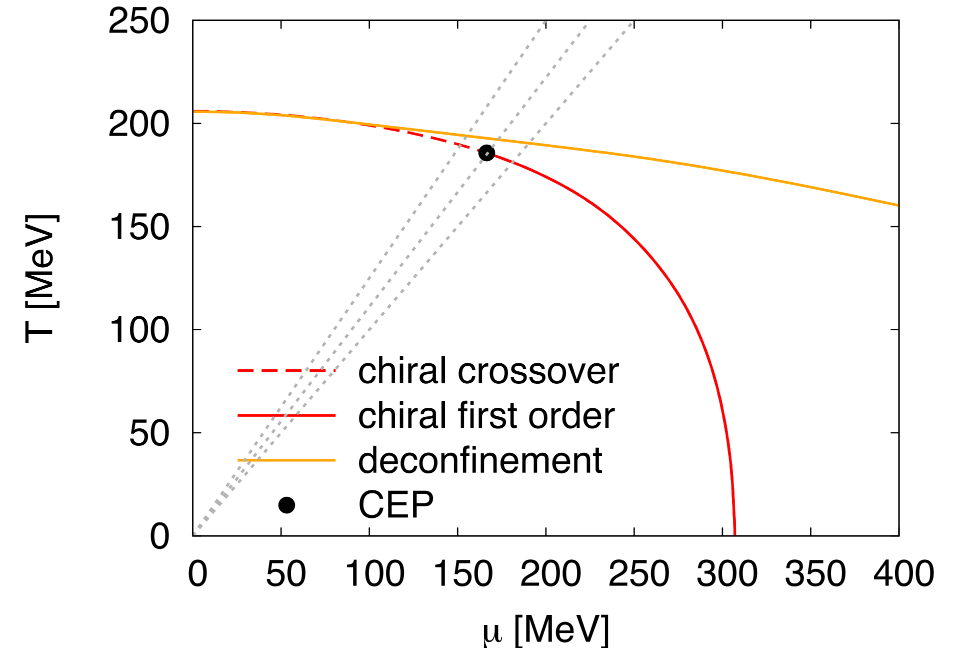
Diverging susceptibility at the CEP

- quark number susceptibility

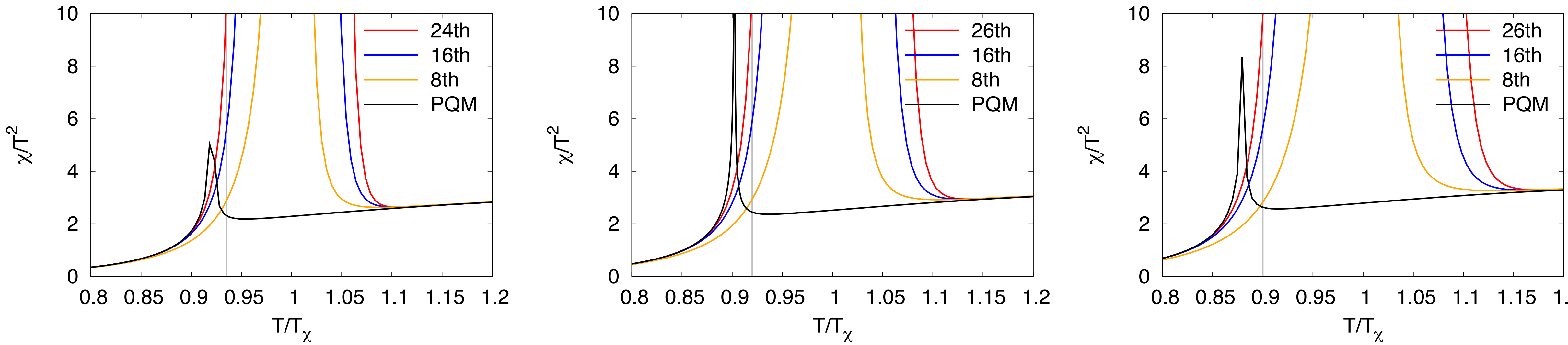
$$\frac{\chi_q(T,\mu)}{T^2} = -\frac{\partial^2\Omega(T,\mu)}{\partial\mu^2}$$

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

F. Karsch, B-J. Schaefer, MW, J. Wambach (in preparation)

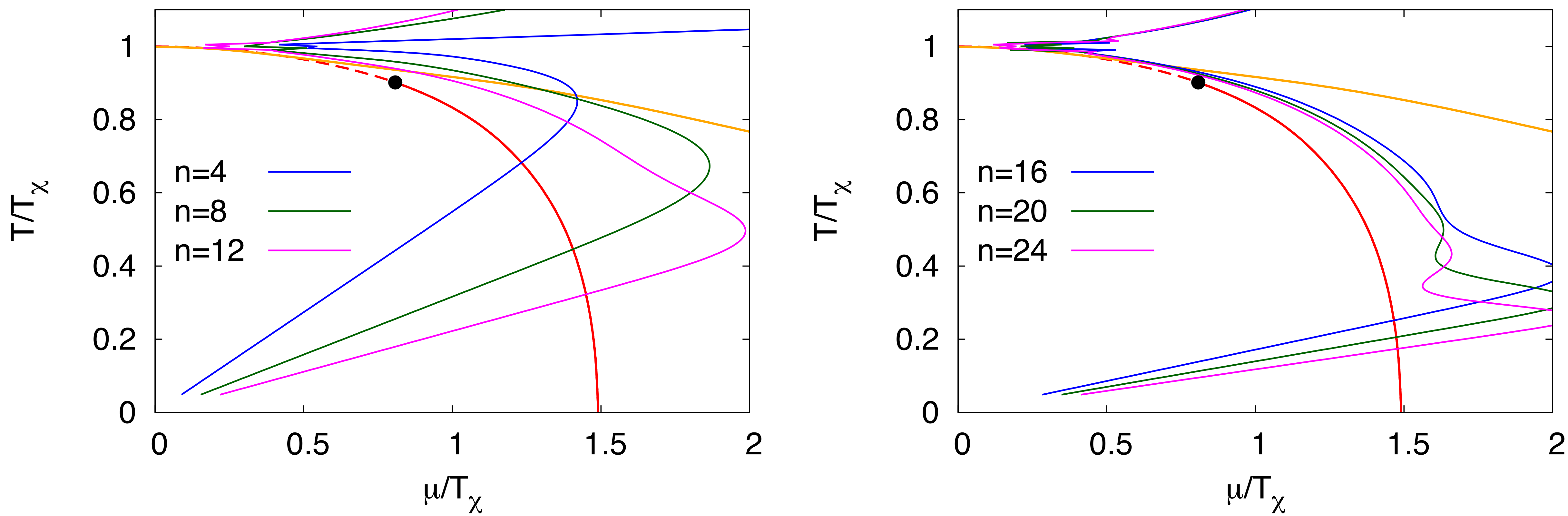


$\mu/T < \mu_c/T_c$ $\mu/T = \mu_c/T_c$ $\mu/T > \mu_c/T_c$



Convergence radii

F. Karsch, B-J. Schaefer, MW, J. Wambach (in preparation)



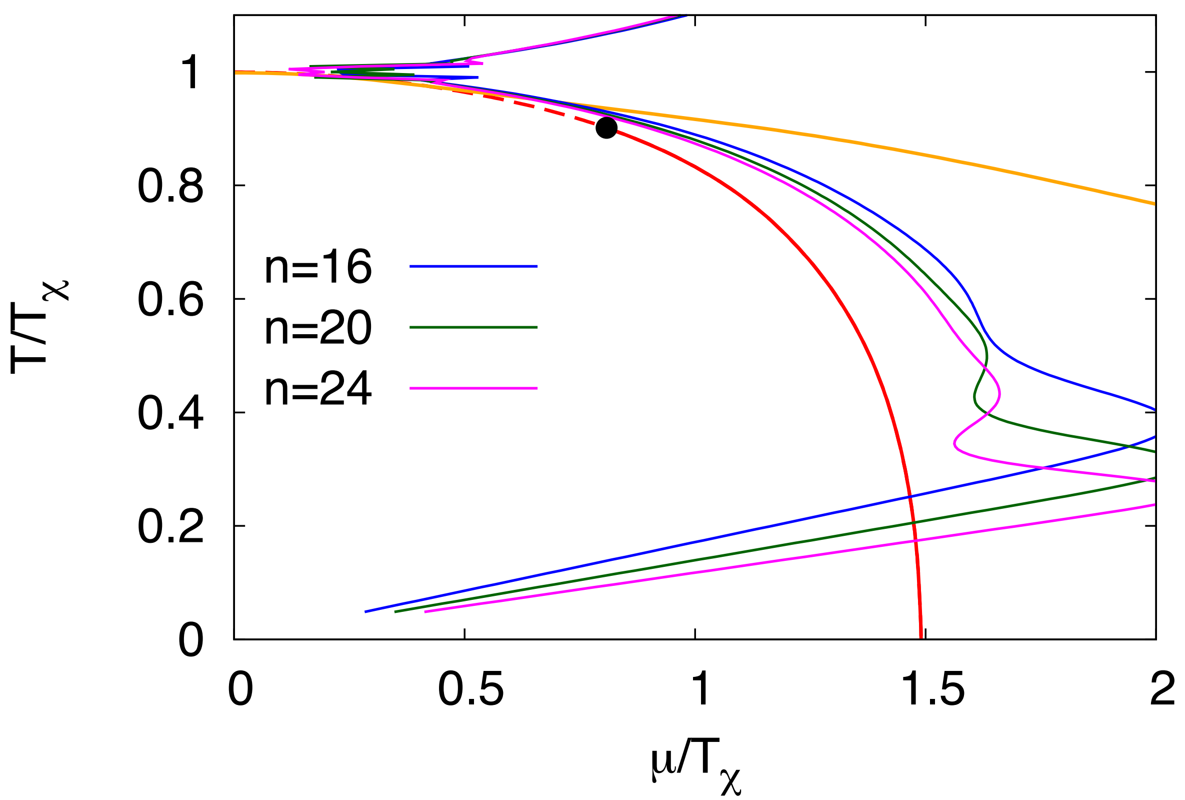
$$r = \lim_{n\to\infty} r_{2n} = \lim_{n\to\infty} \left| \frac{c_{2n}}{c_{2n+2}} \right|^{1/2}$$

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

Relation to phase boundary

- crossover region
  - no divergences
  - oscillations near T_χ
- 2nd order
  - convergence radius close to phase boundary
- 1st order
  - convergence region extends beyond phase boundary

F. Karsch, B-J. Schaefer, MW, J. Wambach (in preparation)

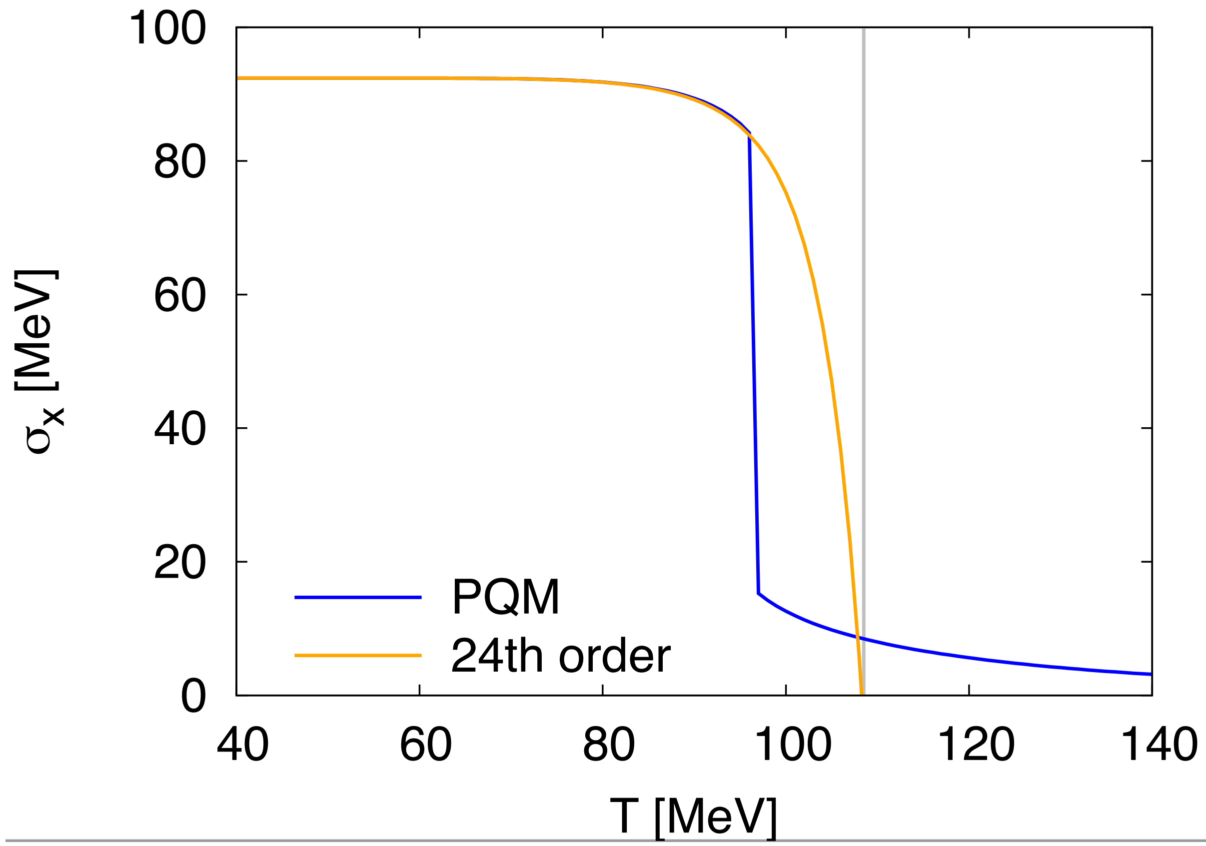


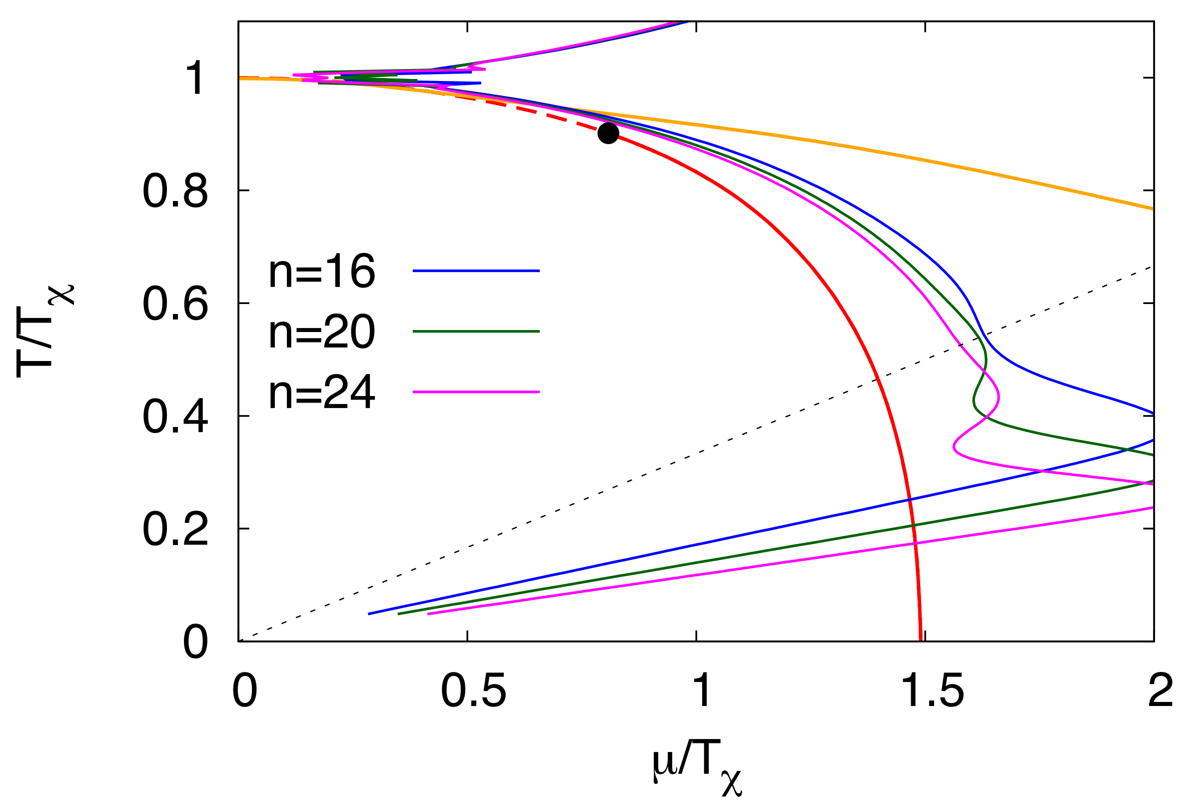
Red line: chiral crossover (dotted), 1st order (solid)
Yellow line: deconfinement crossover
Black dot: chiral critical end point

Closer look at first-order transition

F. Karsch, B-J. Schaefer, MW, J. Wambach (in preparation)

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





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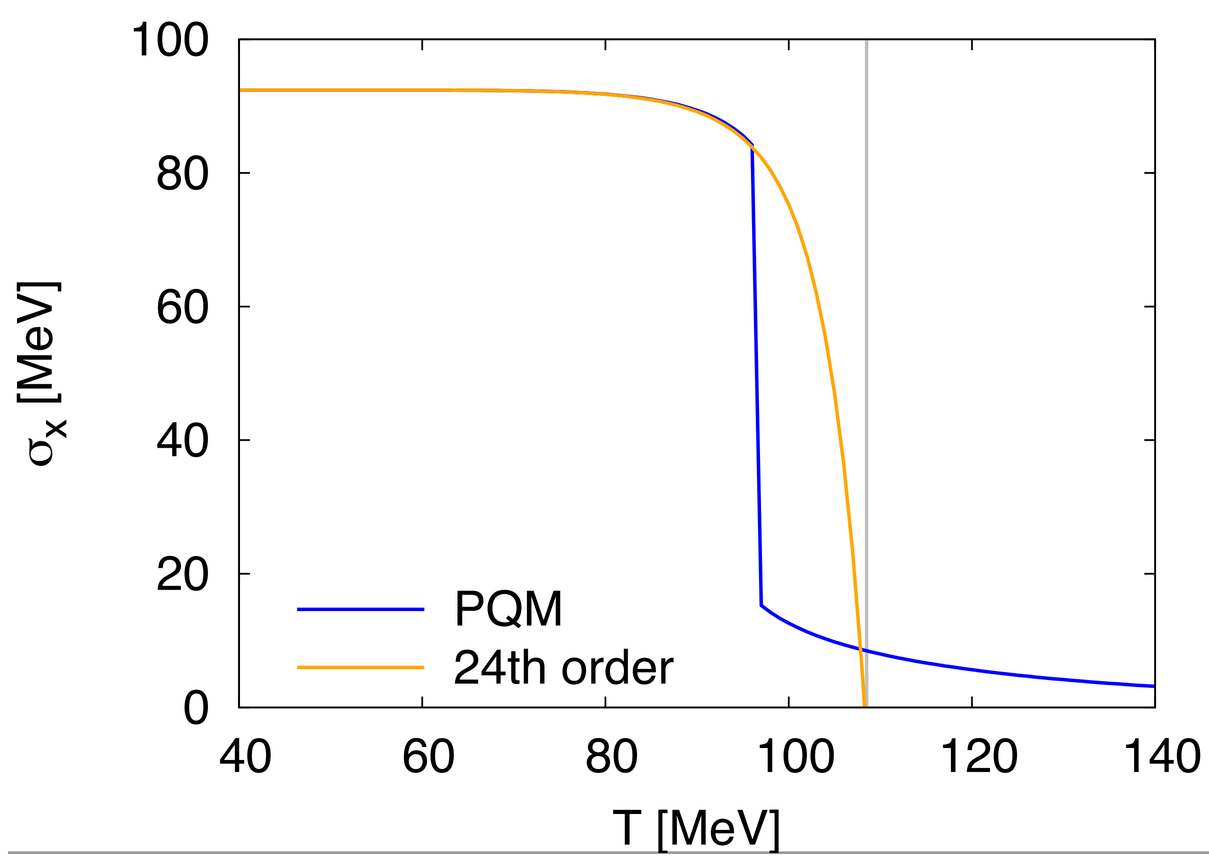
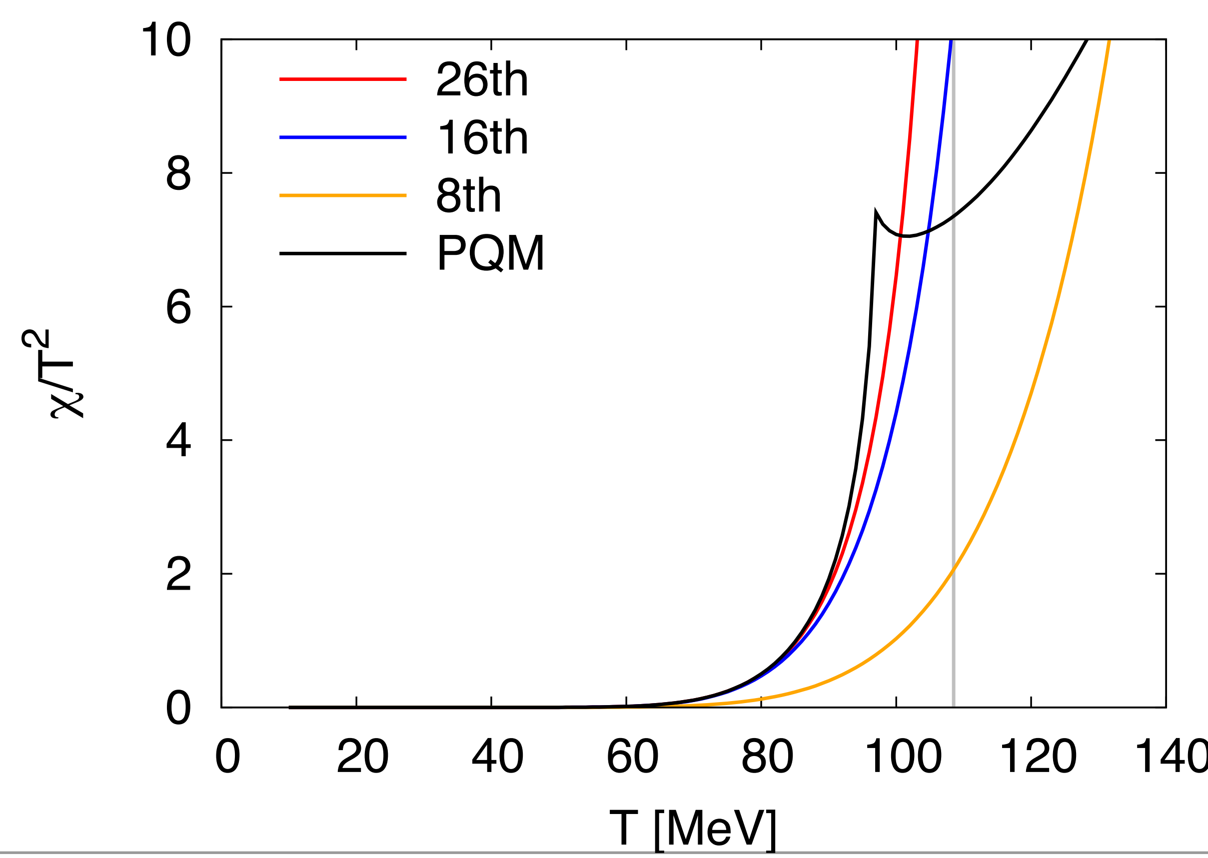


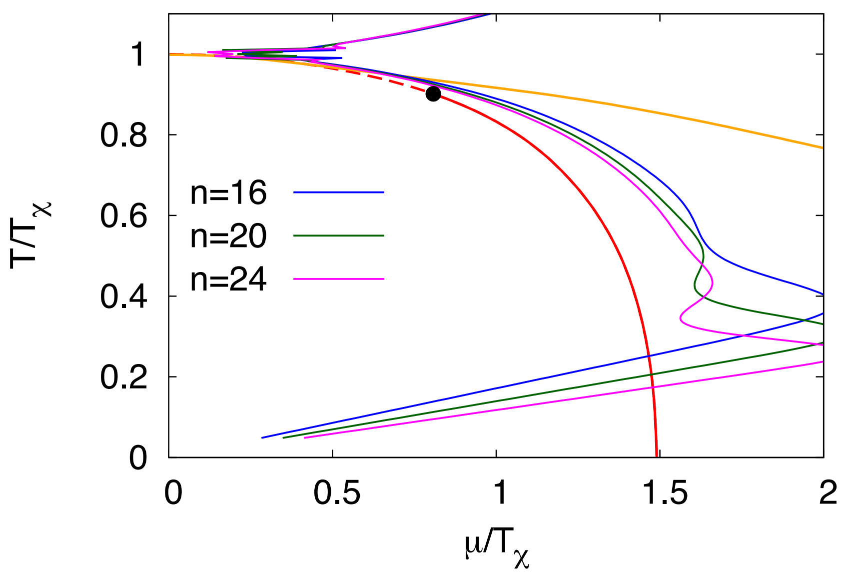


Locating the critical endpoint

- convergence radius close to CEP

$$\lim_{n\to\infty} r_n(T_c) \to \mu_c$$

- need a way to determine T_c:
  sign of coefficients



Locating the critical endpoint

Figure: C. Schmidt (2009)

- convergence radius close to CEP

$$\lim_{n\to\infty} r_n(T_c) \to \mu_c$$

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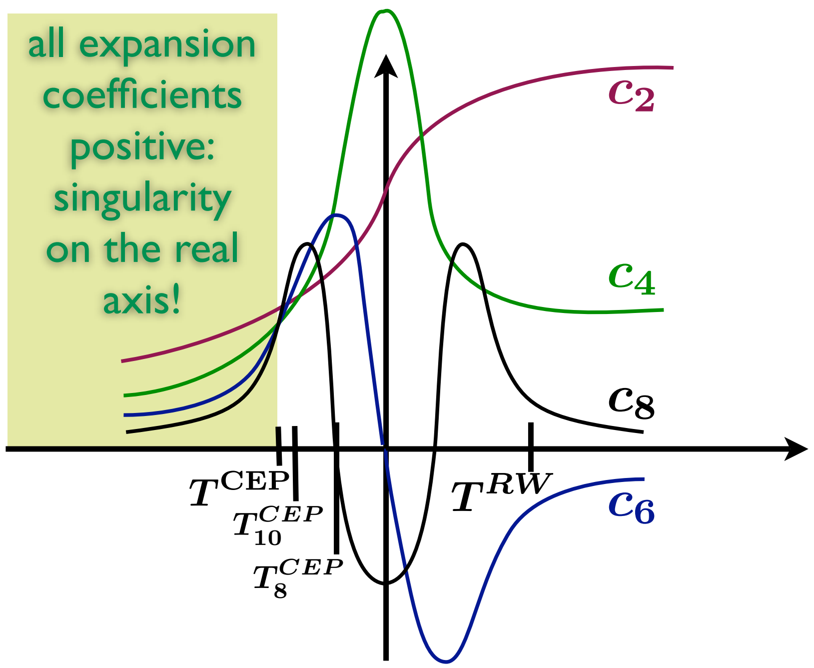
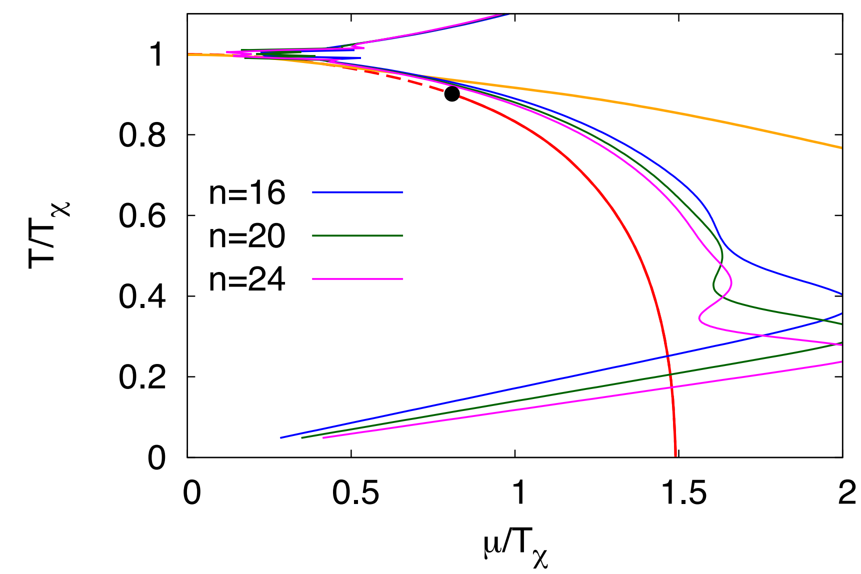


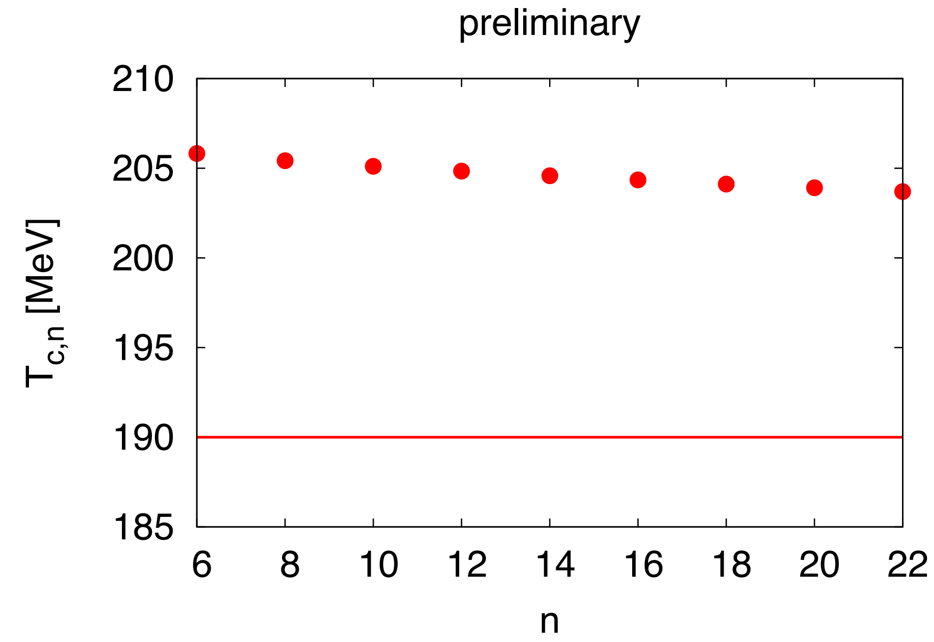
Locating the critical endpoint

- convergence radius close to CEP

$$\lim_{n\to\infty} r_n(T_c) \to \mu_c$$

- need a way to determine T_c : sign of coefficients
- at least n=8 required for non-trivial estimate
- extrapolation required: $T_c = \lim_{n\to\infty} T_{c,n}$
- precise determination and higher orders requires algorithmic differentiation method





Summary & Outlook

- Taylor expansion to higher orders (n=24)
- novel technique for derivatives
- determined convergence region
- relation to phase boundary
- higher orders (n > 12) might locate the CEP

- signals for the critical end point
- Padé approximation
- different model setups, i.e. different location of CEP
- include fluctuations in the hadronic phase (RG)