Location of Yang-Lee edge singularity

Vladi Skokov (Physics Department, NCSU and RBRC, Brookhaven National Laboratory)

Supported by
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Punchline

Decades of research revealed a detailed portrait of a second-order phase transition:

- Critical exponents: $\alpha, \beta, \gamma, \delta, \eta, \nu, \omega$

  Approximate timeline:

  $\beta(\text{vdW}) = 1/2, \quad \beta(1972) = 1/3, \quad \beta(1981) = 0.327(5), \quad \ldots, \beta(2015) = 0.326419(3)$

  Conformal bootstrap → unprecedented precision

- Critical amplitudes: $U_0,\, U_2,\, U_4,\, R_c^{\pm}, R_4^{\pm},\, \underbrace{R_\chi, \ldots}_{19}$

Bielefeld group: J. Engels, F. Karsch, ... for O(2) and O(4) universality classes

Gonzalo De Polsi, Guzmán Hernández-Chifflet, Nicolas Wschebor, 2021

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There is one notable exception: The universal location of the Yang-Lee edge singularity.
The problem was defined by Kortman and Griffiths in 1971.

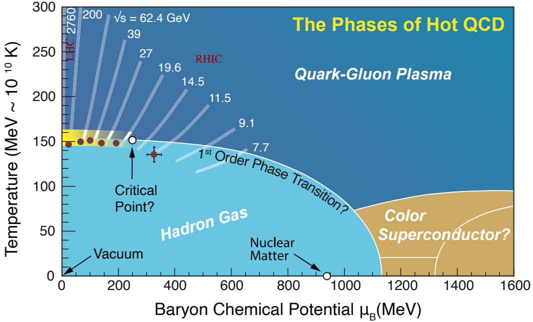
d=3: A. Connelly, G. Johnson, F. Rennecke, and V. S,
Phys.Rev.Lett. 125 19, 191602 (2020) + two follow-up papers

d=2: H.-L. Xu and A. Zamolodchikov
JHEP 08 (2022) 057 (2022)

Outline

- Motivation and introduction: phase transitions and critical phenomena
- Universal features near a second-order phase transition
- Yang-Lee edge singularity
- Application to the phase diagram of strongly interacting matter
- Conclusions

Phase diagram of QCD



- Experiment with relativistic heavy ions: the system is small and has a short lifetime
- Theory: although the underlying theory (QCD) is known, we cannot solve it ✗
- Numerical methods: zero density region only due to the "sign" problem ✗
- Indirect numerical methods: Taylor series coefficients → non-zero baryon density ✓

$$p/T^4 = \sum_{n=0}^{\infty} \frac{\chi_n}{n!}\left(\frac{\mu}{T}\right)^n ; \quad \chi_n = \frac{\partial^n (p/T^4)}{\partial\ (\mu/T)^n} \quad \chi_2 = \frac{\langle(\delta N)^2\rangle}{VT^3} \quad \chi_4 = \frac{\langle(\delta N)^4\rangle - 3\langle(\delta N)^2\rangle^2}{VT^3}$$

Taylor series expansion

$$f(x) = \sum_{i=0}^{\infty} \frac{1}{i!} f^{(i)}(0) x^i$$

- What limits the range of x?

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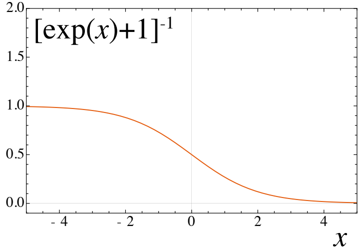
- Example $(a > 0)$

$$\frac{1}{a\, e^x + 1}$$



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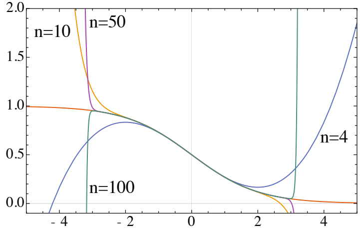

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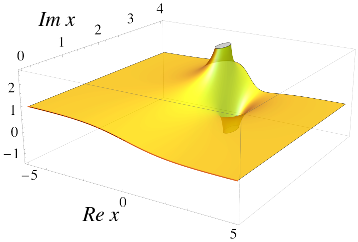

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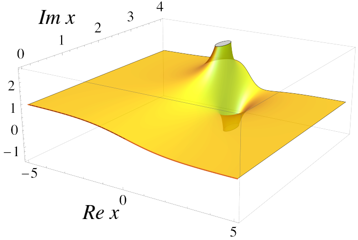
$$\frac{1}{a\,e^x + 1} \rightarrow \frac{1}{e^{\frac{\omega}{T} + \frac{\mu}{T}} + 1}$$



Taylor series expansion

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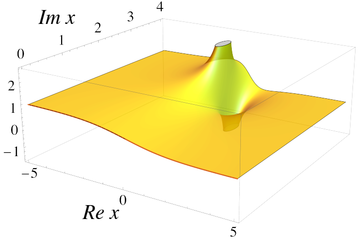
- What limits the range of x?
- Example $(a > 0)$

$$\frac{1}{a\,e^x+1} \to \frac{1}{e^{\frac{\omega}{T}+\frac{\mu}{T}}+1} \xrightarrow{\mu=2\pi T i} -\frac{1}{e^{\frac{\omega}{T}}-1}$$



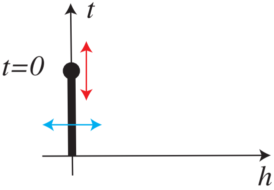
Analytic structure near critical point

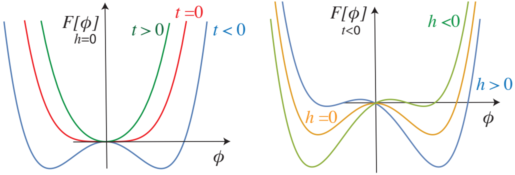
Are there singularities associated with critical point/phase transitions?

L. Landau (1937): Phase transitions $\equiv$ manifestations of broken symmetry; generalized order parameter to measure symmetry breaking

$$F = \int d^d x \left\{ \frac{1}{2} t\phi^2 + \frac{1}{4}\lambda\phi^4 - h\phi \right\}, t = T - T_c$$

Phase diagram:





Minimize $F[\phi] \rightsquigarrow$ equilibrium order parameter

E.g. at zero h, $t\phi + \lambda\phi^3 = 0$ or $\phi = \sqrt{-t/\lambda}$

Magnetic equation of state

- Arbitrary t and h: $t\phi + \lambda\phi^3 = h$

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- Look for solution $\phi = h^{1/3} f_G$: $th^{1/3} f_G + h f_G^3 = h$ or $\frac{t}{h^{2/3}} f_G + f_G^3 = 1$

Magnetic equation of state

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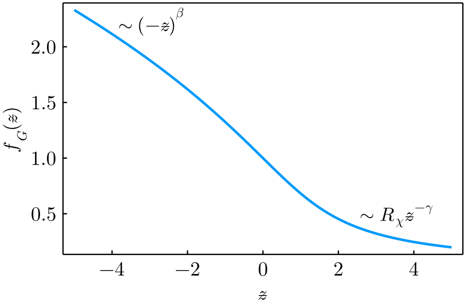
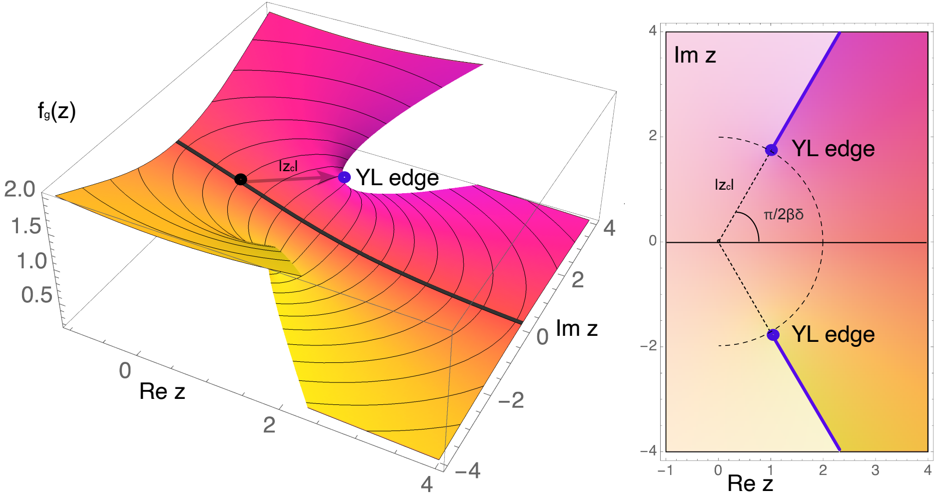
- Look for solution $\phi = h^{1/3} f_G$: $t h^{1/3} f_G + h f_G^3 = h$ or $\frac{t}{h^{2/3}} f_G + f_G^3 = 1$
- Scaling form of "magnetic equation of state"

$$f_G(z + f_G^2) = 1, \quad z = \frac{t}{h^{\frac{1}{\beta\delta}}} \qquad \beta = 1/2, \delta = 3$$



For more details on metric factors, see e.g. F. Rennecke, V.S., Annals Phys. 444 (2022) 169010

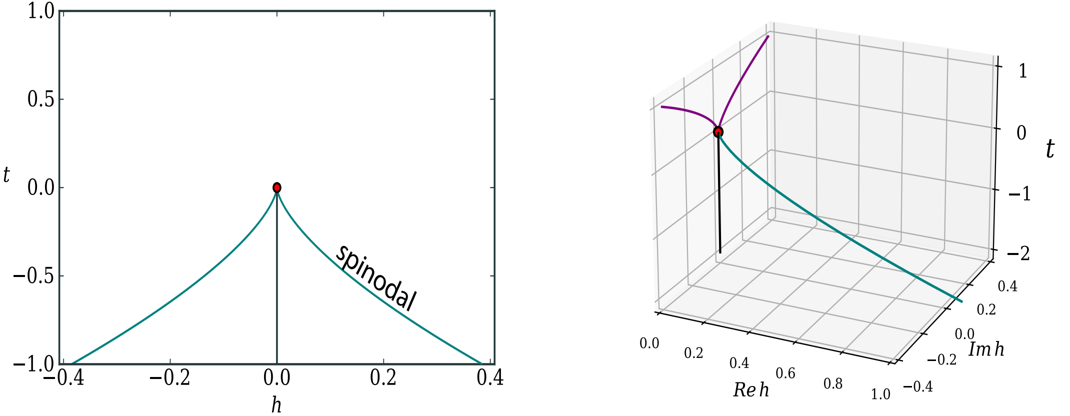
Magnetic equation of state in $\mathbb{C}$: Yang-Lee edge singularity



Defining equations: $\delta F/\delta\phi = 0$ & $\delta^2 F/\delta\phi^2 = 0$

Finite systems: YLE and cuts $\rightsquigarrow$ Lee-Yang zeros

Yang-Lee edge singularity and spinodals



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Yang-Lee edge singularity as a critical point

Number of relevant variables:

	critical	tricritical
	2	4

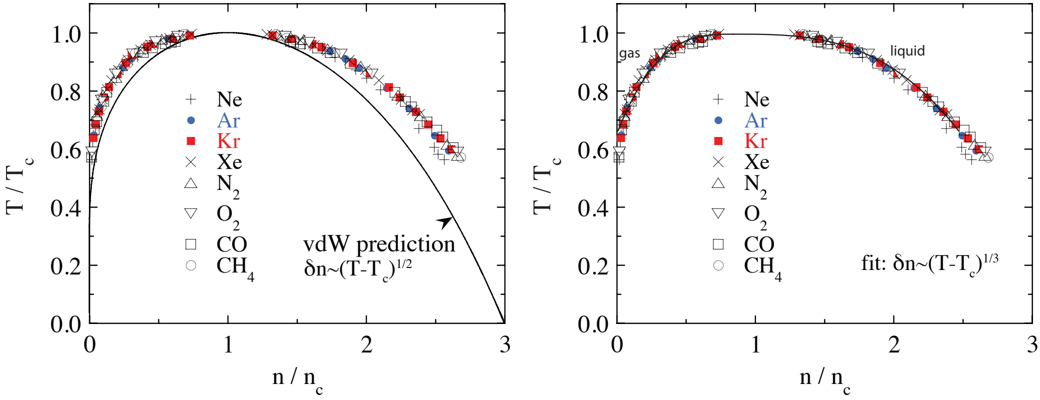
Yang-Lee edge singularity as a critical point

Number of relevant variables:

proto-critical	critical	tricritical
1	2	4

Yang-Lee edge singularity is a proto-critical point with one relevant variable and thus with one relevant critical exponent $\sigma = 1/\delta$.

Limitation of mean-field theories



Ginzburg criterion and ε expansion

- Mean-field approximation: replace fluctuating order parameter with its spatially uniform average
- Fluctuations $\delta\phi(x) = \phi(x) - \phi$ over the coherence volume $\propto \xi^d$ have to be negligible.

Mathematically

$$\frac{1}{\xi^d} \int d^d x \langle \delta\phi(x) \delta\phi(0) \rangle \ll \phi^2$$

$$\left(\frac{\xi}{\xi_0}\right)^{-(d-4)} \ll 1 \qquad \begin{array}{ll} d > 4 & ✓ \\ d < 4 & ✗ \end{array}$$

$d = 4$ – the upper critical dimension for ϕ^4 theory

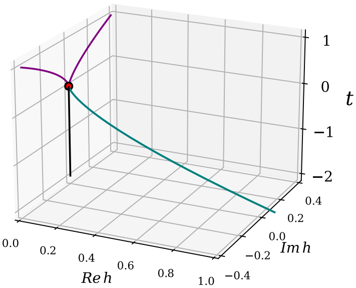
V. Ginzburg, 1960

Perturbation in ε, $d = 4 - \varepsilon$

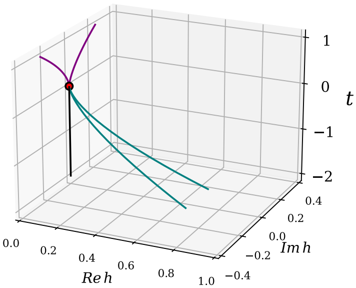
K. Wilson and M. Fisher
"Critical Exponents in 3.99 Dimensions"
Phys. Rev. Lett. 28, 240 (1972)

Inclusion of fluctuations

$d = 4$

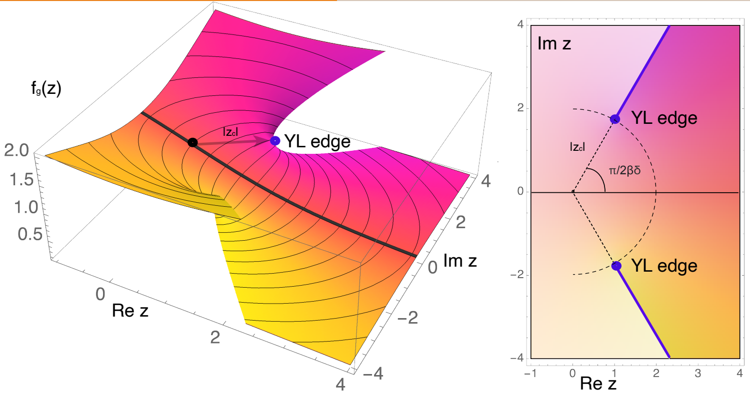


$d = 3$



G. Johnson, F. Rennecke, and V.S., Phys.Rev.D 107 (2023) 11, 116013

Universal location of Yang-Lee edge singularity



Arg of z_c is known owing to the Lee-Yang theorem: $z_c = |z_c| \exp\left[\pm \frac{i\pi}{2\beta\delta}\right]$ $\beta = 0.326419(3)$, $\delta = 4.78984(1)$

T. D. Lee and C. N. Yang, Phys. Rev. 87, 410 (1952)

$|z_c|$ is a universal number; $f(z) \propto (z - z_c)^{\sigma}, \sigma = 1/\delta \approx 0.085(1)$

σ: conformal bootstrap by F. Gliozzi and A. Rago, 2014

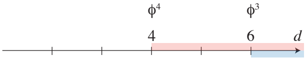
& FRG Studies by X. An, D. Mesterhazy, and M. A. Stephanov, 2016

- Expanding near the upper critical dimension of ϕ^4 theory, $d = 4 - \varepsilon$ $(N = 1)$

$$\beta = \frac{1}{2} - \frac{1}{6}\varepsilon + \underbrace{\#\varepsilon^2 + \#\varepsilon^3 + \#\varepsilon^4 + \#\varepsilon^5 + \dots}_{\text{known or perturbatively computable}}$$

Accidentally, leading correction with $\varepsilon = 1 \rightsquigarrow$ good approximation.

- Near Yang-Lee edge singularity: ϕ^3 theory. The upper critical dimension is 6.
  $\rightsquigarrow$ breakdown of ε-expansion near 4 dimensions



$$|z_c| \approx |z_c^{\mathrm{MF}}| \left[1 + \frac{27\ln\left(\frac{3}{2}\right) - (N-1)\ln 2}{9(N+8)}\epsilon\right] + \epsilon^2 \log\epsilon \times \text{(all loops contribute)}\,.$$

F. Rennecke, and V.S., Annals Phys. 444 (2022) 169010 and Phys.Rev.D 107 (2023) 11, 116013

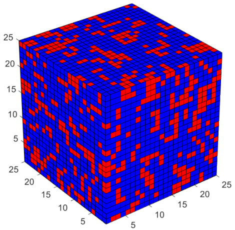
- Properties (e.g. critical exponent) of YLE singularity can be obtained using $d = 6 - \varepsilon$

M. Fisher, "Yang-Lee Edge Singularity and ϕ^3 Field Theory", Phys. Rev. Lett. 40 1610 (1978)

Simulations on the lattice

- Consider d-dimensional lattice

$$\langle O \rangle = \sum_{s \in \text{all possible states}} O[s] \exp(-\beta F[s])$$



- Importance sampling; $\exp(-\beta F[s])$ – probability for s
- Imaginary $h \rightsquigarrow$ "sign problem"
- No practical precision way to circumvent the problem in $d = 3$

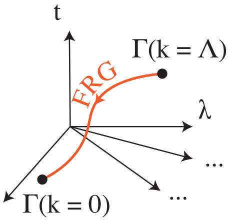
Conventional methods fail

ε-expansion, lattice simulation and, finally, conformal bootstrap

are not equipped to locate YLE.

Functional Renormalization Group

- Start with bare classical action at small distances/large momentum $S_{k=\Lambda}$
- Gradually include fluctuations of larger size/smaller momentum
- Continue until fluctuations of all possible sizes/momenta are accounted for



Equation that does it: Functional Renormalization Group equation (Wetterich, 93)

$$\partial_k \Gamma_k[\phi] = \frac{1}{2}\,\mathrm{STr}\left[\left(\Gamma_k^{(2)}[\phi] + R_k\right)^{-1} \cdot \partial_k R_k\right]$$

Pros: Exact, non-perturbative, no sign problem. Cons: requires truncation.

Truncation: derivative expansion

- Expansion around the uniform field

- First-order derivative expansion

$$\Gamma_k[\phi] = \int d^d x \left(U_k(\phi) + \frac{1}{2} Z_k(\phi) (\partial_i \phi)^2 \right)$$

The average potential

$$\partial_t U_k(\rho) = \frac{1}{2} \int \bar{d}^d q \, \partial_t R_k \left(q^2\right) \left[G_k^{\parallel} + (N-1) G_k^{\perp} \right], \quad \rho = \frac{\phi^2}{2}$$

with

$$G_k^{\perp} = \frac{1}{Z_k^{\perp}(\rho) q^2 + U_k'(\rho) + R_k(q^2)}, \quad G_k^{\parallel} = \frac{1}{Z_k^{\parallel}(\rho) q^2 + U_k'(\rho) + 2\rho U_k''(\rho) + R_k(q^2)}.$$

Truncation: derivative expansion

Wave function renormalization:

$$\partial_t Z_{\parallel}(\phi) = \int \bar{d}^d q \partial_t R_k(q^2) \Bigg\{ G_{\parallel}^2 \Big[\gamma_{\parallel}^2 \big(G'_{\parallel} + 2G''_{\parallel}\frac{q^2}{d}\big) + 2\gamma_{\parallel} Z'_{\parallel}(\phi)\big(G_{\parallel} + 2G'_{\parallel}\frac{q^2}{d}\big)$$
$$+ (Z'_{\parallel}(\phi))^2 G_{\parallel}\frac{q^2}{d} - \frac{1}{2} Z''_{\parallel}(\phi)\Big]$$
$$+ (N-1)G_{\perp}^2 \Big[\gamma_{\perp}^2 \big(G'_{\perp} + 2G''_{\perp}\frac{q^2}{d}\big) + 4\gamma_{\perp} Z'_{\perp}(\phi) G'_{\perp}\frac{q^2}{d} + (Z'_{\perp}(\phi))^2 G_{\perp}\frac{q^2}{d}$$
$$+ 2\frac{Z_{\parallel}(\phi) - Z_{\perp}(\phi)}{\phi}\gamma_{\perp} G_{\perp} - \frac{1}{2}\left(\frac{1}{\phi} Z'_{\parallel}(\phi) - \frac{2}{\phi^2}(Z_{\parallel} - Z_{\perp})\right)\Big]\Bigg\}$$

with

$$\gamma_{\parallel} = q^2 Z'_{\parallel}(\phi) + U^{(3)}(\phi), \quad \gamma_{\perp} = q^2 Z'_{\perp}(\phi) + \frac{\partial}{\partial\phi}\left(\frac{1}{\phi}U'(\phi)\right), \quad G' = \frac{\partial G}{\partial q^2}, \ldots$$

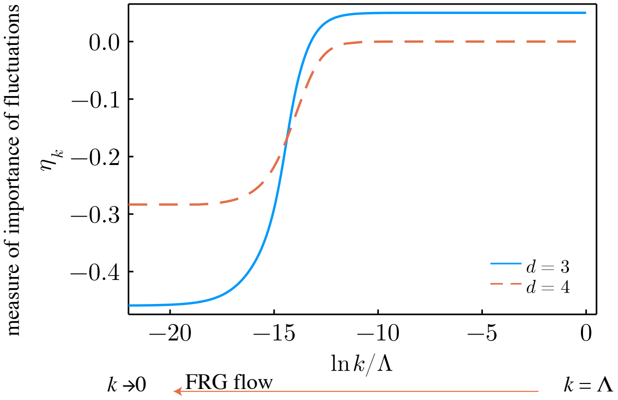
G. Johnson, F. Rennecke, and V.S., Phys.Rev.D 107 (2023) 11, 116013

Truncation: derivative expansion

- Taylor series expansion of $U_k(\phi)$ and $Z_k(\phi)$ (orders 12 and 6 respectively)
  Traditionally: expand near k-dependent minimum: $U_k'[\phi_k] = h = \text{const.}$
  To locate YLE: expand near $U_k''[\phi_k] = m^2 \to 0$.
    $\rightsquigarrow$ $U_k'[\phi_k] = h_k \neq \text{const}$
    $\rightsquigarrow$ Calculations in the broken phase are not feasible

- We use Litim regulator $\rightsquigarrow$ we cannot go beyond first order DE

Results: importance of fluctuations



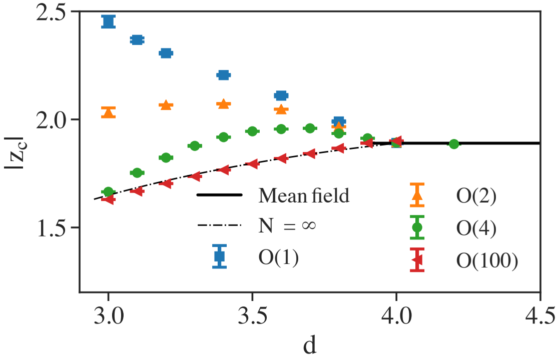
F. Rennecke and V. S, Annals Phys. 444 (2022) 169010

At YLE fixed point, independently compute ν through the stability matrix.

For $d = 3$, the hyperscaling relation $\frac{1}{\nu} \stackrel{!}{=} \frac{d-2+\eta}{2}$ is satisfied modulo numeric precision.

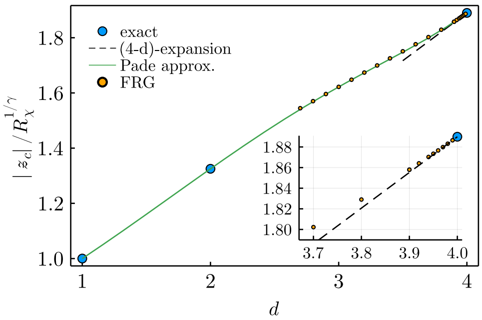
C.f. X. An, D. Mesterhazy, and M. Stephanov, JHEP 07 (2016) 041

Results: LPA’



A. Connelly, G. Johnson, F. Rennecke, and V. S,
Phys.Rev.Lett. 125 19, 191602 (2020)

Results: first-order derivative expansion $N = 1$



d	1	2	3	4
$\lvert z_c\rvert/R_\chi^{1/\gamma}$	1	1.32504(2)	1.621(3)	$3/2^{2/3}$

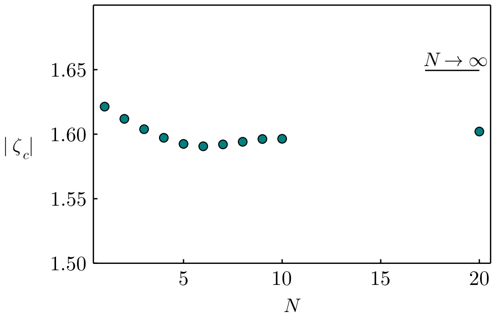
F. Rennecke and V. S, Annals Phys. 444 (2022) 169010

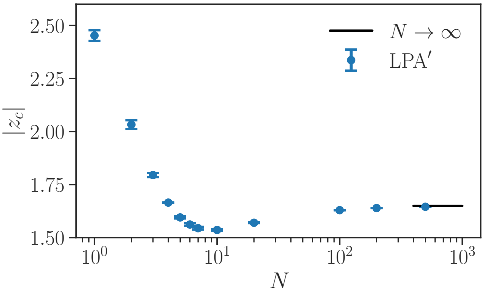
$d = 2$:

H.-L. Xu and A. Zamolodchikov, JHEP 08 (2022) 057

H.-L. Xu and A. Zamolodchikov, 2304.07886

Results: first-order derivative expansion, arbitrary N and $d = 3$





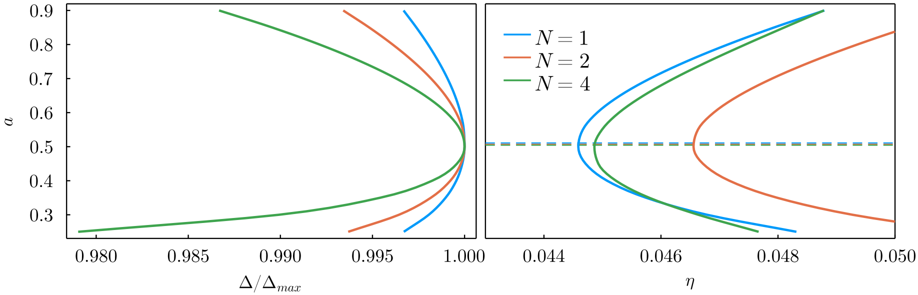
N	1	2	3	4	5
$\lvert\zeta_c\rvert = \lvert z_c\rvert / R_\chi^{1/\gamma}$	1.621(4)(1)	1.612(9)(0)	1.604(7)(0)	1.597(3)(0)	1.5925(2)(1)

G. Johnson, F. Rennecke, and V. S, Phys.Rev.D 107 (2023) 11, 116013

Error-estimate: truncation error and minimal sensitivity analysis

Truncation error is estimated by varying the truncation order of Taylor expansion for $U(\phi)$ and $Z(\phi)$

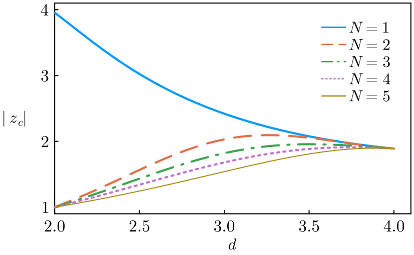
Regulator function is parameter dependent: $R_k(p) = a(k^2 - p^2)\theta(k^2 - p^2)$



Fix a to minimize sensitivity of Δ or h_c

Results: $d = 3$

N	1	2	3	4
$\|z_c\|$	2.43(4)	2.04(8)	1.83(6)	1.69(3)



Schofield's parametrization based on the data for real h from

F. Karsch, M. Neumann, and M. Sarkar, 2304.01710:

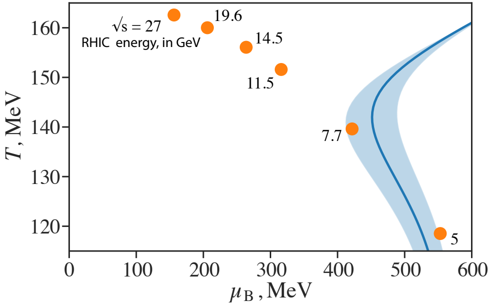
$z_c(N = 1) \approx 2.364$

$z_c(N = 2) \approx 2.26$

$z_c(N = 4) \approx ...$

Can parameterization be improved using $|z_c|$ as an input?!

Application to QCD phase diagram



- Near the chiral critical point

$$p(T,\mu_B)/T^4 = -\#h^{(2-\alpha)/\beta\delta} f_f(z) - f_{\text{regular}}(T,\mu_B)$$

$$z = z_0 t h^{-1/\beta\delta} = z_0 \left[\frac{T-T_c}{T_c} + \kappa_B \left(\frac{\mu_B}{T}\right)^2\right] \left(\frac{m_{u,d}}{m_s}\right)^{-1/\beta\delta}$$

$$t = \frac{T-T_c^0}{T_c^0} + \kappa_B \left(\frac{\mu_B}{T}\right)^2 ; \quad h = \frac{m_{u,d}}{m_s} .$$

O(4) critical exponents: $\alpha = -0.21$, $\beta = 0.38$, $\delta = 4.82$

- LQCD: $T_c = 132^{+3}_{-6}$ MeV; $\kappa_B = 0.012(2)$; $z_0 = 1-2$

H. T. Ding et al. (2019), 1903.04801

S. Mukherjee and V. S., Phys.Rev.D 103 7, L071501 (2021)

Application to QCD phase diagram: Taylor series coefficients

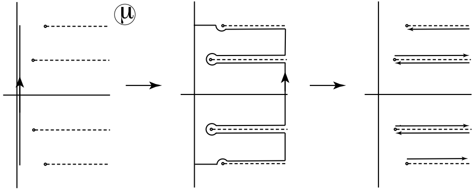
YLE defines the behavior of

the higher order Taylor expansion coefficients (Darboux's theorem) of $f_G(z)$:

$$f_G^{(n)} \sim 2B_0 |z_c|^{-n} \frac{n^{\sigma-1}}{\Gamma(\sigma)} \cos\left(\beta_0 - \frac{\pi n}{2\Delta}\right), \quad B_0 \exp(i\beta_0) = \lim_{z \to z_c} \frac{f_G(z) - f_G(z_c)}{(1 - z/z_c)^{\sigma}}$$

A more efficient program: talk by Gokce Basar

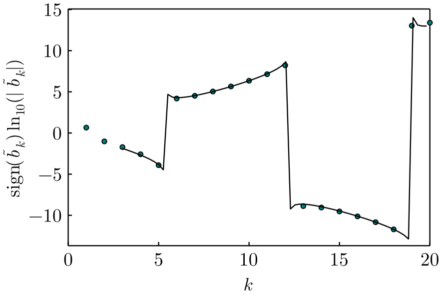
Application to QCD phase diagram: Fourier coefficients



Fourier coefficients:

$$b_k = |\tilde{A}_{\mathrm{YLE}}| \frac{e^{-\hat{\mu}_r^{\mathrm{YLE}} k}}{k^{1+\sigma}} \cos(\hat{\mu}_i^{\mathrm{YLE}} k + \phi_a^{\mathrm{YLE}}) + |\hat{A}_{\mathrm{RW}}| (-1)^k \frac{e^{-\hat{\mu}_r^{\mathrm{RW}} k}}{k^{1+\sigma}} + \dots$$

Application to quark-meson/NJL model beyond mean-field:



Fit: $\hat{\mu}_{\mathrm{YLE}}^{\mathrm{fit}} = 1.483(7) + i\,0.446(6)$

Actual value: $\hat{\mu}_{\mathrm{YLE}} = 1.553 + i\,0.4794$

C. Schmidt-Sonntag and V. S., 2309.xxxx

Conclusions & Outlook

- Conventional methods which were successful in extracting most of the critical statics (exponents, amplitudes, equations of state) fail to locate YLE
- Functional Renormalization Group is uniquely poised to find the location of YLE
- First-order derivative expansion FRG to extract location for classical 3-d Ising universality class (N=1), X-Y model (N=2), Heisenberg model (N=3), and relevant for QCD N=4
- Importance for QCD: high-order coefficients of Taylor series, Fourier coefficients, direct application to LQCD results
- Beyond first-order derivative expansion?!


BACKUP