Frontier of Universality: Yang-Lee edge singularity

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

G. Johnson, F. Rennecke, and V.S., 2211.00710

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

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

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

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

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

There is one notable exception! The universal location of the Yang-Lee edge singularity.
The problem was defined by Kortman and Griffiths in 1971. 5 decades later, it was solved.

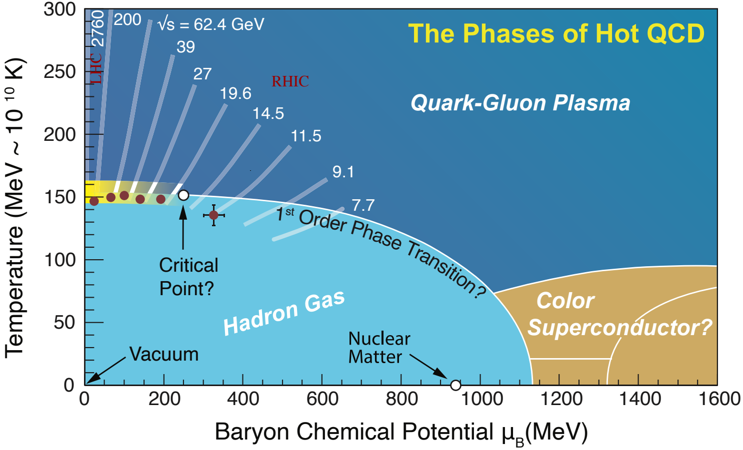
d=3: A. Connelly, G. Johnson, F. Rennecke, and V. S, Phys.Rev.Lett. 125 19, 191602 (2020)

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

Outline

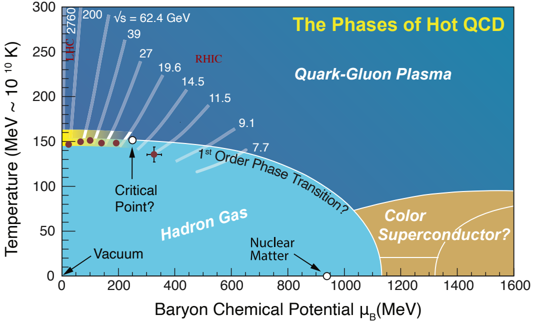
- Motivation and introduction: phase transitions and critical phenomena
- Universal features near a second-order phase transition
- Yang-Lee edge singularity
- Application to the phase diagram of strongly interacting matter
- Conclusions

Phase diagram of QCD



- The only phase diagram of the Standard model of particle physics that can be studied theoretically and also probed experimentally in the laboratory

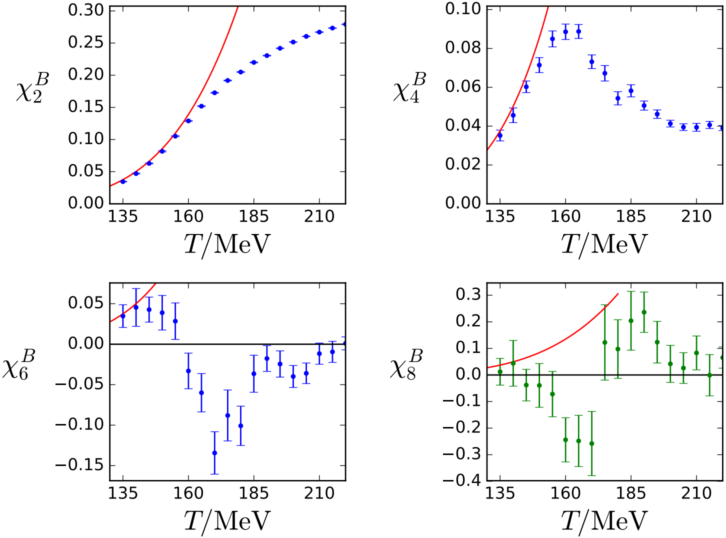
Phase diagram of QCD



- 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 ✗
- Lattice QCD: zero density region only due to the “sign” problem ✗
- Indirect: Taylor series coefficients → non-zero baryon density ✓

Taylor series coefficients from LQCD

S. Borsanyi, Z. Fodor, ... JHEP 10 (2018) 205



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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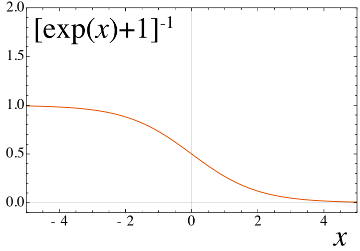
- Example $(a > 0)$

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



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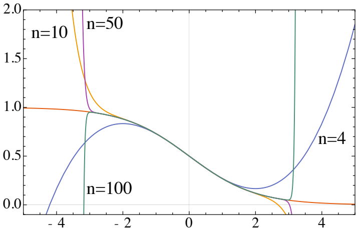

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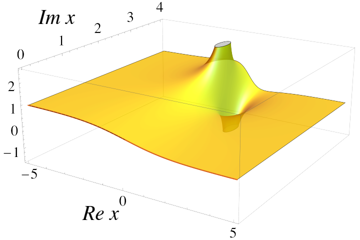

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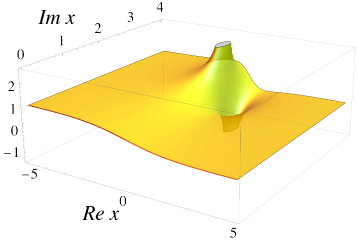
$$\frac{1}{a\, e^{x}+1} \to \frac{1}{e^{\frac{\omega}{T}+\frac{\mu}{T}}+1}$$



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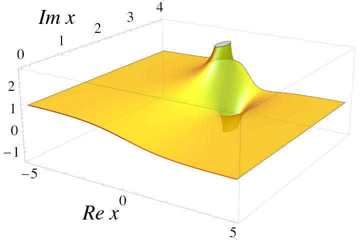

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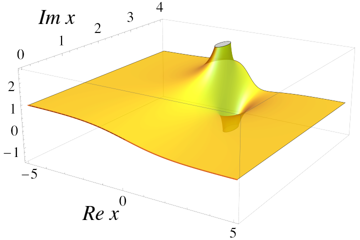


Yang-Mills with adjoint Weyl quark on $R^3 \times S^1$

Mithat Unsal's papers on weak coupling confinement in QCD-like theories

Analytic structure near critical point

Are there singularities associated with critical point/phase transitions?

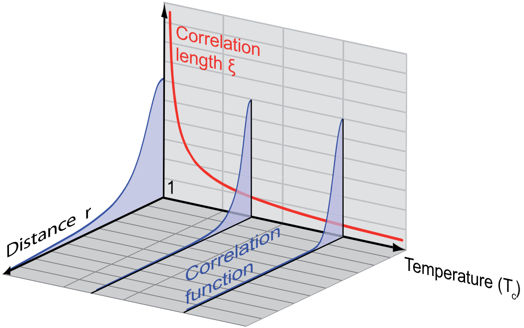
Analytic structure near critical point

Are there singularities associated with critical point/phase transitions?

Are they universal?

Correlation length, ξ

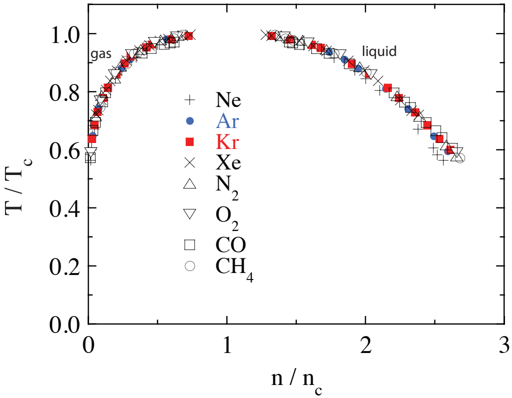
ξ = distance over which fluctuations of microscopic degrees of freedom are correlated



Universality

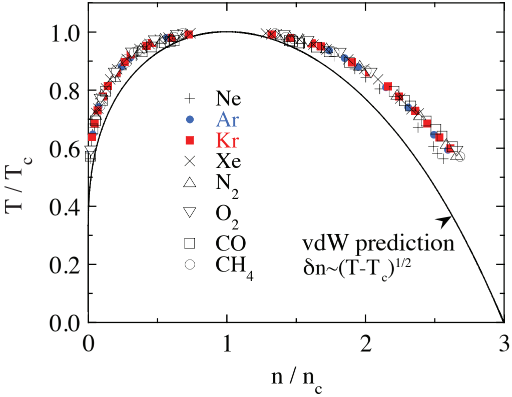
Divergent ξ: a large number of degrees of freedom are strongly correlated;
normal perturbative methods fail

Divergent ξ: no sensitivity to microscopic details $\rightsquigarrow$ universality



Reploted from E. Guggenheim, J. Chem. Phys. 13, 253 (1945); D. Johnston, 2014

Van Der Waals equation of state (1873): $\left(P + a\frac{N^2}{V^2}\right)(V - Nb) = NRT.$



Critical exponent $\beta_{\mathrm{vdW}} = 1/2$

D. Johnston, 2014

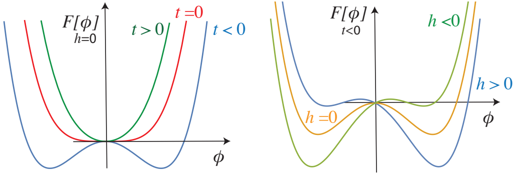
Landau free energy: the cornerstone of universality

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

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

Order parameters ϕ:

- Ferromagnet $\rightsquigarrow$ magnetization
- Fluid $\rightsquigarrow$ density of gas - density of fluid
- Confinement in Yang-Mills theory $\rightsquigarrow$ Polyakov loop



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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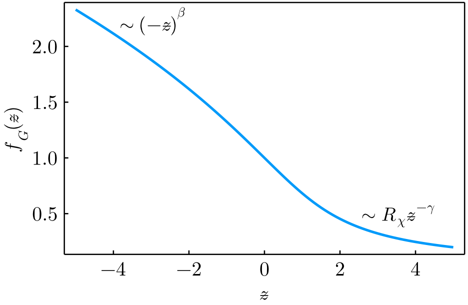
Magnetic equation of state

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

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

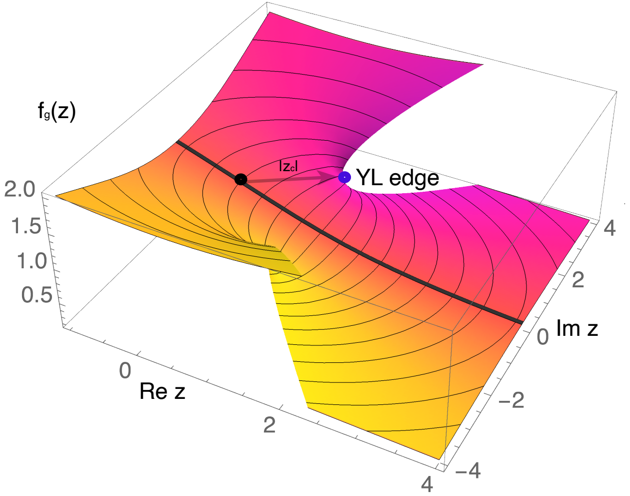


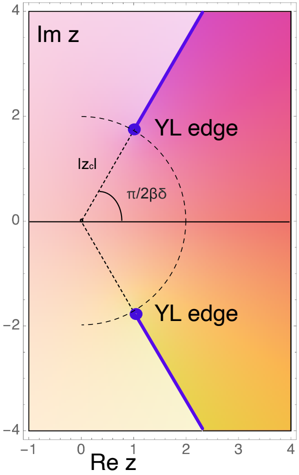
In general: $\phi = h^{1/\delta} f_G(z)$.

$$\phi = B(-t)^\beta \quad \rightsquigarrow \quad \phi = (-t)^\beta$$

$$\phi = B_c h^{1/\delta} \quad \rightsquigarrow \quad \phi = h^{1/\delta}$$

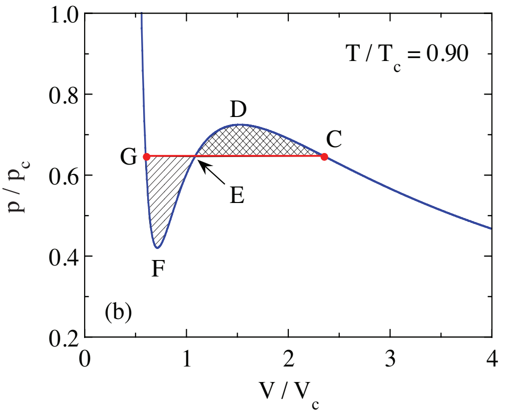
Magnetic equation of state in ℂ: Yang-Lee edge singularity





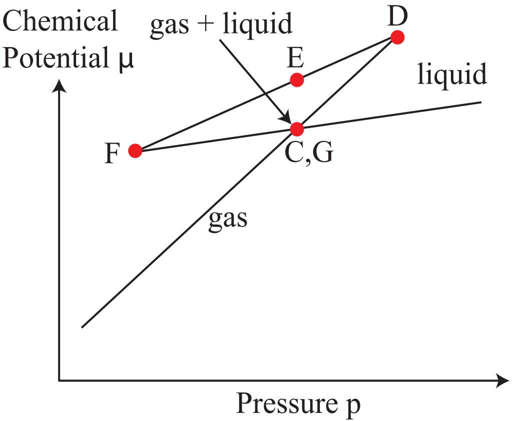
Finite size: YLE and cuts ⇝ Lee-Yang zeros

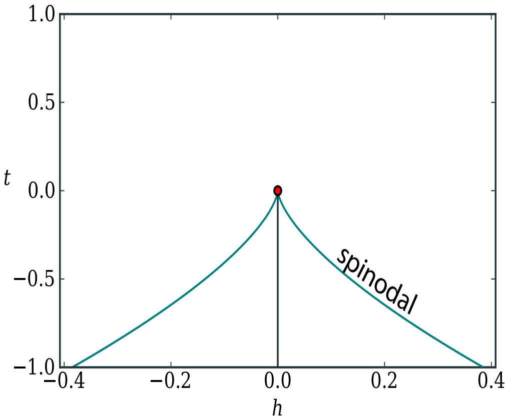
Yang-Lee edge singularity and spinodals



Spinodal points: F and D.

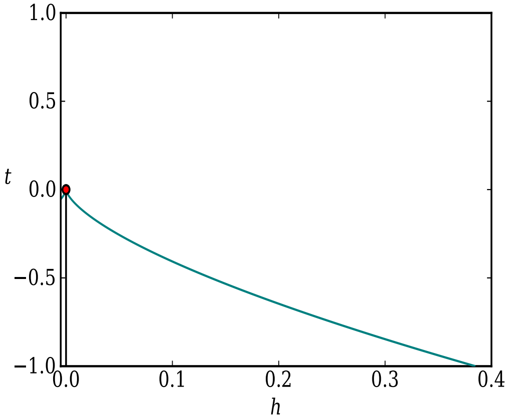
Yang-Lee edge singularity and spinodals





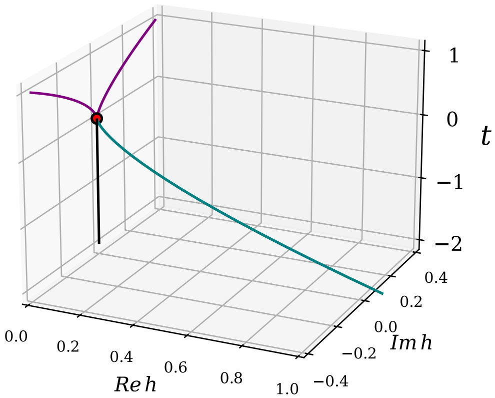
Spinodal points: F and D. As a function of T $\rightsquigarrow$ spinodal lines

Yang-Lee edge singularity and spinodals

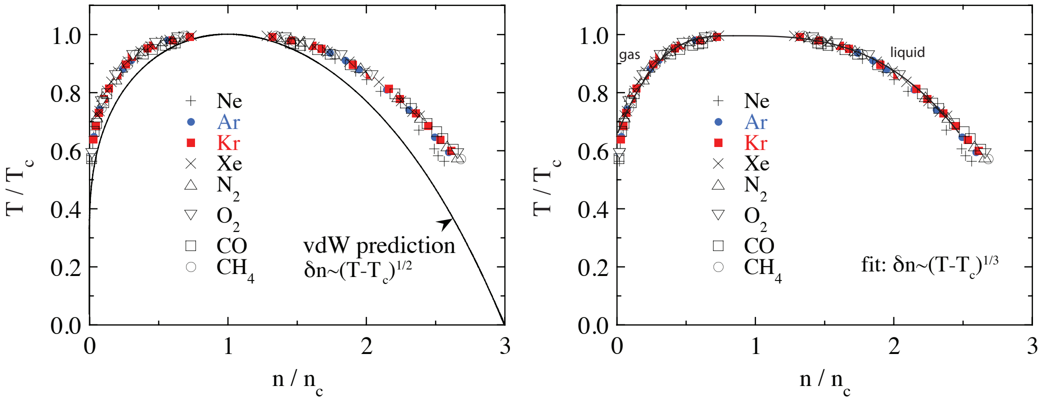


Defining equations: $\delta F/\delta\phi = 0$ & $\delta^2 F/\delta\phi^2 = 0$

Yang-Lee edge singularity and spinodals



Limitation of mean-field theories



The discrepancy was ignored until 1960

Ginzburg criterion and ε expansion

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

Mathematically

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

$$\frac{1}{\xi^d}\int d^dx\, x^{-(d-2)}\, g(x/\xi) \ll \frac{t}{\lambda}, \qquad \xi \propto t^{-1/2}$$

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

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

V. Ginzburg, 1960

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Idea: perturbation in ε, $d = 4 - \varepsilon$

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

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

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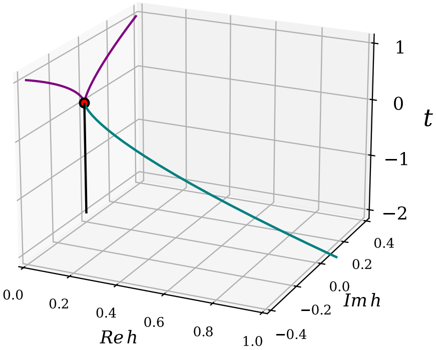
V. Ginzburg, 1960

Gradual inclusion of fluctuations

$d = 4$

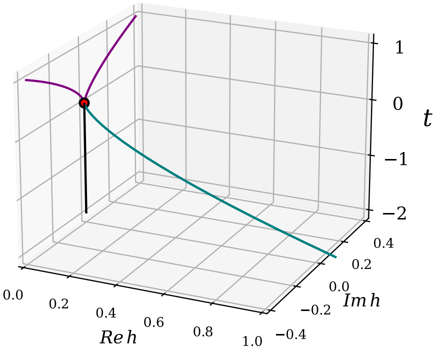


F. Rennecke, and V.S., Annals Phys. 444 (2022) 169010

G. Johnson, F. Rennecke, and V.S., 2211.00710

Gradual inclusion of fluctuations

$d = 3.99$

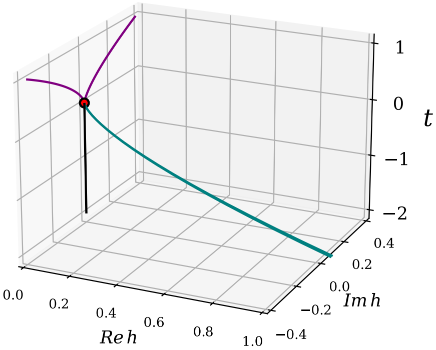


F. Rennecke, and V.S., Annals Phys. 444 (2022) 169010

G. Johnson, F. Rennecke, and V.S., 2211.00710

Gradual inclusion of fluctuations

$d = 3.9$

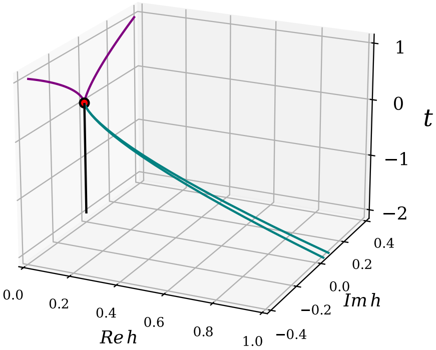


F. Rennecke, and V.S., Annals Phys. 444 (2022) 169010

G. Johnson, F. Rennecke, and V.S., 2211.00710

Gradual inclusion of fluctuations

$d = 3.8$

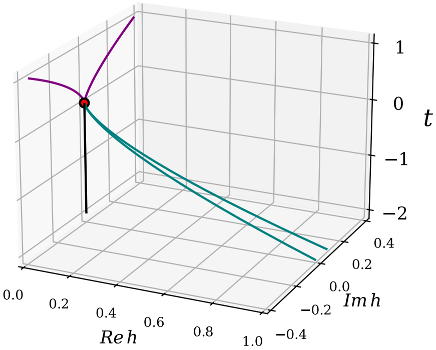


F. Rennecke, and V.S., Annals Phys. 444 (2022) 169010

G. Johnson, F. Rennecke, and V.S., 2211.00710

Gradual inclusion of fluctuations

$d = 3.7$



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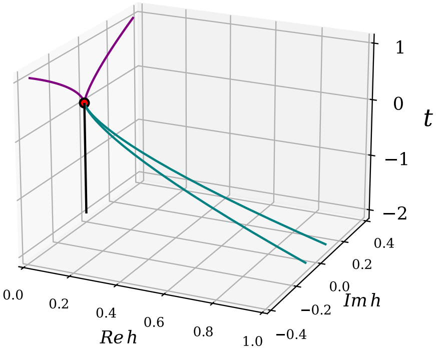
G. Johnson, F. Rennecke, and V.S., 2211.00710

Gradual inclusion of fluctuations

$d = 3.6$

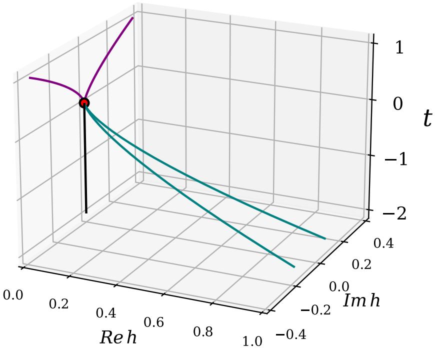


F. Rennecke, and V.S., Annals Phys. 444 (2022) 169010

G. Johnson, F. Rennecke, and V.S., 2211.00710

Gradual inclusion of fluctuations

$d = 3.5$

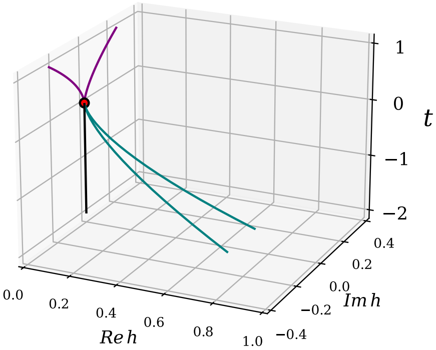


F. Rennecke, and V.S., Annals Phys. 444 (2022) 169010

G. Johnson, F. Rennecke, and V.S., 2211.00710

Gradual inclusion of fluctuations

$d = 3$



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

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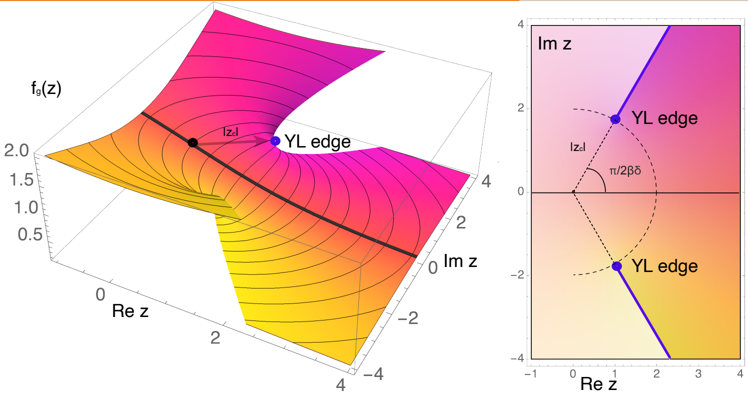
Universal location of Yang-Lee edge singularity



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

Attempts to locate $|z_c|$ started with the work of Kortman and Griffiths, Phys. Rev. Lett. 27 1439 (1971)

The ε-expansion: non-perturbative contributions

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

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

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.

$$|z_c| \approx |z_c^{\mathrm{MF}}| \left[1 + \frac{27 \ln\left(\frac{3}{2}\right) - (N-1)\ln 2}{9(N+8)}\epsilon\right] + \text{non-perturbative terms}\,.$$

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

G. Johnson, F. Rennecke, and V.S., 2211.00710

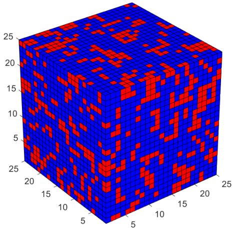
- Properties of YLE singularity (not the location) can be obtained using $d = 6 - \varepsilon$

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

Simulations on the lattice: sign problem

- Consider d-dimensional lattice

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

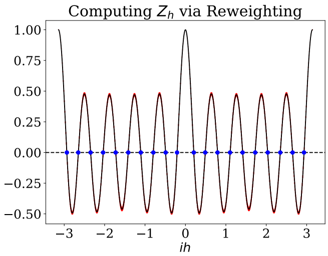


- 1d Ising model with 100 spins: sum over 2^{100} states

- Importance sampling; $\exp(-\beta F[s])$ – probability for s

- Imaginary $h \rightsquigarrow$ "sign problem"

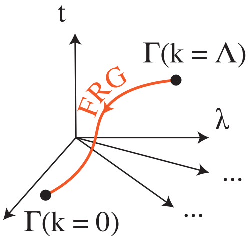
- No practical way to circumvent the problem in $d = 3$



Lee-Yang zeroes in 1-d Ising model, PY525 NCSU's students, 2021

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: infinite tower of coupled functional PDEs.

Truncation scheme

Critical phenomena $\rightsquigarrow$ long-distance properties

This suggests truncation scheme: derivative expansion:

- Local potential approximation (LPA): unrenormalized $(\partial\phi)^2$
- LPA': field-independent wave-function renormalization $Z(\partial\phi)^2$
- Next-to-leading order: $Z(\phi)(\partial\phi)^2$
- Next-to-next-to-leading order: $Z(\phi)(\partial\phi)^2 + W(\partial^2\phi)^2 + \ldots$
- ...

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- ...

Critical exponent $(N = 1)$	FRG $\mathcal{O}(\partial^6)$: fixed point "$\partial_k \Gamma_k[\phi] = 0$"	Conformal Bootstrap
η	0.0358(6)	0.0362978(20)
ν	0.6300(2)	0.629971(4)

G. De Polsi, I. Balog, M. Tissier and N. Wschebor, Phys. Rev. E 101, 042113 (2020)

Next-to-leading order in derivative expansion

In this talk: next-to-leading order

$$\Gamma_k = \int d^dx \left[\frac{1}{2} Z_k(\rho)\,\partial^\mu \phi_a \partial_\mu \phi_a + \frac{1}{4} Y_k(\rho)\,\partial^\mu \rho \partial_\mu \rho + U_k(\rho)\right], \quad \rho = \frac{1}{2}\phi_a\phi_a$$

The flow equation for the average potential

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

with “dressed” Green functions ($Z_k^{\perp} = Z_k$, $Z_k^{\parallel} = Z_k + \rho Y_k$, $\phi = \sqrt{2\rho}$)

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

Wave function renormalization

$$\partial_t Z_{\|}(\phi) = \int \bar{d}^d q\, \partial_t R_k(q^2) \Bigg\{ G_{\|}^2 \left[\gamma_{\|}^2 \left(G_{\|}' + 2G_{\|}'' \frac{q^2}{d} \right) + 2\gamma_{\|} Z_{\|}'(\phi) \left(G_{\|} + 2G_{\|}' \frac{q^2}{d} \right) + (Z_{\|}'(\phi))^2 G_{\|} \frac{q^2}{d} - \frac{1}{2} Z_{\|}''(\phi) \right]$$

$$+ (N-1) G_{\perp}^2 \left[\gamma_{\perp}^2 \left(G_{\perp}' + 2G_{\perp}'' \frac{q^2}{d} \right) + 4\gamma_{\perp} Z_{\perp}'(\phi) G_{\perp}' \frac{q^2}{d} + (Z_{\perp}'(\phi))^2 G_{\perp} \frac{q^2}{d} + 2 \frac{Z_{\|}(\phi) - Z_{\perp}(\phi)}{\phi} \gamma_{\perp} G_{\perp} \right.$$

$$\left. - \frac{1}{2} \left(\frac{1}{\phi} Z_{\|}'(\phi) - \frac{2}{\phi^2} (Z_{\|} - Z_{\perp}) \right) \right] \Bigg\}$$

$$\partial_t Z_k^{\perp}(\phi) = \int \bar{d}^d q\, \partial_t R_k(q^2) \Bigg\{ G_{\|}^2 \left[\bar{\gamma}_{\perp}^2 \left(G_{\perp}' + 2G_{\perp}'' \frac{q^2}{d} \right) + 2\bar{\gamma}_{\perp} Z_{\perp}'(\phi) \left(G_{\perp} + 2G_{\perp}' \frac{q^2}{d} \right) + (Z_{\perp}'(\phi))^2 G_{\perp} \frac{q^2}{d} - \frac{1}{2} Z_{\perp}''(\phi) \right]$$

$$+ G_{\perp}^2 \left[\bar{\gamma}_{\perp}^2 \left(G_{\|}' + 2G_{\|}'' \frac{q^2}{d} \right) + 4\bar{\gamma}_{\perp} \left(\frac{Z_{\|} - Z_{\perp}}{\phi} - Z_{\perp}'(\phi) \right) G_{\|}' \frac{q^2}{d} + \left(2 \frac{Z_{\|} - Z_{\perp}}{\phi} - Z_{\perp}'(\phi) \right)^2 G_{\|} \frac{q^2}{d} \right.$$

$$\left. + 2 \frac{Z_{\|} - Z_{\perp}}{\phi} \bar{\gamma}_{\perp} \left(G_{\|} + 2G_{\|}' \frac{q^2}{d} \right) - \frac{Z_{\|} - Z_{\perp}}{\phi^2} - \frac{1}{2} (N-1) \frac{1}{\phi} Z_{\perp}'(\phi) \right] \Bigg\}$$

$$\gamma_{\|} = q^2 Z_{\|}'(\phi) + U^{(3)}(\phi), \quad \gamma_{\perp} = q^2 Z_{\perp}'(\phi) + \frac{\partial}{\partial \phi} \left(\frac{1}{\phi} U'(\phi) \right),$$

$$\bar{\gamma}_{\|} = q^2 \frac{Z_{\|} - Z_{\perp}}{\phi} + U^{(3)}(\phi), \quad \bar{\gamma}_{\perp} = q^2 \frac{Z_{\|} - Z_{\perp}}{\phi} + \frac{\partial}{\partial \phi} \left(\frac{1}{\phi} U'(\phi) \right).$$

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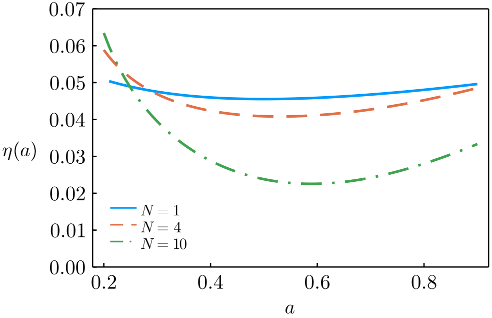
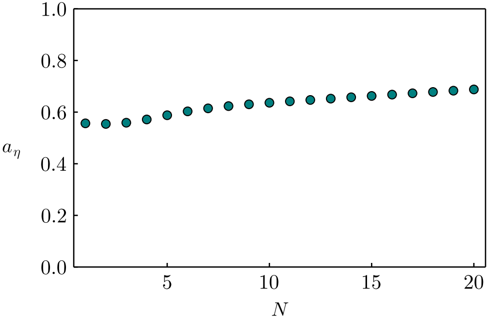
Regulator function

- To simplify numerics – choose $R_k(q)$ which leads to analytical expressions for momentum integrals $R_k(q^2) = a\ Z_k^{||}\ (k^2 - q^2)\theta(k^2 - q^2)$.
- Without truncation: FRG IR solution is independent of the form of R & the value of a
- Any truncation $\rightsquigarrow$ spurious dependence; the principle of minimal sensitivity to fix a





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Numerics

Challenge: Analytical expressions are very lengthy
Solution: Symbolic manipulation program (Mathematica; equations in text form $\approx$ 2 Gb)

Challenge: The problem reduces to stiff differential equations
Solution: Implicit solvers

Challenge: Computationally difficult
Solution: modular design, optimized data management, HPC

Numerics: broken phase

- Calculations in broken phase are possible, but numerically expensive

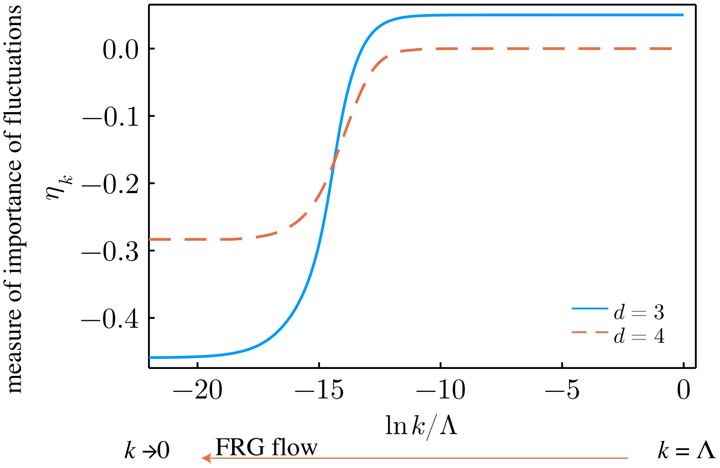
- Why do we need broken phase to study what is primarily the property of symmetric phase?

$$z = \left(\frac{B}{B_c}\right)^{1/\beta} \frac{\hat{t}}{\hat{h}^{1/\beta\delta}}$$

- Instead

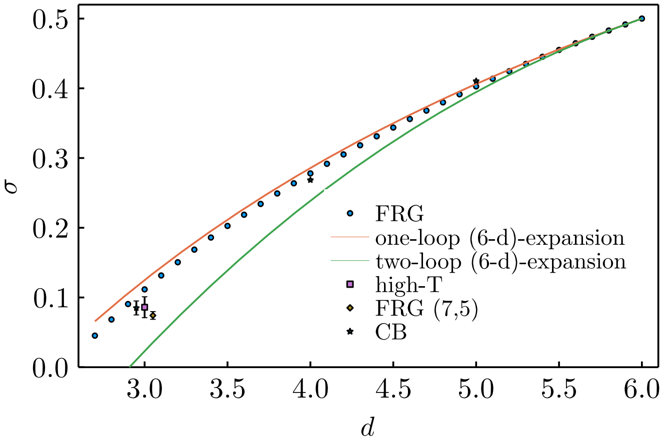
$$\zeta = z/R_\chi^{1/\gamma} = \left(\frac{B_c}{C_+}\right)^{1/\gamma} \frac{\hat{t}}{\hat{h}^{1/\beta\delta}}, \qquad \chi = C_+ \hat{t}^{-\gamma}$$

Results: importance of fluctuations



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

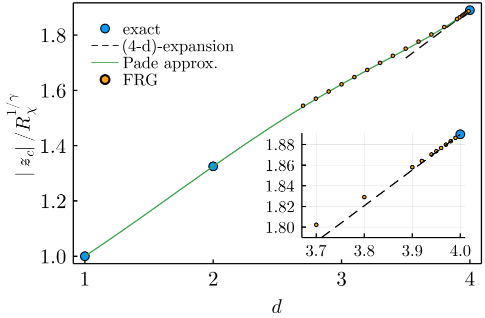
Edge critical exponent



$\sigma = \frac{d-2+\eta}{d+2-\eta}$

F. Rennecke and V. S, Annals Phys. 444 (2022) 169010
FRG (5,7): X. An, D. Mesterhazy and M. A. Stephanov, JHEP 07, 041 (2016)
*CB: F. Gliozzi and A. Rago, JHEP **10**, 042 (2014)*

Results: precision calculation $N = 1$

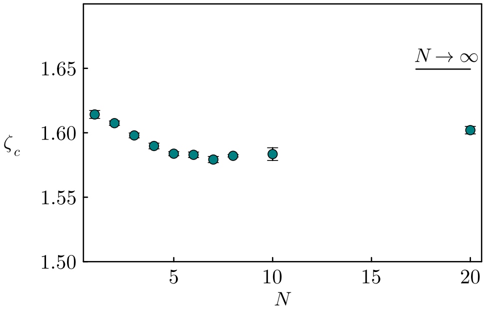


d	1	2	3	4
$\lvert z_c\rvert/R_\chi^{1/\gamma}$	1	1.32504(2)	1.614(4)	$3/2^{2/3}$

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

$d = 2$ from H.-L. Xu and A. Zamolodchikov, "2D Ising Field Theory in a magnetic field: the Yang-Lee singularity" JHEP 08 (2022) 057

Results: precision calculation arbitrary N and $d = 3$



N	1	2	3	4	5
$\lvert\zeta_c\rvert$	1.614(4)(0)	1.607(2)(1)	1.597(2)(1)	1.589(2)(0)	1.583(2)(1)

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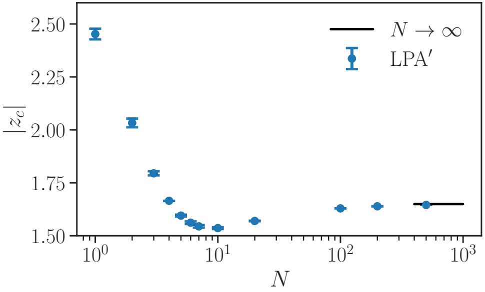
Results: precision calculation arbitrary N and $d = 3$



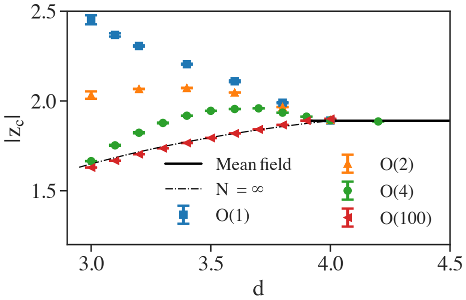
N	1	2	3	4	5
$\lvert z_c \rvert$	2.42(4)	2.03(8)	1.82(5)	1.68(3)	1.54(4)

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

G. Johnson, F. Rennecke, and V. S, 2211.00710

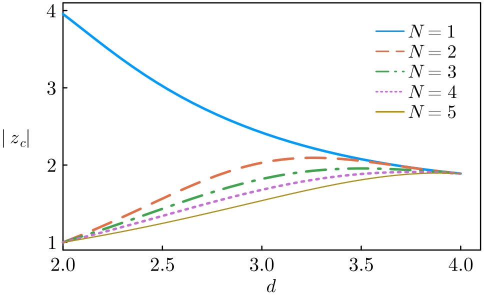
Results

LPA'



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

Next-to-leading order



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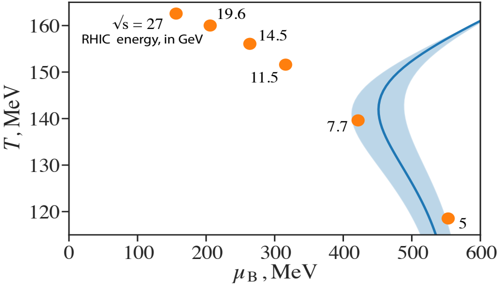
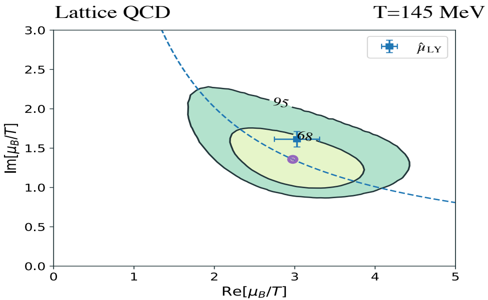
Application to QCD phase diagram





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

Bielefeld Lattice QCD: P. Dimopoulos et al., Phys.Rev.D 105, 034513 (2022)

"Universality, Lee-Yang Singularities, and Series Expansions", G. Basar, Phys. Rev. Lett. 127 17, 171603 (2021)

Conclusions

- FRG approach to locating Yang-Lee edge singularity for a range of N and d

- Towards precision results for three-dimensional classic universality classes

N	1	2	4
$\lvert z_c\rvert$	2.42(4)	2.03(8)	1.68(3)
$\lvert z_c\rvert/R_\chi^{1/\gamma}$	1.614(4)(0)	1.607(2)(1)	1.589(2)(0)