Lee-Yang singularities, series expansions and the critical point

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 Based on:

 GB PRL 127 (2021) 17, 171603

 GB, G. Dunne (UConn), Z. Yin (UNC→ Stanford) PRD 105 (2022) 10, 105002

Motivations



Motivations

Strongly correlated fermions, ultra-cold atoms

• At high *T*/low density, *Virial expansion*

$$\Omega = -T \log \mathscr{Z} \sim -T \sum_{n=0}^{N} b_n e^{n\mu/T}$$



Motivations

EXAMPLE 1017 (2022) 1222421
$$\begin{pmatrix} r \\ h \end{pmatrix} = \mathbb{M} \begin{pmatrix} T - T_c \\ \mu - \mu_C \end{pmatrix} = \begin{pmatrix} r_T & r_\mu \\ h_T & h_\mu \end{pmatrix} \begin{pmatrix} T - T_c \\ \mu - \mu_C \end{pmatrix}$$



Given the e.o.s. as truncated Taylor series around μ =0, what can we say about *the critical e.o.s* ? More generally how much of the e.o.s. we can reconstruct?



Given a finitely many terms in the series expansion the equation of state, obtained away from a critical point, what can we say about *the critical phenomena* ?

How much of the critical e.o.s can we reconstruct?

Mathematically: reconstructing a function near a singularity from a truncated local expansion at a regular point.

 $f(x) \sim c_0 + c_1 x + c_2 x^2 + \dots + c_n x^n$

Gross-Neveu Model

$$S = \int d^2x \sum_{a=1}^{N_F} \left(i\bar{\psi}_a(\partial - m_q)\bar{\psi}_a + \frac{g^2}{2}(\bar{\psi}_a\psi_a)^2 \right)$$

[Gross, Neveu, '74]

- Solvable in large N_f limit (mean field is exact at $N_f = \infty$)
- Asymptotically free, dimensional transmutation
- Chiral symmetry breaking $(\mathbb{Z}_2 : \psi \to \gamma^5 \psi)$
- Toy model for QCD
- Condensed matter: model for *trans-polyacetylene*

$$\frac{\pi}{Ng^2} = \log \frac{\Lambda}{m}$$

Dimensional transmutation



$$\gamma \equiv \frac{\pi}{Ng^2} \frac{m_q}{m} = \log \frac{m[m_q]}{m[0]}$$

Explicit χ SB parameter

Thermodynamics:

$$\Omega[T,\mu] = \min_{\phi} \left(\frac{\phi^2}{2\pi} \left(\log \phi - \frac{1}{2} + \gamma \right) - \frac{\gamma}{\pi} \phi - T \int \frac{dk}{2\pi} \log \left[\left(1 + e^{-\left(\sqrt{k^2 + \phi^2} - \mu\right)/T} \right) \left(1 + e^{-\left(\sqrt{k^2 + \phi^2} + \mu\right)/T} \right) \right] \right]$$

Gross-Neveu Model

"homogeneous" phase diagram (toy example for QCD)* [Barducci et al. '95]



- Assume m_q ≠ 0
 Near the critical p.t
 ⇒ Z₂ Ising e.o.s
 mean field exponents
 β = 1/2, δ = 3, σ_{LY} = 1/2
- Focus on the crossover

 $T\gtrsim T_c$

• T, μ normalized to m

*for the phase diagram including crystalline phases see [Schnetz ,Thies, Ulrichs '05 ; GB, Dunne, Thies '08]

Lee-Yang edge singularities

- The equation of state has complex singularities
- Zeroes of partition function $\mathscr{Z}(\zeta)$ ($\zeta = e^{\mu/T}$: fugacity)
- Coalesce into branch cuts in thermodynamic limit
- Pinch the real axis at a second order transition

[Lee-Yang, 52']



[See talk by Skokov]

In the context of QCD see eg. [Halasz, Jackson Verbaarshot '97, Ejiri '05, Stephanov '06, Mukherjee, Skokov '20,...]

Lee Yang edge singularity

• The scaling e.o.s, $f_s(w)$, has singularities at $w = \pm i w_{LY}$ ($w := hr^{-\beta\delta}$)

$$\mu_{LY}(T) \approx \mu_c - \frac{h_T}{h_{\mu}}(T - T_c) \pm iw_{LY} \frac{\left(\det \mathbb{M}\right)^{\rho o}}{h_{\mu}^{\beta \delta + 1}}(T - T_c)^{\beta \delta}$$

$$(\tan \alpha_1)^{-1} \qquad \det \mathbb{M} \propto (\tan \alpha_2 - \tan \alpha_1)$$

$$relative \ angle$$

$$between \ r, \ h \ axes$$

$$see$$

$$[Pradeep, Stephanov '19]$$

 $T = T_c$

• The e.o.s. near the LY singularity: $M(w) \sim (w \pm iw_{LY})^{\sigma_{LY}}$, (*M* : magnetization) $\sigma_{LY,d=3} \approx 0.1$, $\sigma_{LY,d=6} = 1/2$ (mean field)

[Fisher, '74; An, Stephanov, Mesterházy '16; Connelly, Johnson, Mukherjee, Skokov '20]

Large order behavior e.g. $\chi(T,\mu) = \sum_{n} c_{2n}(T)\mu^{2n} \to c_{2n}/c_{2n+2} \sim |\mu_{LY}^2|, \quad n \to \infty$

• Singularities are complex conjugate pairs: *interference* effect in large order behavior

• Difficult to extract the radius of convergence



Large order behavior e.g. $\chi(T,\mu) = \sum_{n} c_{2n}(T)\mu^{2n} \to c_{2n}/c_{2n+2} \sim |\mu_{LY}^2|, \quad n \to \infty$

We can do better!

- I Extract the location of $\mu_{LY}(T)$
- II Reconstruct the equation of state beyond the radius of convergence
- III Reconstruct the equation of state beyond the leading Riemann sheet (globally!)

When life gives you Taylor series...



When life gives you Taylor series...

Spurious poles are unavoidable in Padé when there are conjugate pair of singularities...



Conformal Maps

We can still do better!



Do Padé resummation in the ζ plane (unit circle)

"conformal Padé"
$$P\chi(T,\phi(\zeta)) = \frac{\tilde{p}_0(T) + \tilde{p}_1(T)\zeta + \dots + \tilde{p}_{N/2}(T)\zeta^N}{\tilde{q}_0(T) + \tilde{q}_1(T)\zeta + \dots + \tilde{q}_{N/2}(T)\zeta^N} \Big|_{\zeta = \phi^{-1}(\mu^2)}$$

Results: susceptibility



Results: susceptibility



Results: skewness, kurtosis



Results: Lee-Yang trajectory

• Find $\mu_{LY}^2(T)$ from conformal- Padé for different temperatures



Results

$$\mu_{LY}(T) \approx \mu_c - \frac{h_T}{h_{\mu}}(T - T_c) + iw_{LY}\frac{r_{\mu}^{3/2}}{h_{\mu}} \left(\frac{r_T}{r_{\mu}} - \frac{h_T}{h_{\mu}}\right)^{3/2}(T - T_c)^{3/2} \qquad w_{LY} = \frac{2}{3\sqrt{3}}$$

$$\boxed{T_c \quad \mu_c \quad h_T/h_{\mu} \quad c}$$

$$\boxed{exact \quad 0.192 \quad 0.717 \quad 0.249 \quad 4.684}$$

$$\boxed{conf. \ Padé (N=21) \quad 0.195 \quad 0.716 \quad 0.248 \quad 4.323}$$

$$\boxed{conf. \ Padé (N=11) \quad 0.185 \quad 0.707 \quad 0.225 \quad 3.666}$$

Crossing the branch cuts...

 $w = hr^{-\beta\delta}$ $z = Mr^{-\beta}$ Ising model: w = F(z) $F(z) = z + z^3$ (mean field)

High Temperature (T>T_c)

Low Temperature $(T < T_c)$



Uniformization



$$\lambda(\tau) = \frac{\theta_2^4(\tau)}{\theta_3^4(\tau)} \quad \text{(elliptic modular function)}$$

$$\theta_2(\tau) = \sum_{n=1}^{\infty} e^{2\pi i \tau (n+1/2)^2}, \quad \theta_3(\tau) = \sum_{n=1}^{\infty} e^{2\pi i \tau n^2}$$



High T



Uniformization



Uniformization



Uniformization: higher Riemann sheets



Moving within unit circle (smooth)



Jumping through sheets

Uniformization: higher Riemann sheets





Low T





- Combined with conformal maps, Padé approximants provide a powerful tool to extract information from truncated Taylor series.
- In the crossover region by using this tool it is possible to pin down the location of the *Lee-Yang edge singularity* and also extract information on the *mapping parameters to critical Ising e.o.s.*
- Conformal Padé gives a significantly better approximation to the e.o.s than than the Taylor series, going beyond the radius of convergence .
- Uniformizing map allows one to reconstruct the e.o.s globally. *Physically: crossover to 1st order region.*
- All of this comes with no more cost than the Taylor series!



- Beyond mean field
- •Numerical uncertainties in coefficients
- Extrapolation from imaginary μ, pairing with other resummation schemes
 [with V. Skokov, F. Rennecke]
 [e.g. Ratti et al '21-22, Mukherjee et al '22,...]
- Singularity elimination

