Complex-valued degrees of freedom in the analysis of phase diagrams: Lefschetz thimbles, Pade approximants and all that

Francesco Di Renzo (University of Parma and INFN)

GAUGE TOPOLOGY, FLUX TUBES AND HOLOGRAPHIC MODELS:
THE INTRICATE DYNAMICS OF QCD IN VACUUM AND EXTREME ENVIRONMENTS

ECT* Trento, 25/05/2022

In collaboration with P. Dimopoulos, S. Singh (Parma), K. Zambello (Parma -> Pisa),
L. Dini, J. Goswami, D. Clarke, G. Nicotra, C. Schmidt, F. Zieschè (Bielefeld)

I teach students that it is better to regard real functions as restrictions to the real axis of (analytic) complex functions rather than regarding complex functions as extensions of real functions to complex plane …

As annoyed as we can be of complex actions (and the sign problem), we always have to surrender to the complex plane as the real arena for the study of phase diagrams…

We will look at a couple of examples of *interesting physics going on in the complex plane*.

We will be concerned with **Lefschetz Thimbles** (doing better that what we had been able to do previously) and **Lattice QCD at imaginary values of the baryonic chemical potential**.

A unifying tool will be (**multi-point**) **Padè analysis**.

Thimble regularisation in a nutshell (via a toy model)

Aurora Coll. (2012) Y. Kikukawa et al (2013)

$$\langle O \rangle = Z^{-1} \int dx e^{-S(x)} O(x)$$

$$S(x) = S_R(x) + iS_I(x)$$

complex action … SIGN PROBLEM!

Thimble regularisation in a nutshell (via a toy model)

$$\langle O \rangle = Z^{-1} \int dx e^{-S(x)} O(x)$$

$$= \frac{\sum_\sigma n_\sigma e^{-iS_I(p_\sigma)} \int_{\mathcal{J}_\sigma} dz e^{-S_R(z)} O(z) e^{i\omega(z)}}{\sum_\sigma n_\sigma e^{-iS_I(p_\sigma)} \int_{\mathcal{J}_\sigma} dz e^{-S_R(z)} e^{i\omega(z)}}$$

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$\mathcal{J}_\sigma$ union of solutions of the SA equations attached to STATIONARY POINTS where $\partial_z S = 0$

$$\frac{d}{dt} z_i = \frac{\partial \bar{S}}{\partial \bar{z}_i}$$ complex DOF!

$$e^{-iS_I(p_\sigma)}$$ constant!

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$$= \frac{\sum_\sigma n_\sigma e^{-iS_I(p_\sigma)} Z_\sigma \langle O e^{i\omega} \rangle_\sigma}{\sum_\sigma n_\sigma e^{-iS_I(p_\sigma)} Z_\sigma \langle e^{i\omega} \rangle_\sigma}$$

with $\langle X \rangle_\sigma \equiv \frac{\int_{\mathcal{J}_\sigma} dz e^{-S_R} X}{\int_{\mathcal{J}_\sigma} dz e^{-S_R}} \equiv \frac{\int_{\mathcal{J}_\sigma} dz e^{-S_R} X}{Z_\sigma}$

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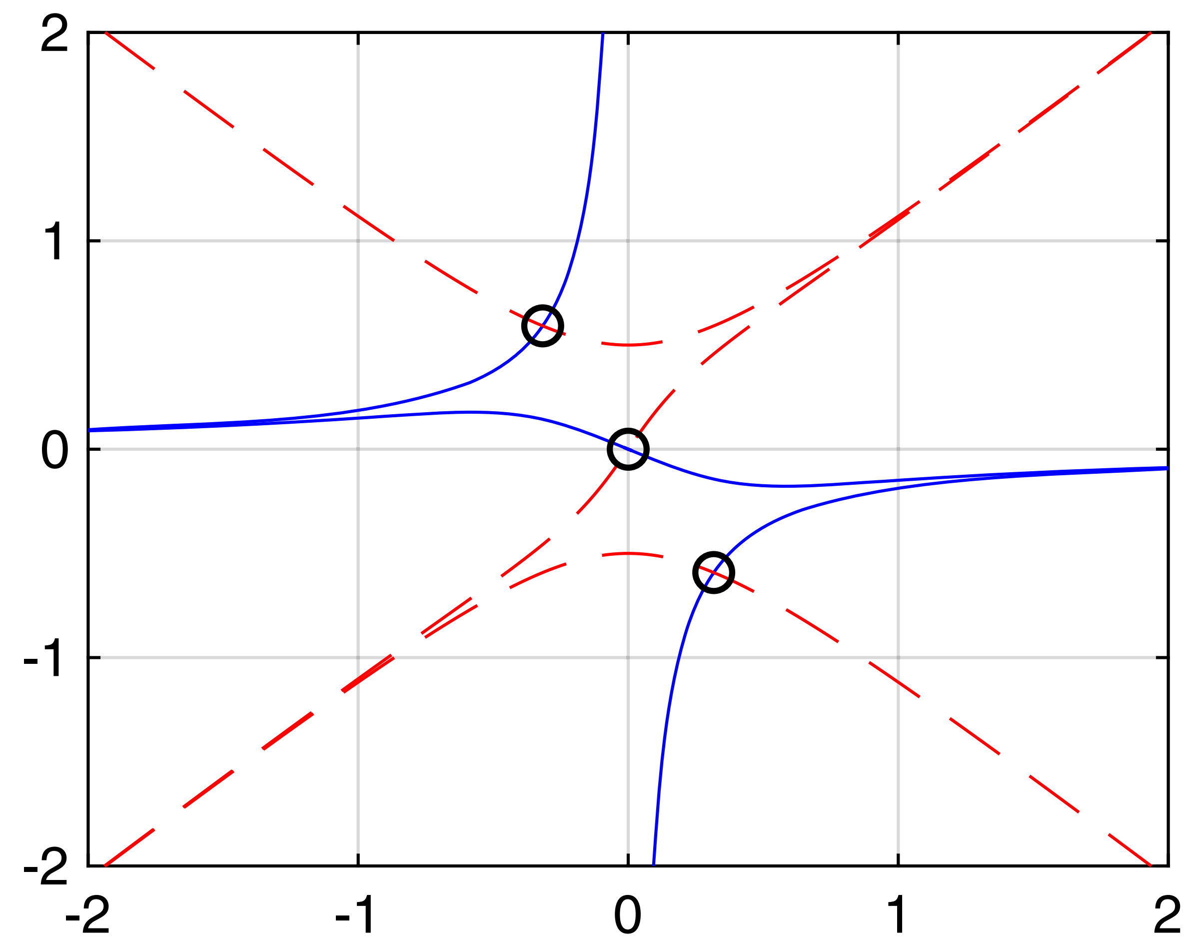
<u>concrete example</u>

$$Z = \int_{\mathbb{R}} \mathrm{d}\phi e^{-S(\phi)} \qquad S(\phi) = \frac{1}{2}\sigma\phi^2 + \frac{1}{4}\lambda\phi^4$$

STABLE (SA) and UNSTABLE (SD) thimbles



Only thimbles associated to critical points whose unstable thimble intersects the original domain of integration enter the THIMBLE DECOMPOSITION!

I am cheating you …

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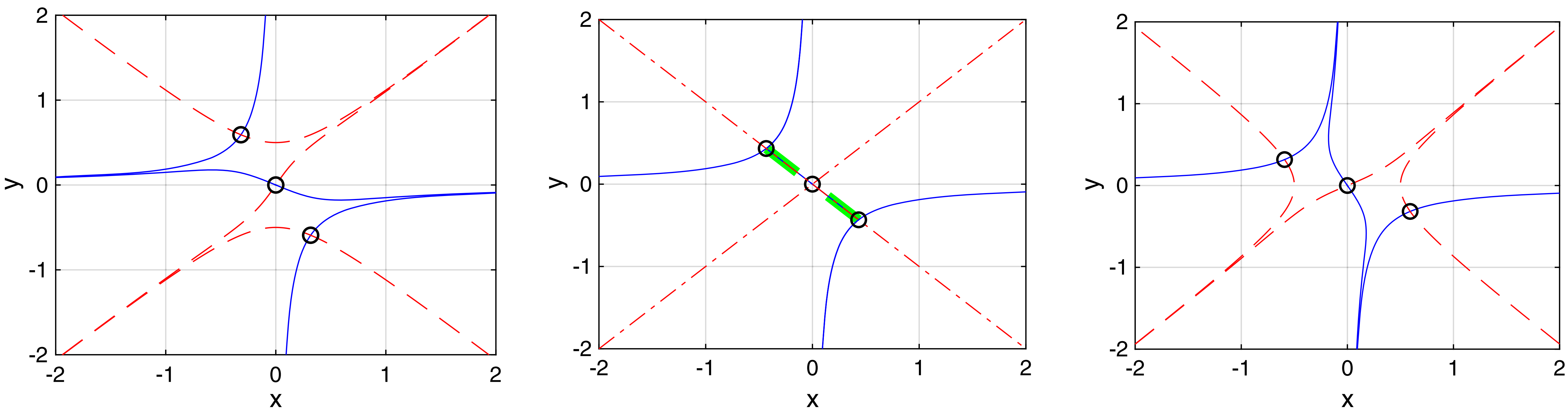
THIMBLE DECOMPOSITION does not hold the same once and forever!
It is different in different region of the parameters space!



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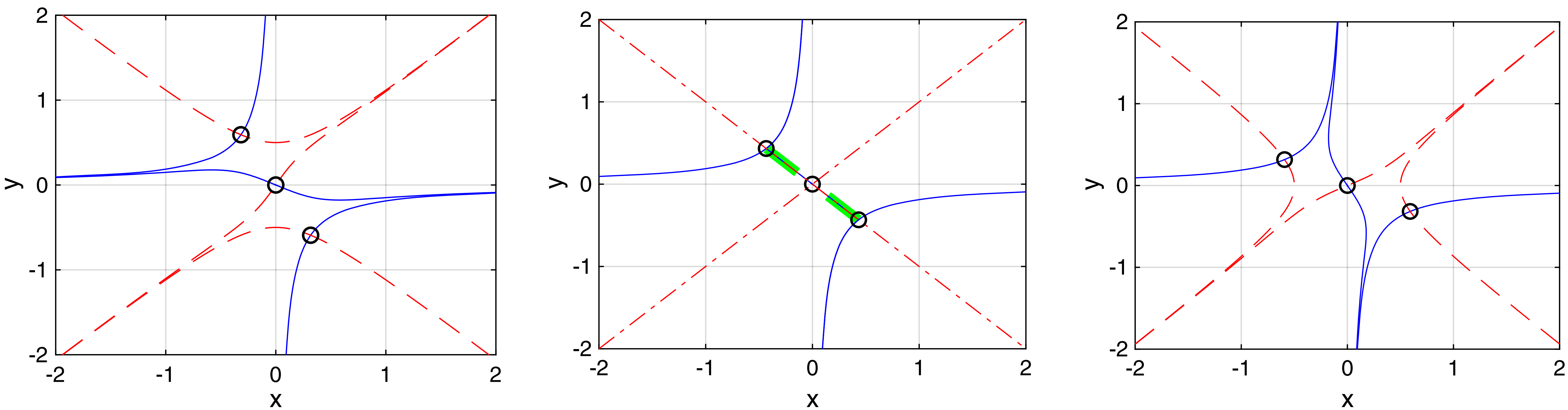

One single thimble contributing

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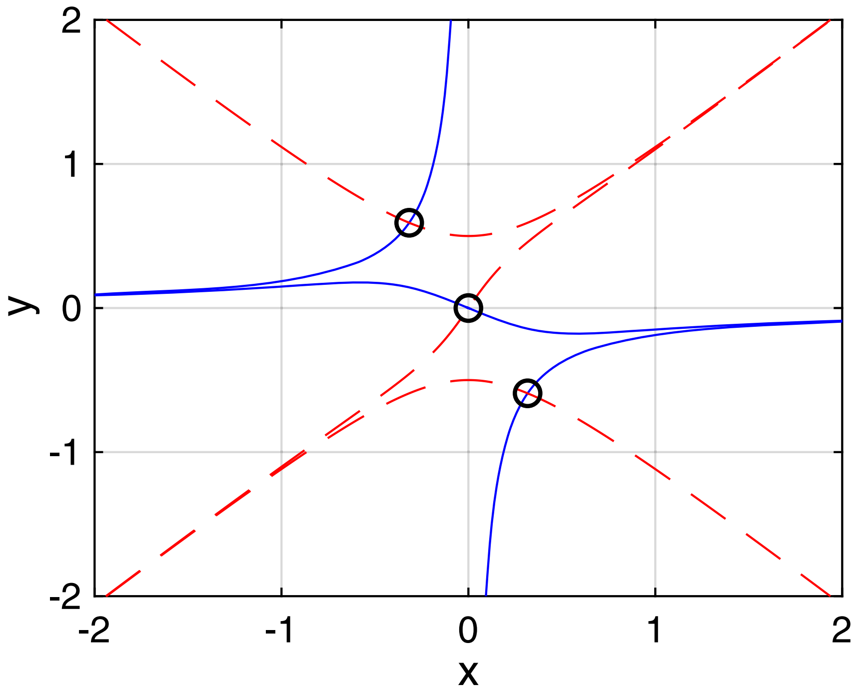

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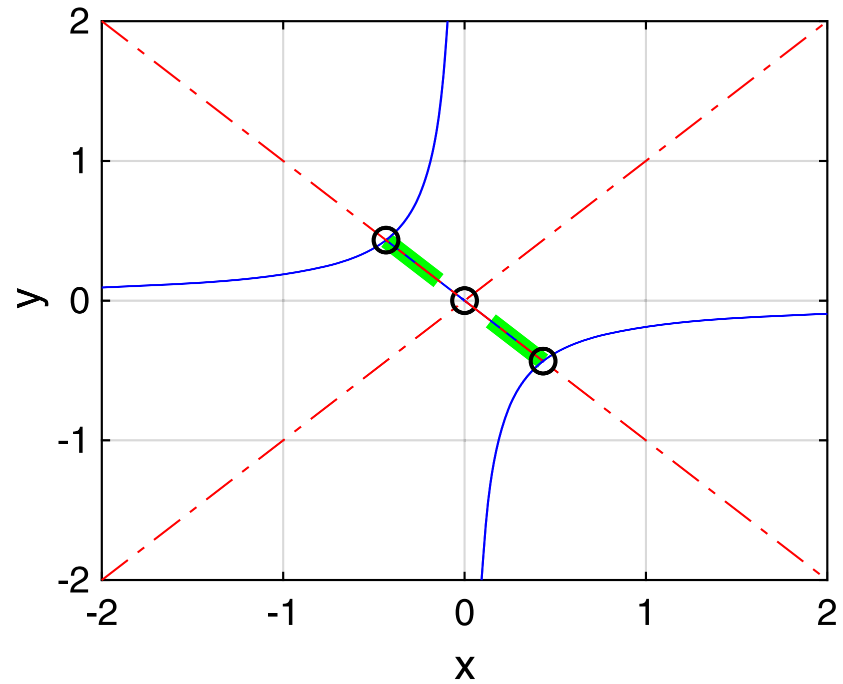

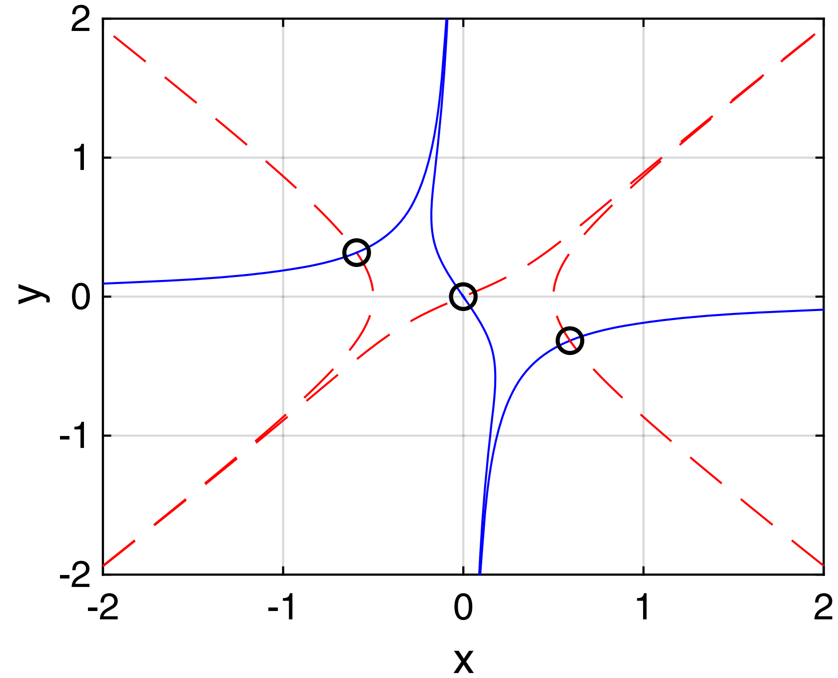

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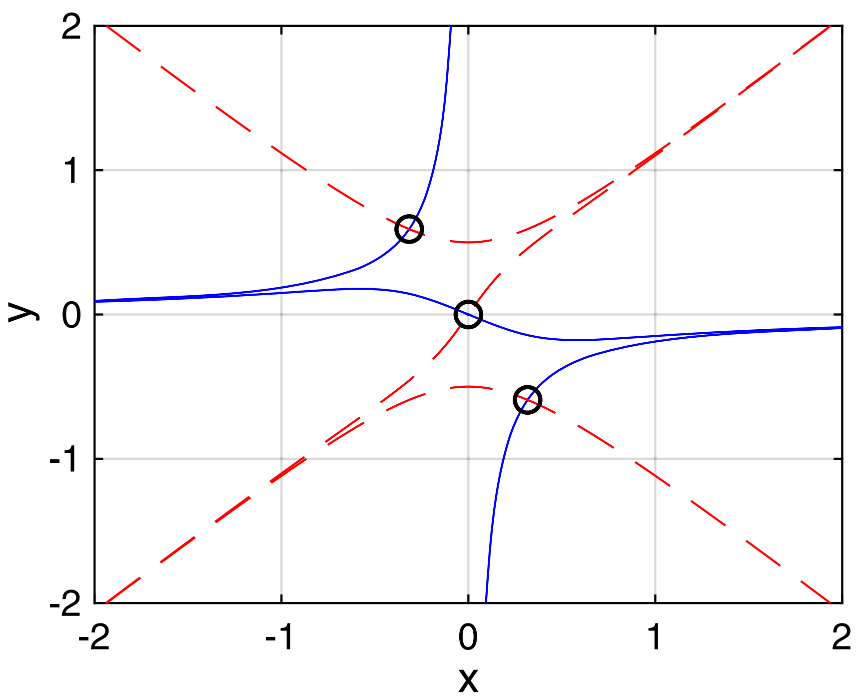

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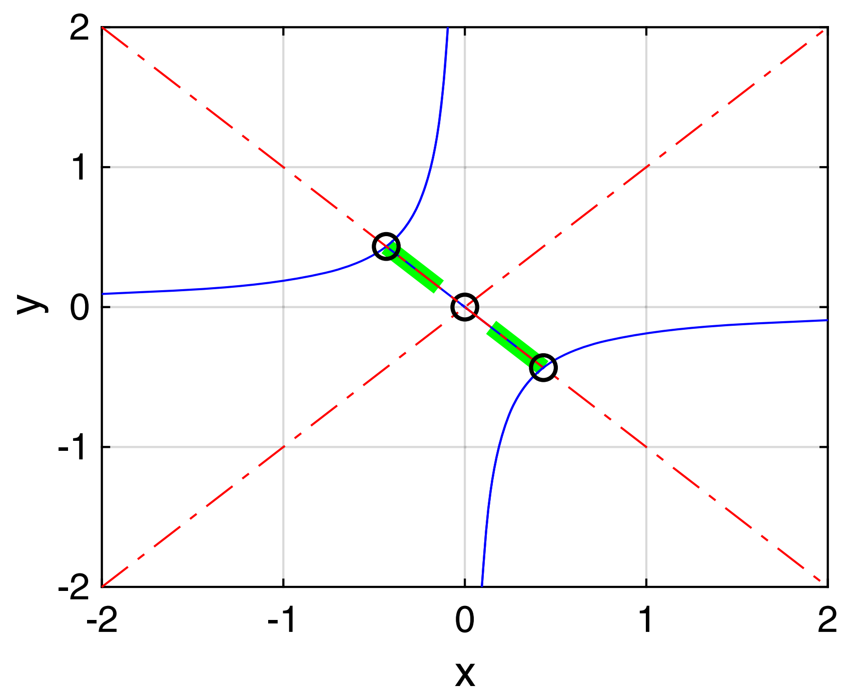
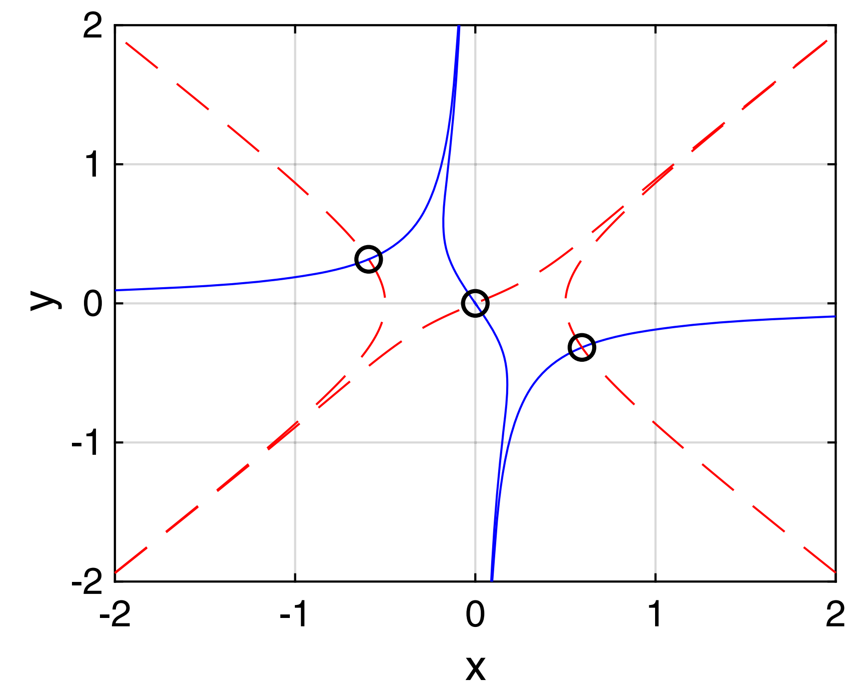


Stokes phenomenon



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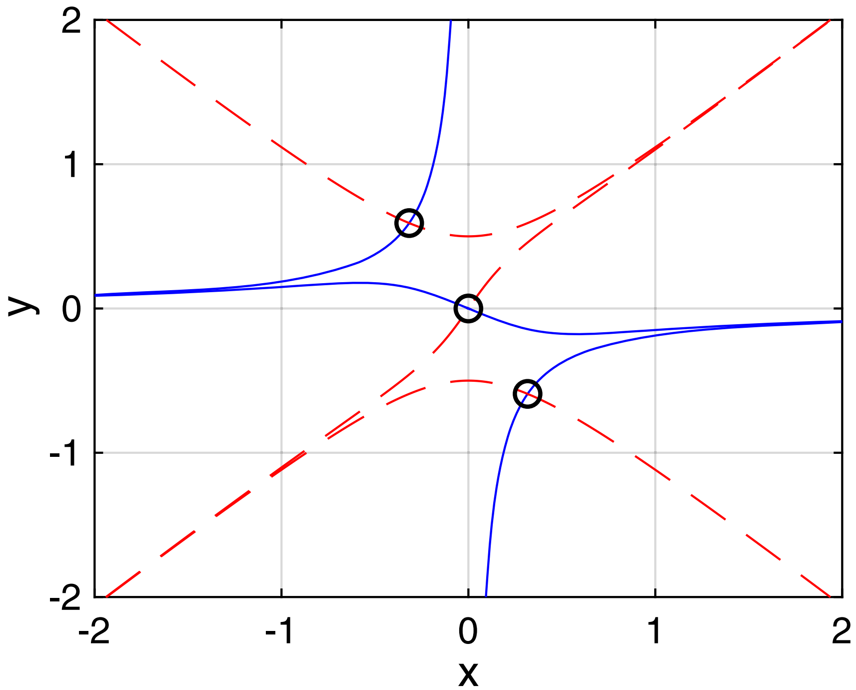

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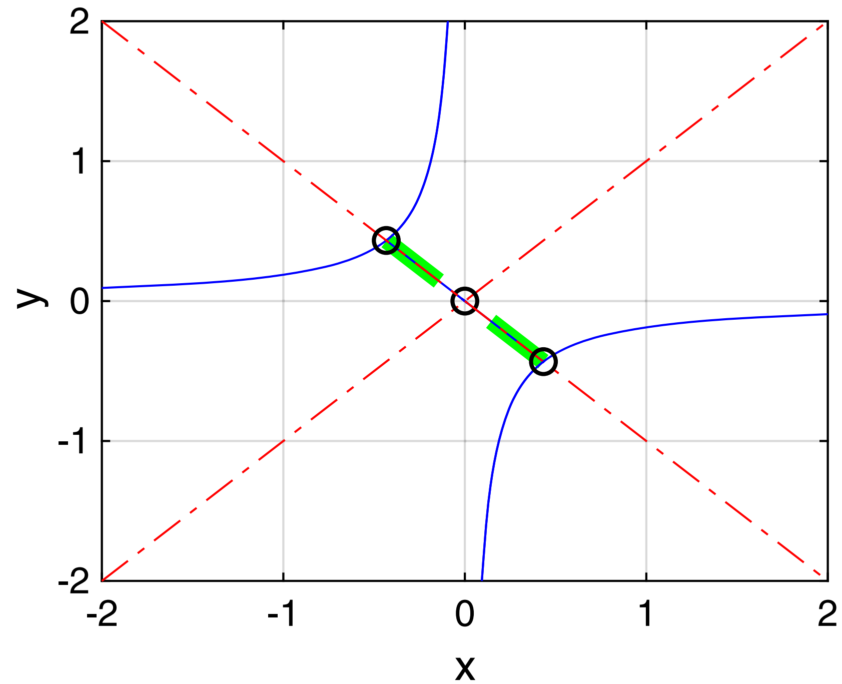

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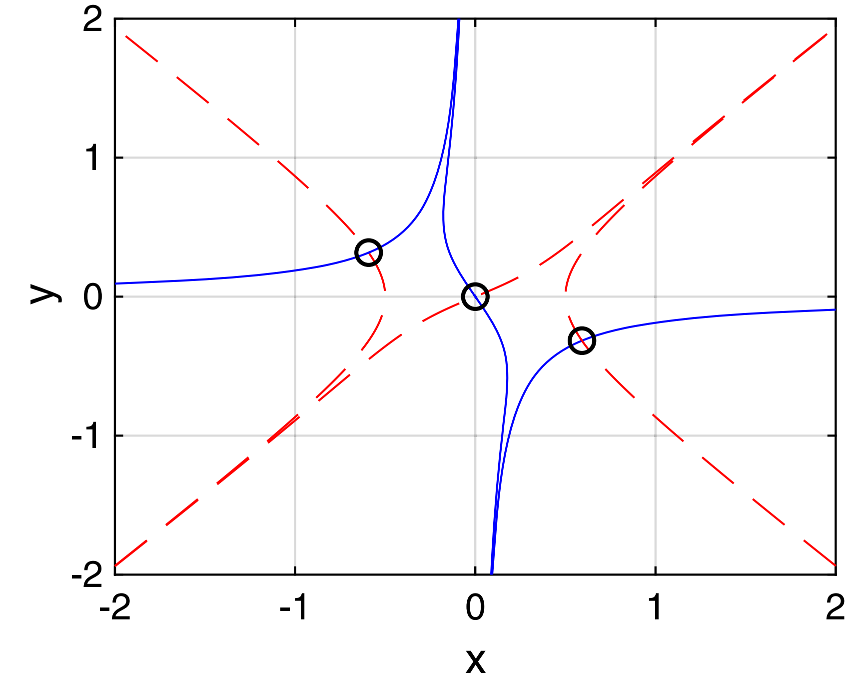


More thimbles contributing

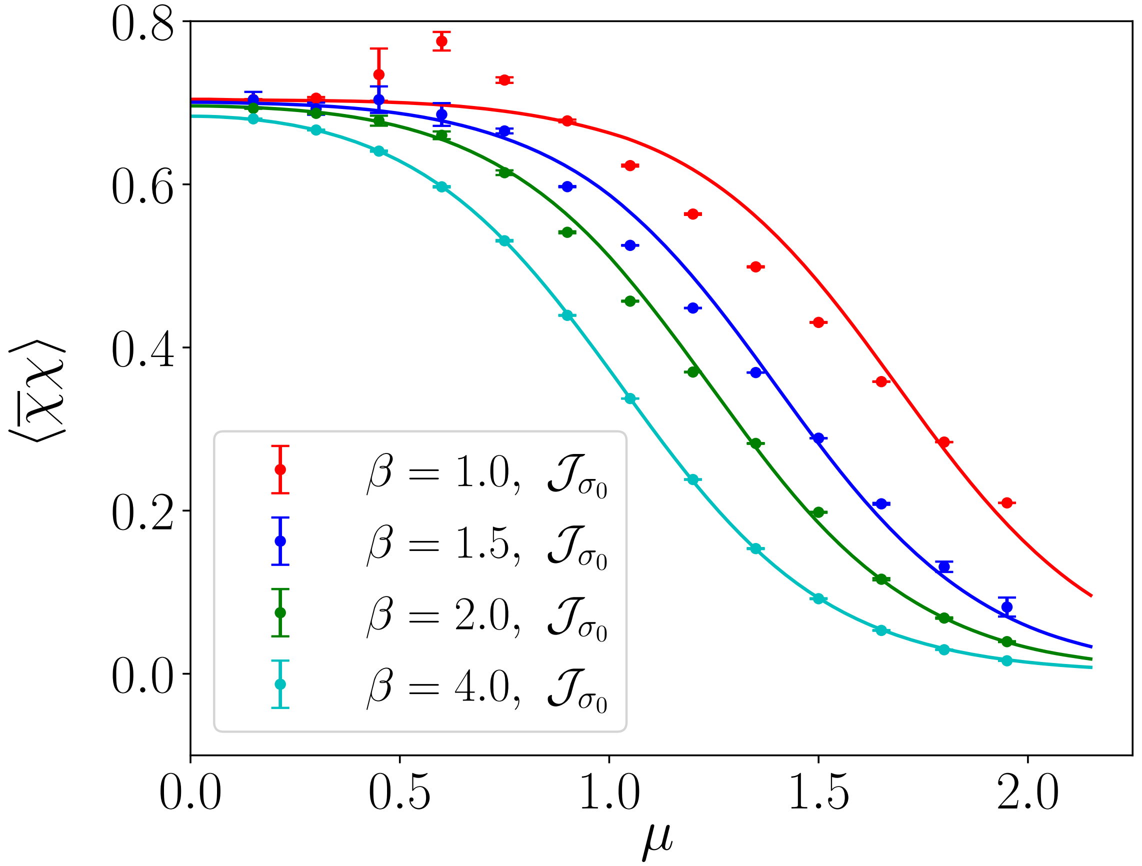
SINGLE THIMBLE DOMINANCE has been a dream for a while …

Sometimes it holds true, in general it fails

Thirring model first clear counterexample

Thirring model: from failure to new opportunity

$$S = \beta \sum_{n=1\dots L} (1 - \cos(\phi_n)) - \log\ \det\ D$$



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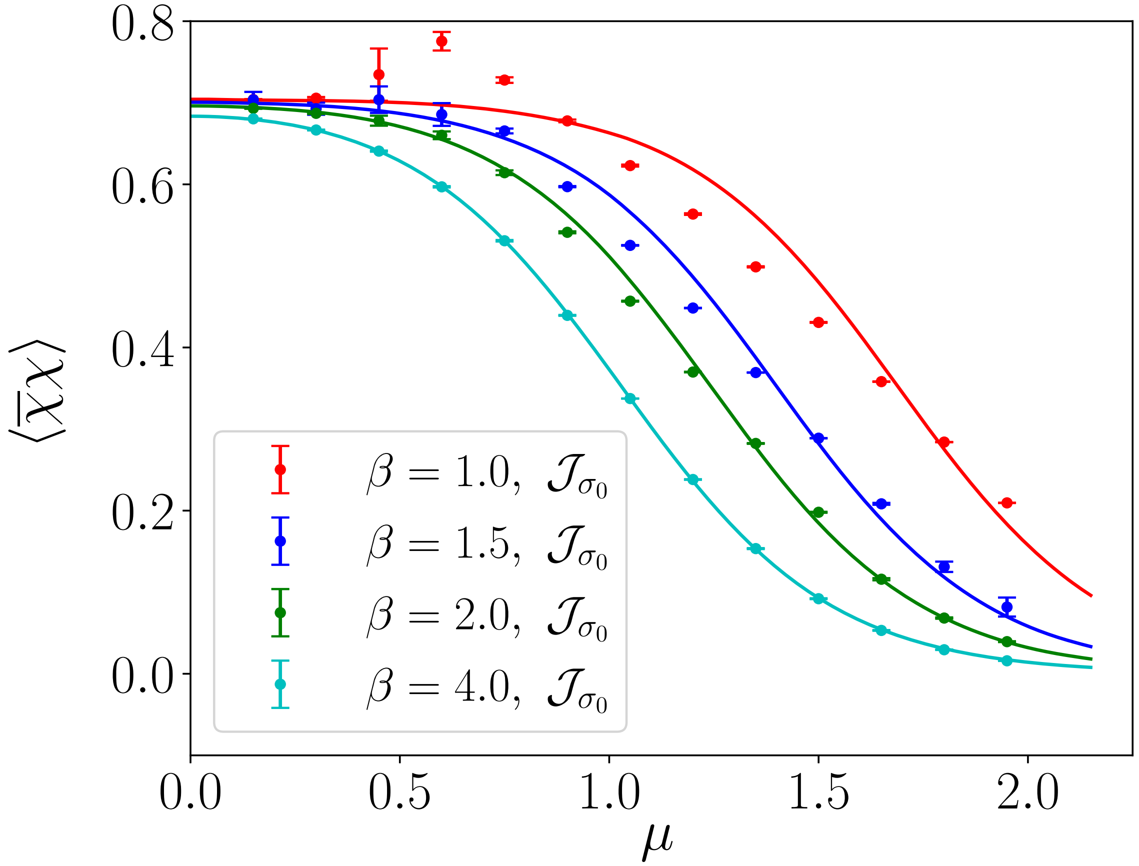

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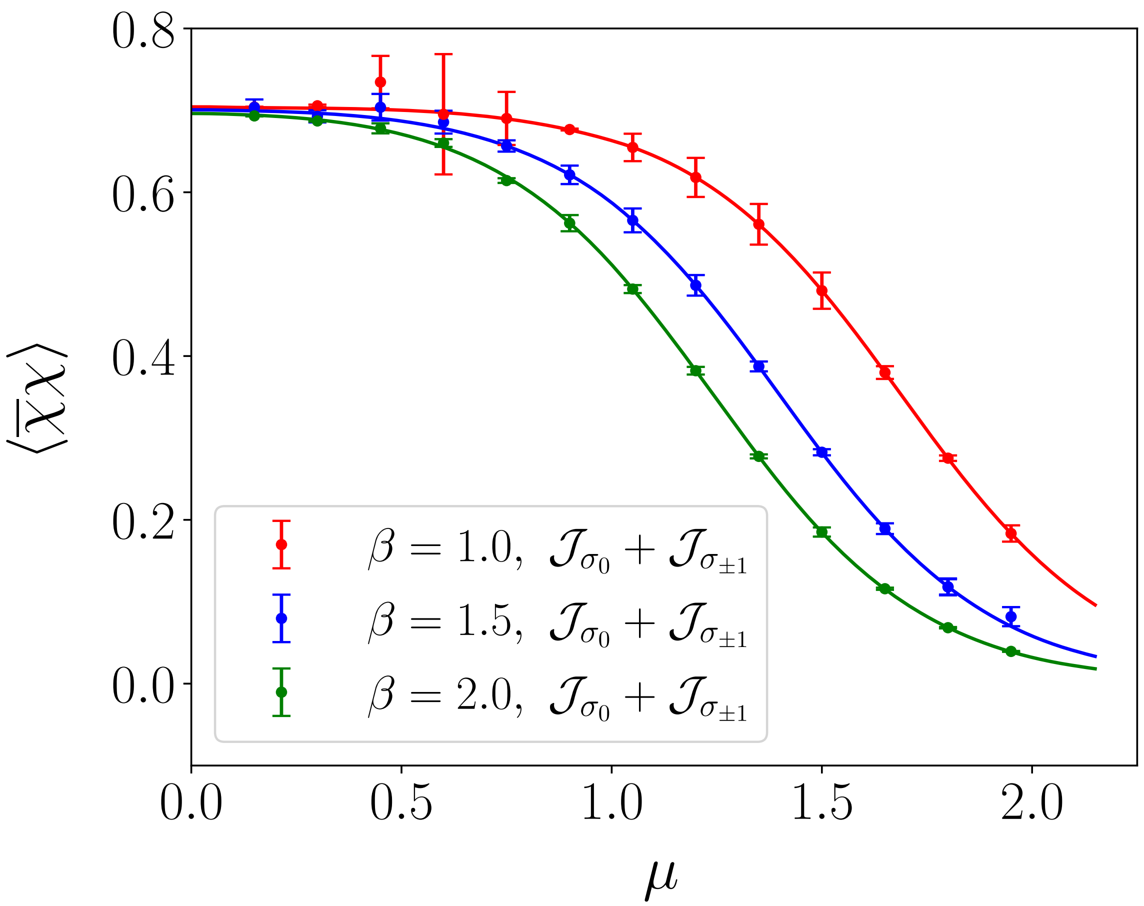
Two can be enough …

F. Di Renzo, K. Zambello (2022)

$$\langle O \rangle = \frac{\langle O e^{i\omega} \rangle_{\sigma_1} + \alpha \langle O e^{i\omega} \rangle_{\sigma_2}}{\langle e^{i\omega} \rangle_{\sigma_1} + \alpha \langle e^{i\omega} \rangle_{\sigma_2}}$$



Taylor expansions on Lefschetz thimbles

Di Renzo, Singh, Zambello (2021)

THIMBLE DECOMPOSITION is DISCONTINUOUS across STOKES points, but PHYSICAL OBSERVABLES are NOT!

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First idea: compute TAYLOR EXPANSIONS in regions where single decomposition holds and BRIDGE!

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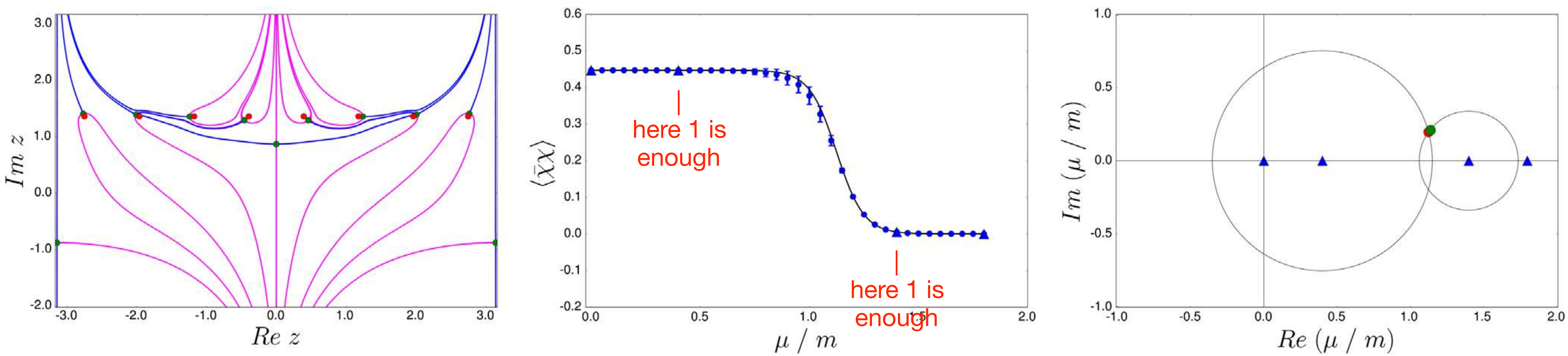

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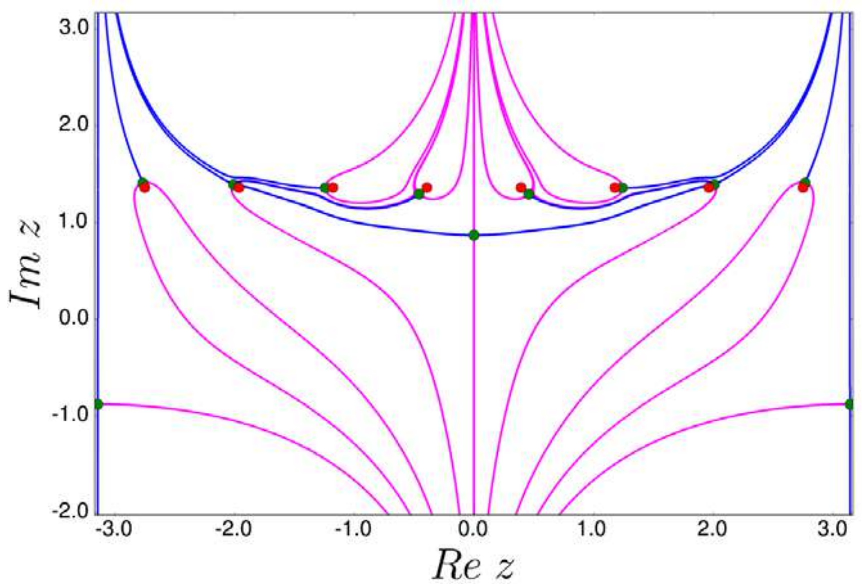
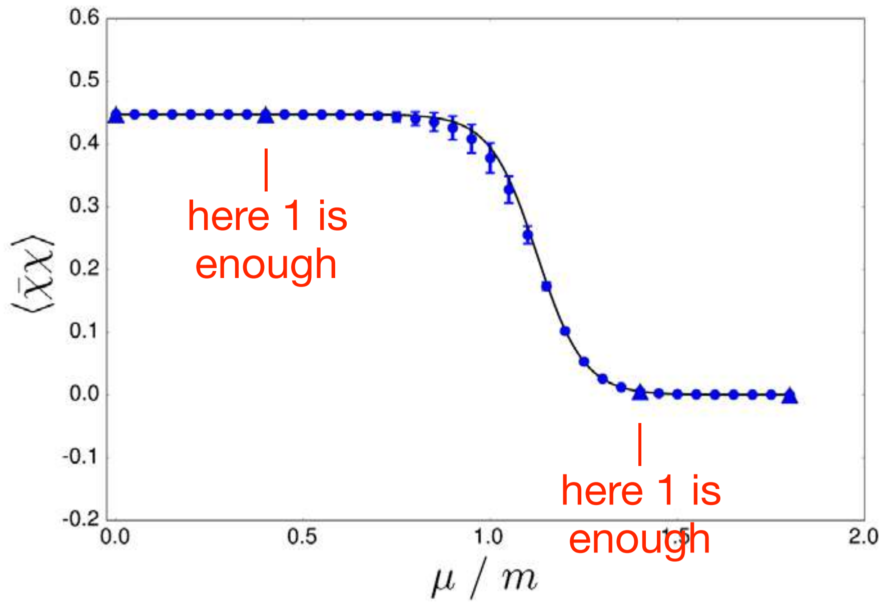
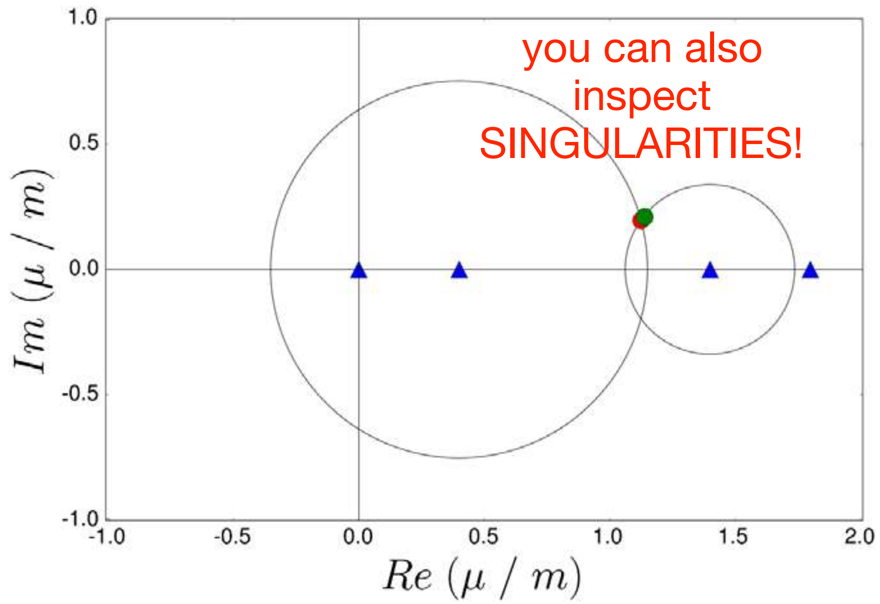




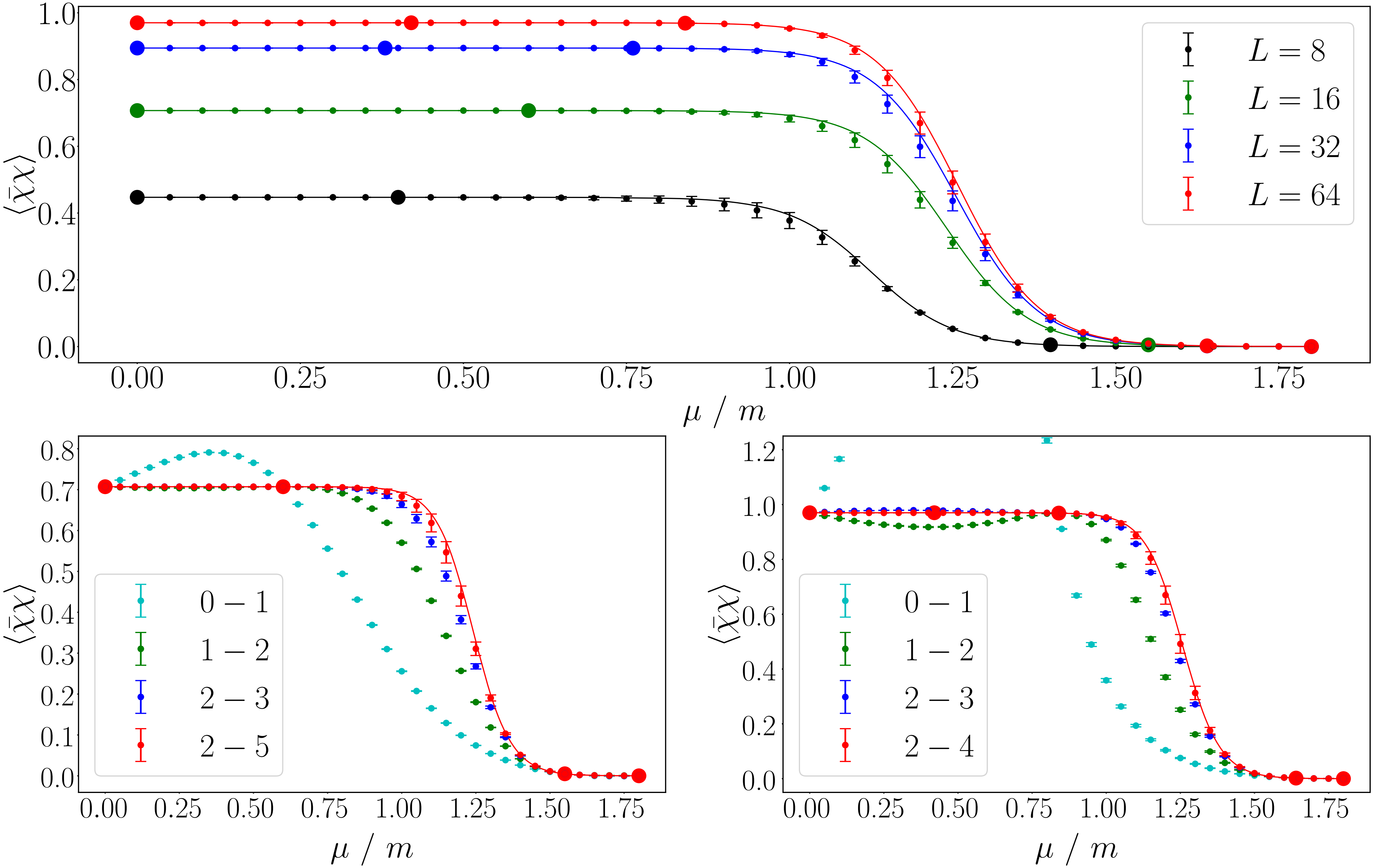


Taylor expansions on Lefschetz thimbles

Di Renzo, Zambello (2022)

$L = \frac{1}{Ta}$ $\beta = (2g^2 a)^{-1}$ increasing

We could take the continuum limit at fixed $L\hat{m} = 16$ $\beta\hat{m} = 2$



PADÈ approximants for dense QCD (and forgetting about thimbles…)

Bielefeld Parma (2022)

What can we compute in dense lattice QCD, given the sign problem?

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Let's merge the two and then go for a (multi-point) PADÈ !

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$$\chi_n^B(T,V,\mu_B) = \left(\frac{\partial}{\partial \hat{\mu}_B}\right)^n \frac{\ln Z(T,V,\mu_l,\mu_s)}{VT^3}$$
$$= \left(\frac{1}{3}\frac{\partial}{\partial \hat{\mu}_l} + \frac{1}{3}\frac{\partial}{\partial \hat{\mu}_s}\right)^n \frac{\ln Z(T,V,\mu_l,\mu_s)}{VT^3}$$

cumulants of the net baryon density are computed at a number of imaginary values of μ_B (including zero...)

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cumulants of the net baryon density are computed at a number of imaginary values of μ_B (including zero…)

and approximated by rational functions

$$R_n^m(x) = \frac{P_m(x)}{\tilde{Q}_n(x)} = \frac{P_m(x)}{1+Q_n(x)} = \frac{\sum_{i=0}^m a_i x^i}{1+\sum_{j=1}^n b_j x^j}$$

A bit more on multi-point PADÈ

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which we want to hold at many points for a function $f(x)$ and its derivatives

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Solve a linear system …

$$P_m(x_1) - f(x_1)Q_n(x_1) = f(x_1),$$
$$P'_m(x_1) - f'(x_1)Q_n(x_1) - f(x_1)Q'_n(x_1) = f'(x_1),$$
$$\cdots,$$
$$P_m(x_2) - f(x_2)Q_n(x_2) = f(x_2),$$
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- $$R_n^m(x) = \frac{\sum_{i=0}^{m'} a_{2i+1} x^{2i+1}}{1+\sum_{j=1}^{n/2} b_{2j} x^{2j}},$$
  $$(m = 2m'+1,\, a_1 = \chi_2^B(T,V,0))$$

  odd function…

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$$c_j^{(k)} \equiv \frac{\partial^j f}{\partial x^j}(x_k) \simeq \frac{\partial^j R_n^m}{\partial x^j}(x_k)$$

* minimise $$\tilde{\chi}^2 = \sum_{j,k} \frac{|\frac{\partial^j R_n^m}{\partial x^j}(x_k) - c_j^{(k)}|^2}{|\Delta c_j^{(k)}|^2}$$

2+1 HISQ, first around Roberge Weiss transition temperature, N_t=4

PHYSICAL REVIEW D **105,** 034513 (2022)

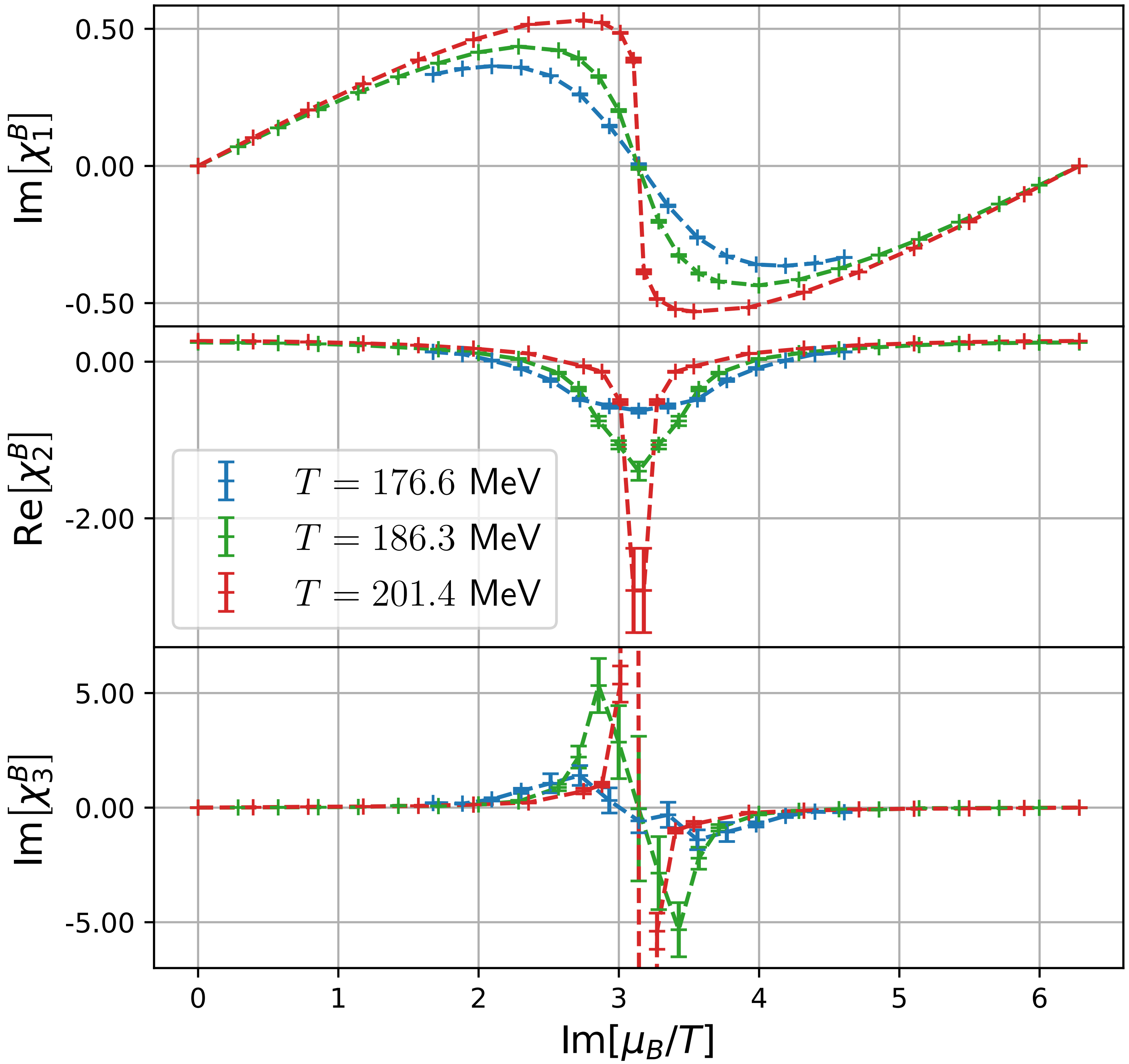

FIG. 2. Cumulants of the net baryon number fluctuations as a function of a purely imaginary chemical potential, for three different temperatures, obtained on $24^3 \times 4$ lattices. Shown are Im[χ_1^B] (top), Re[χ_2^B] (middle), and Im[χ_3^B]. Data points are connected by dashed lines to guide the eye.

2+1 HISQ, first around Roberge Weiss transition temperature, N_t=4

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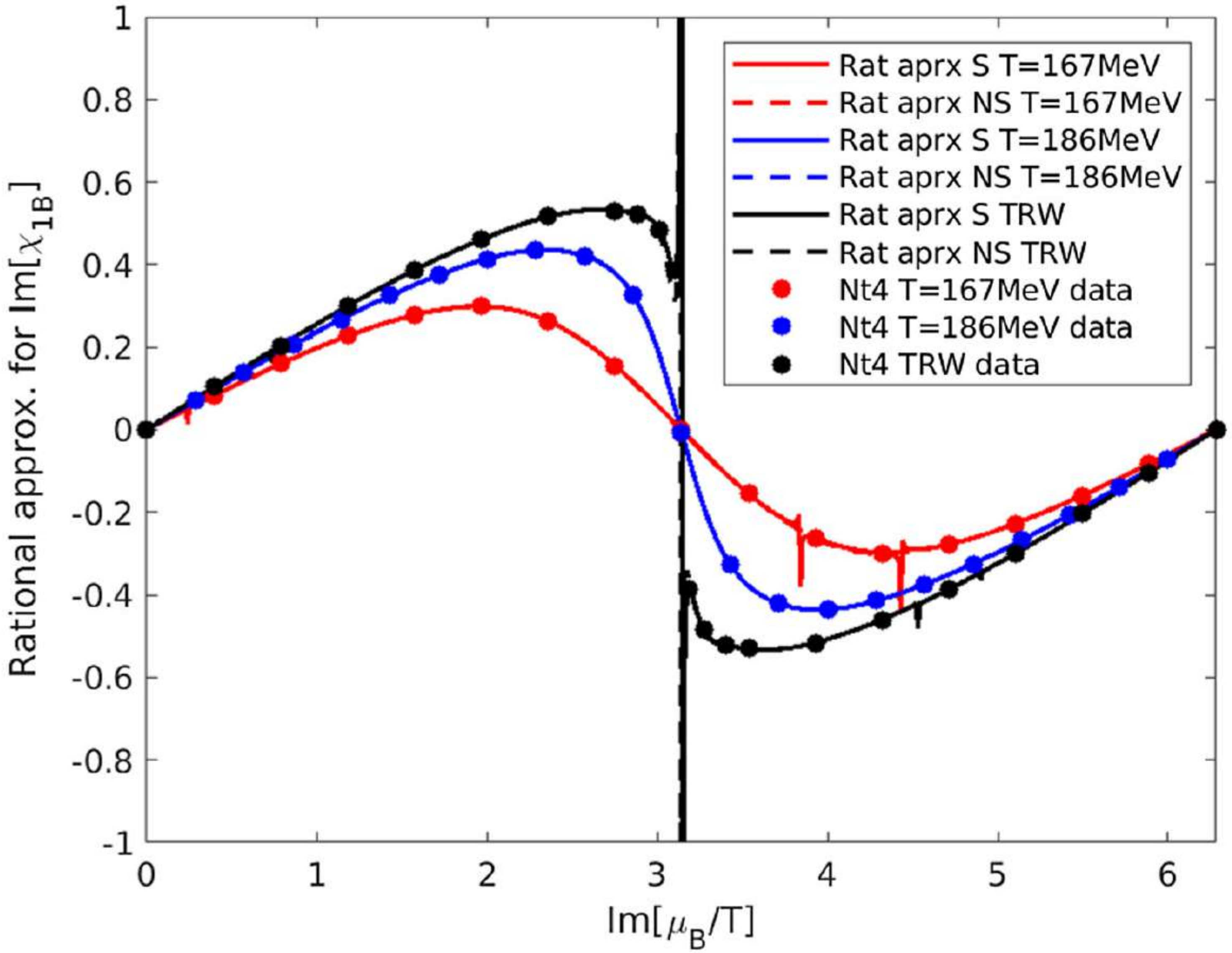
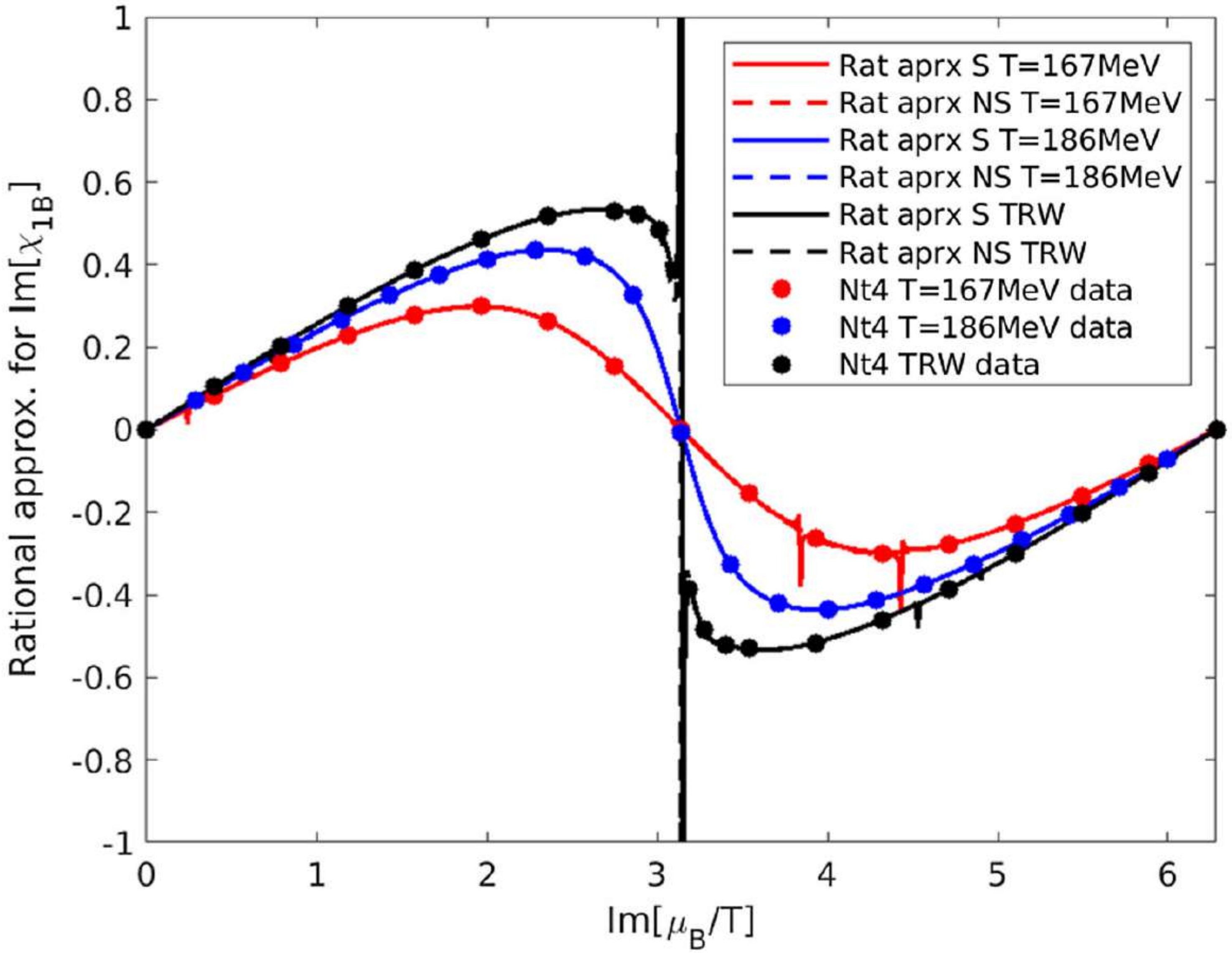


Rational approximations
describing data

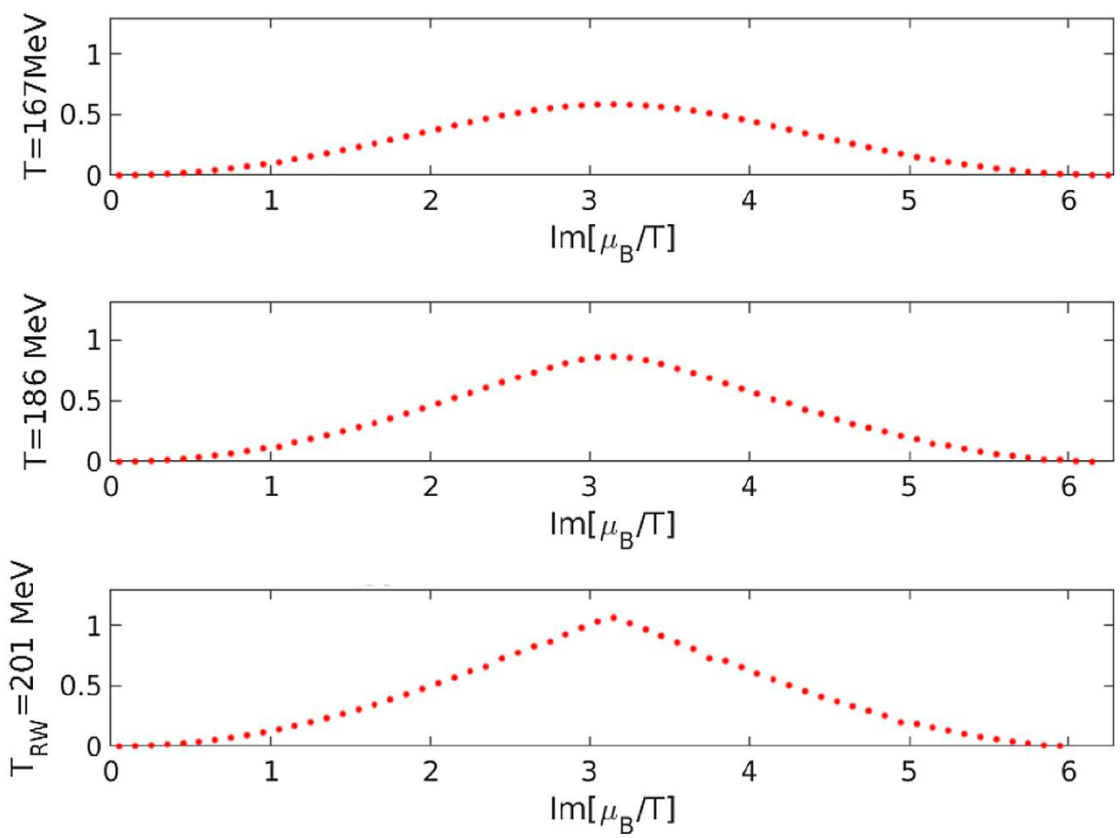
2+1 HISQ, first around Roberge Weiss transition temperature, N_t=4

PHYSICAL REVIEW D **105,** 034513 (2022)



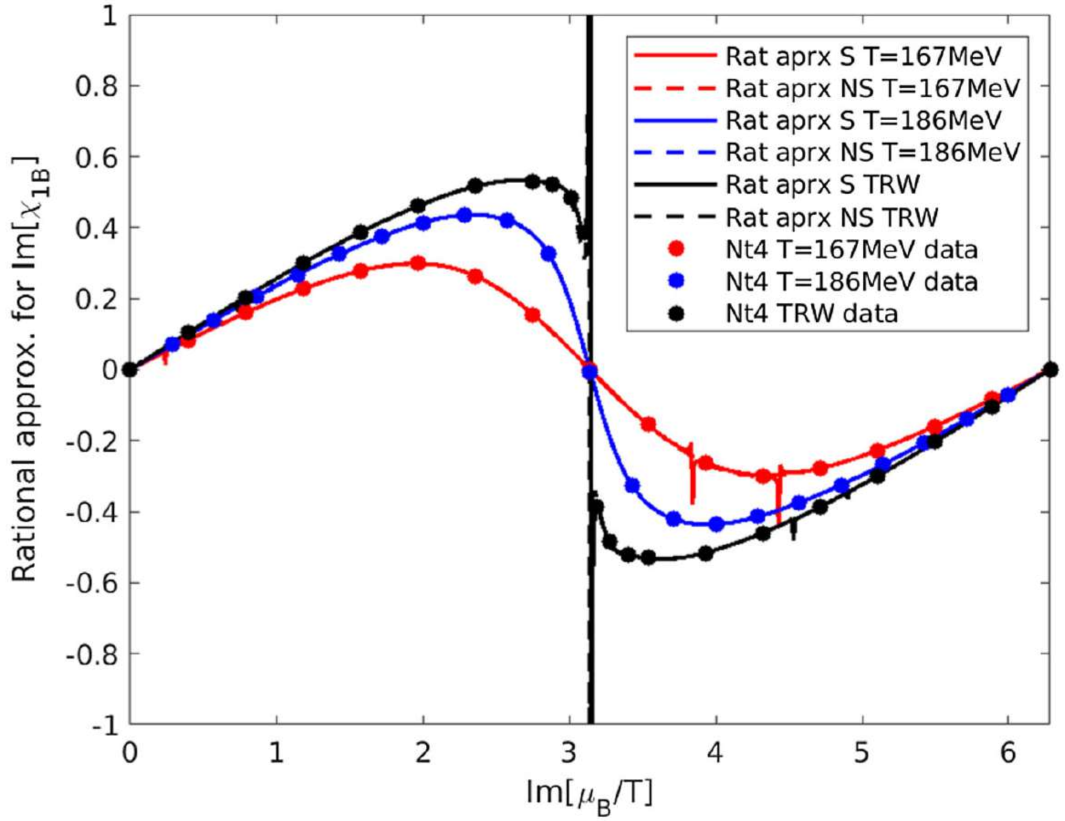
Rational approximations
describing data

Free energy
by integration…



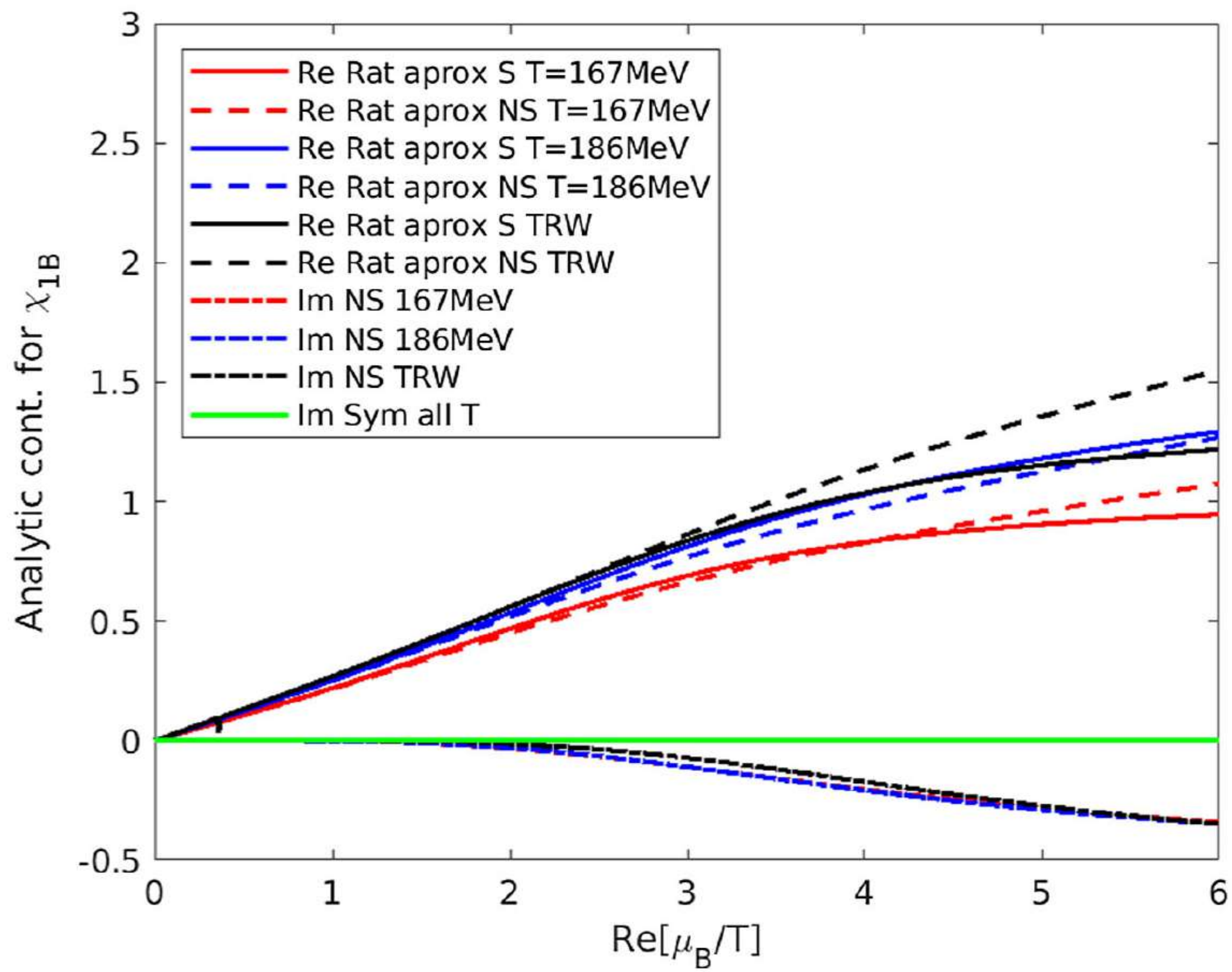
2+1 HISQ, first around Roberge Weiss transition temperature, N_t=4

PHYSICAL REVIEW D **105,** 034513 (2022)



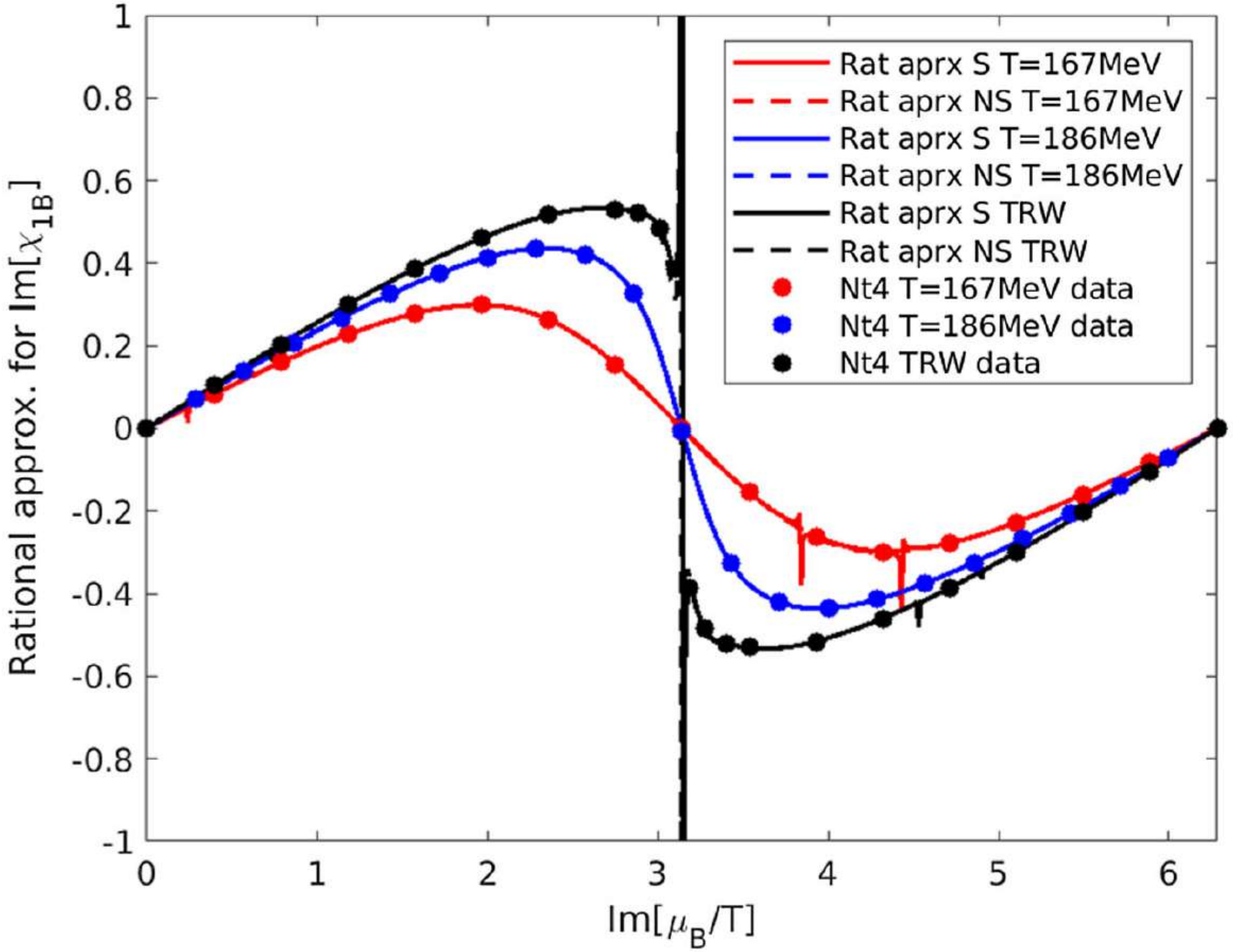
Rational approximations describing data

next thing we want to do is analytic continuation



2+1 HISQ, first around Roberge Weiss transition temperature, $N_t=4$

PHYSICAL REVIEW D **105,** 034513 (2022)



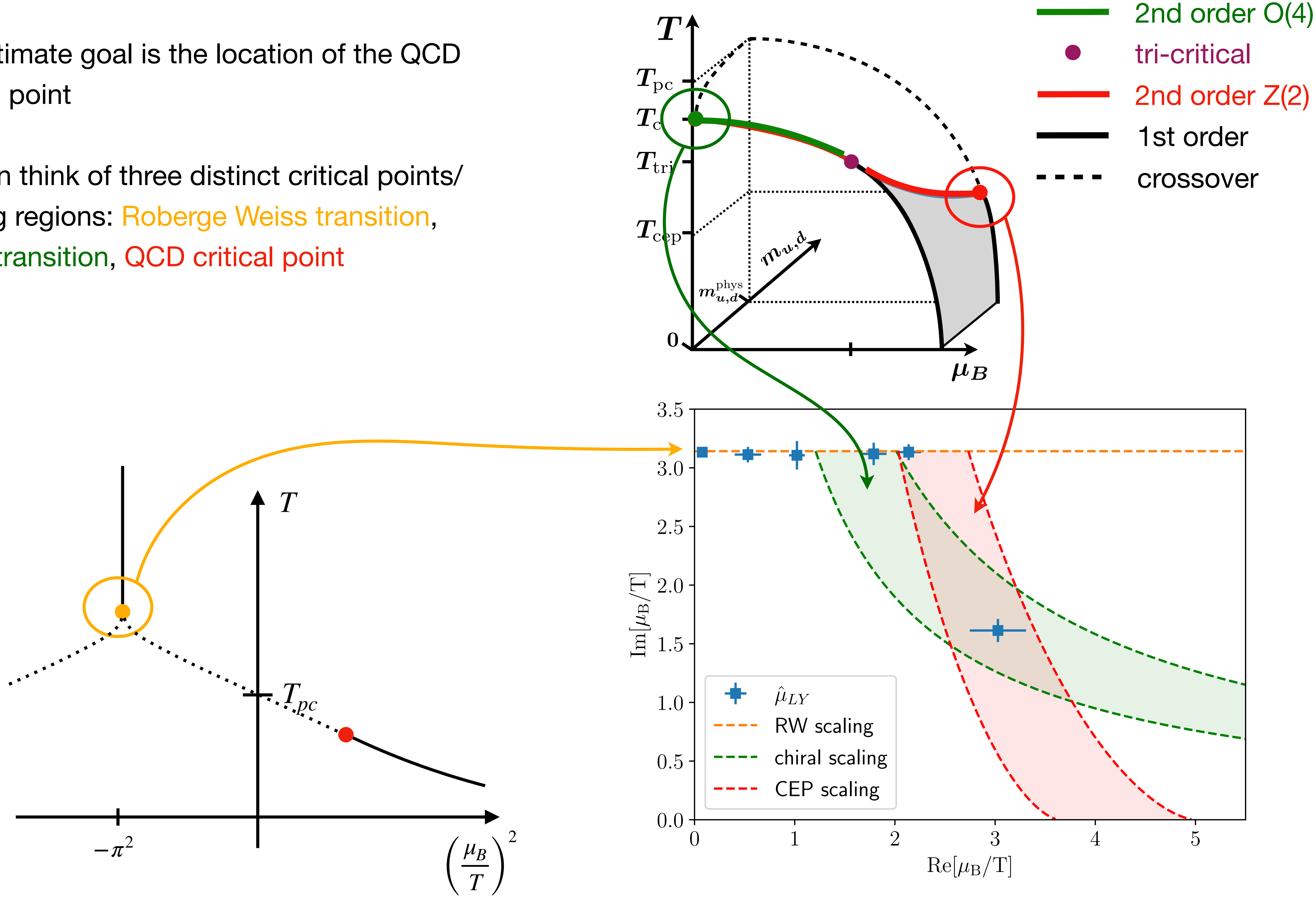
We have already seen SPIKES …

Let's now look for the SINGULARITY STRUCTURE
(we hunt for LEE YANG ZEROS, i.e. zeros of the partition function)

The big picture of Lee Yang edge singularities in QCD

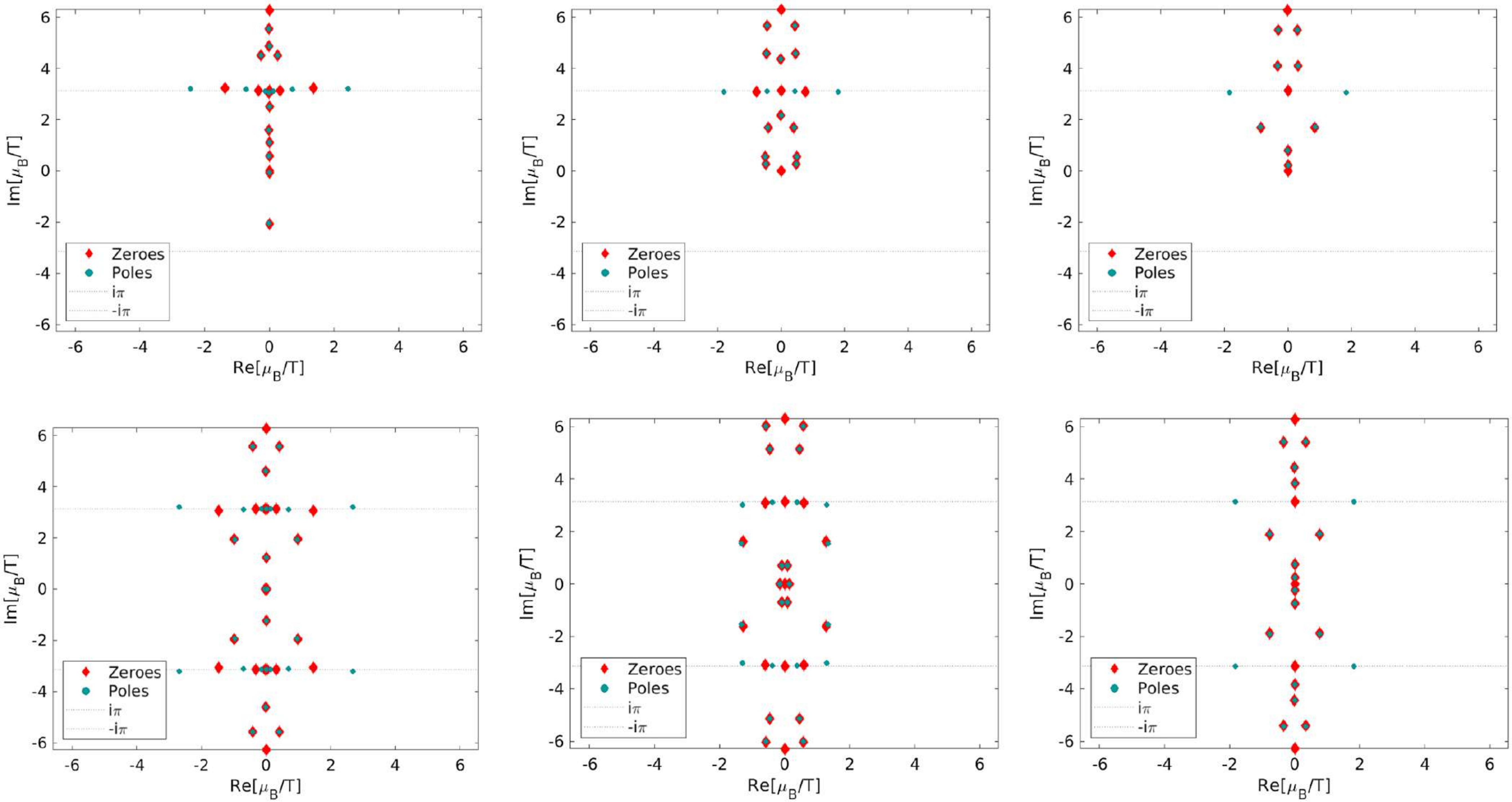
Slide produced by Christian Schmidt

- The ultimate goal is the location of the QCD critical point
- We can think of three distinct critical points/ scaling regions: Roberge Weiss transition, chiral transition, QCD critical point



2+1 HISQ, first around Roberge Weiss transition temperature, N_t=4

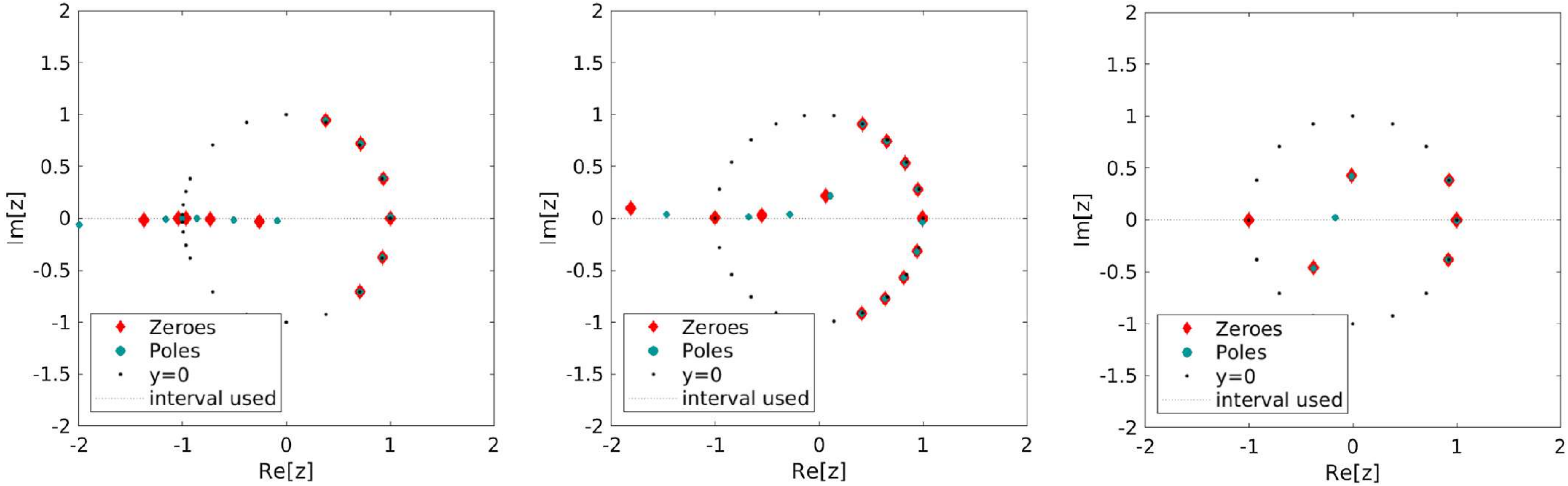
PHYSICAL REVIEW D **105,** 034513 (2022)



zeros and poles show up where they are expected || large number of cancelations || relevant vs NON relevant pieces of informations

2+1 HISQ, first around Roberge Weiss transition temperature, N_t=4

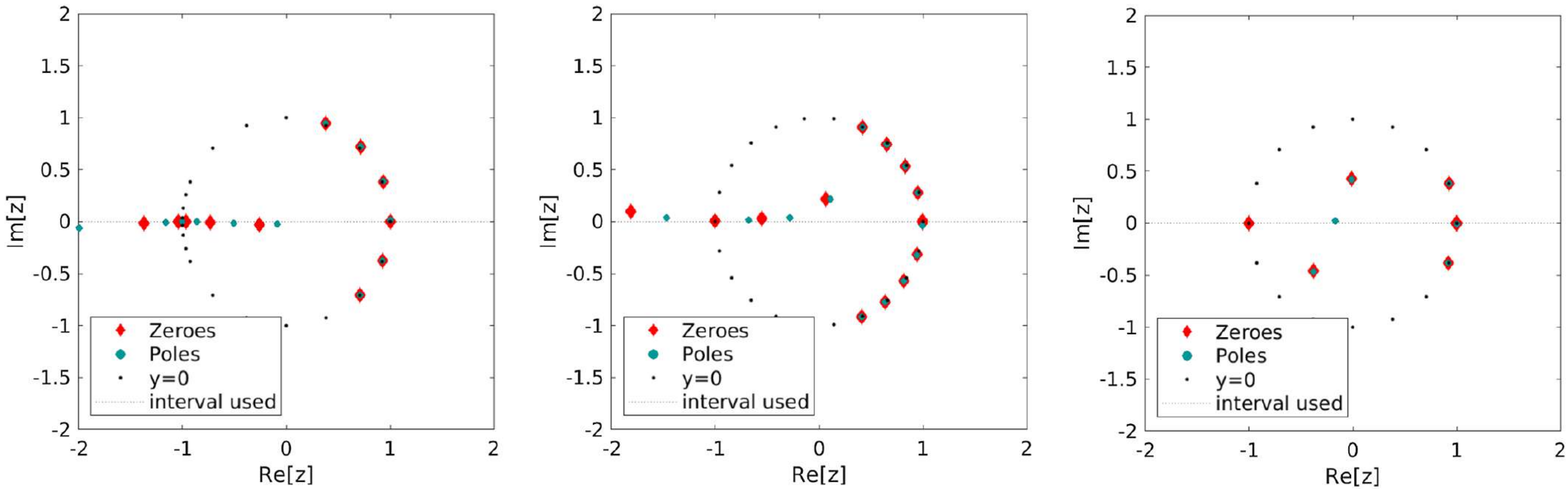
PHYSICAL REVIEW D **105,** 034513 (2022)



The same in the fugacity plane

2+1 HISQ, first around Roberge Weiss transition temperature, $N_t=4$

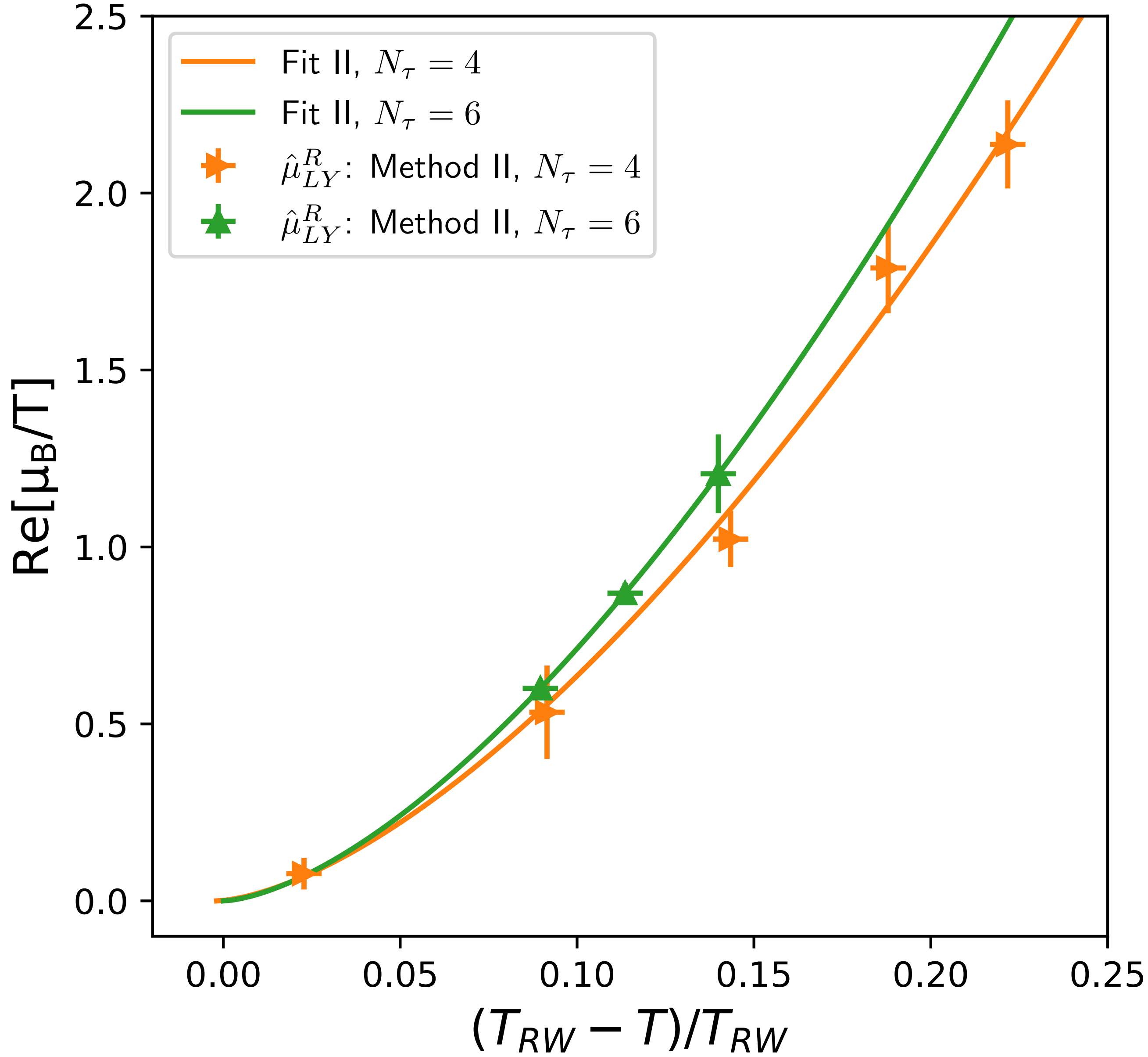
PHYSICAL REVIEW D **105,** 034513 (2022)



The same in the fugacity plane

SHALL WE TRUST ALL THIS?

2+1 HISQ, first around Roberge Weiss transition temperature, N_t=4,6



Order parameter near a 2nd order phase transition

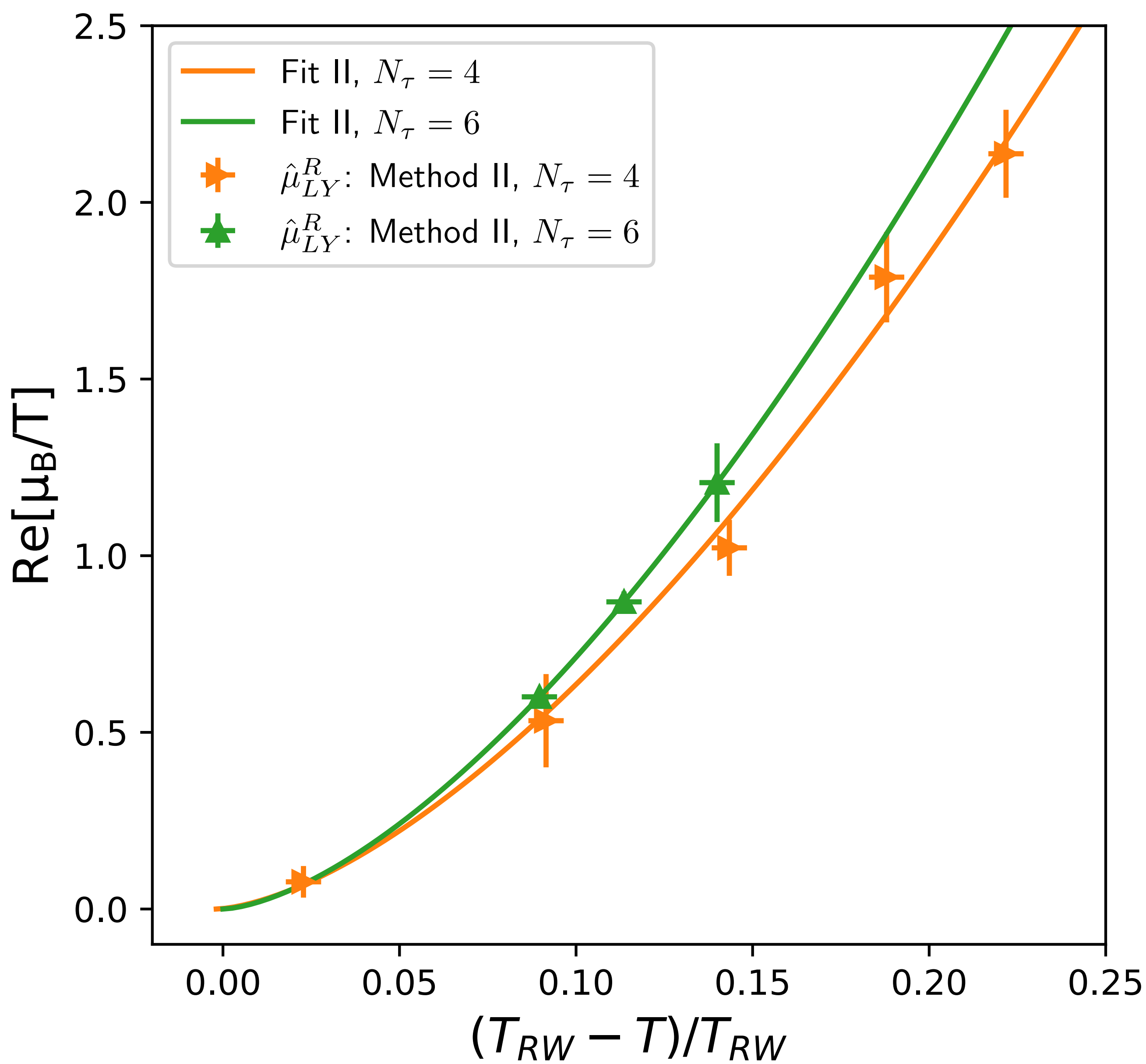
$$M = h^{1/\delta} f_G(z) + M_{\mathrm{reg}} \qquad z \equiv t/|h|^{1/\beta\delta}$$

$$t = t_0^{-1}\left(\frac{T_{\mathrm{RW}} - T}{T_{\mathrm{RW}}}\right)$$

scaling fields

$$h = h_0^{-1}\left(\frac{\hat{\mu}_B - i\pi}{i\pi}\right) \qquad \hat{\mu}_B = \mu_B/T$$

2+1 HISQ, first around Roberge Weiss transition temperature, N_t=4,6



Order parameter near a 2nd order phase transition

$$M = h^{1/\delta} f_G(z) + M_{\rm reg} \qquad z \equiv t/|h|^{1/\beta\delta}$$

$$t = t_0^{-1} \left(\frac{T_{\rm RW} - T}{T_{\rm RW}} \right)$$

scaling fields

$$h = h_0^{-1} \left(\frac{\hat{\mu}_B - i\pi}{i\pi} \right) \qquad \hat{\mu}_B = \mu_B/T$$

$$\hat{\mu}^R_{\rm LY} = \pm\pi \left(\frac{z_0}{|z_c|} \right)^{\beta\delta} \left(\frac{T_{\rm RW} - T}{T_{\rm RW}} \right)^{\beta\delta}$$

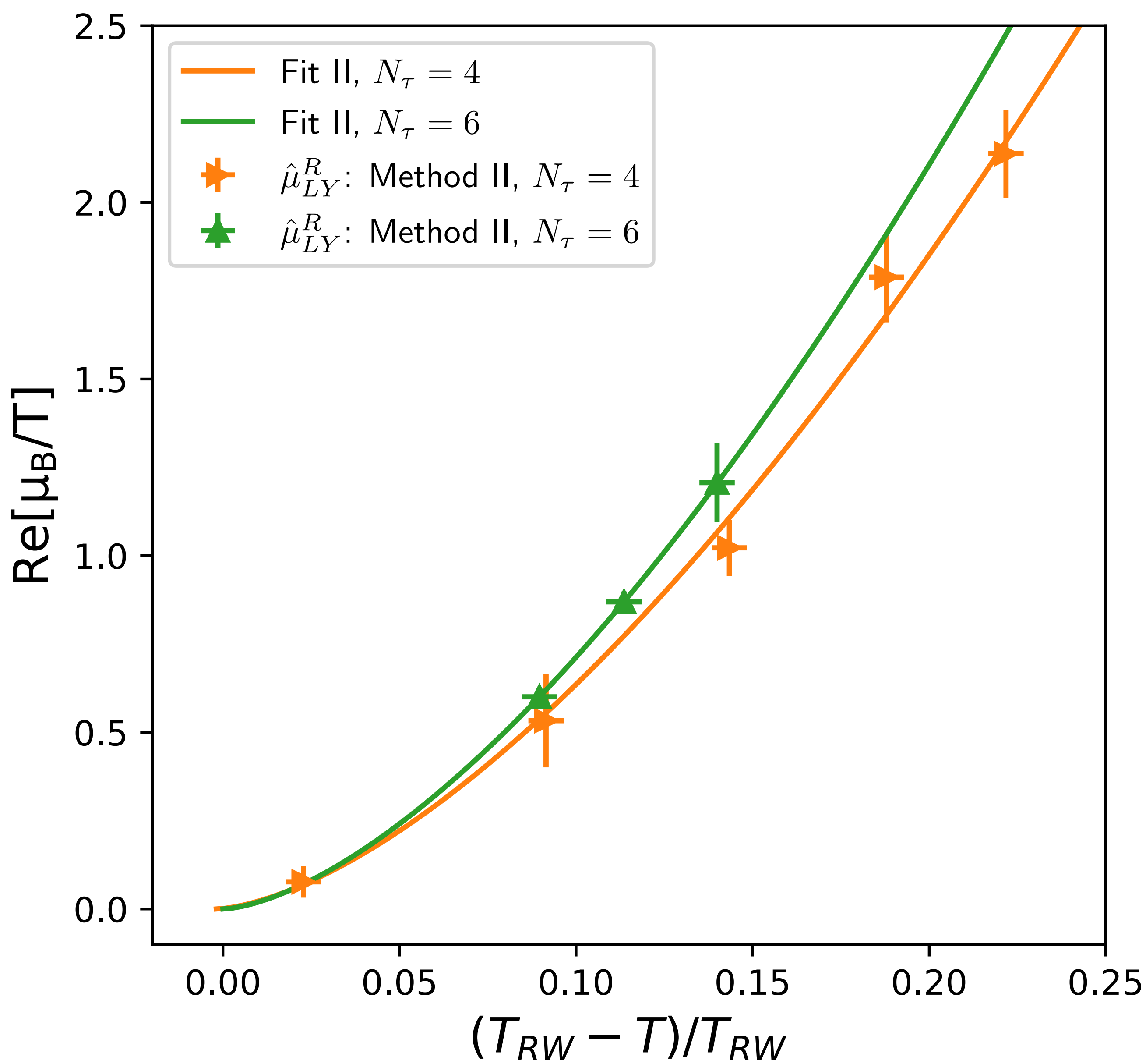
$$\hat{\mu}^I_{\rm LY} = \pm\pi,$$

From the fit we get

$T_{\rm RW}$ = 206.7(2.6) MeV

$T_{\rm RW}$ = 208.705(0.002) MeV

2+1 HISQ, first around Roberge Weiss transition temperature, N_t=4,6



Order parameter near a 2nd order phase transition

$$M = h^{1/\delta} f_G(z) + M_{\rm reg} \qquad z \equiv t/|h|^{1/\beta\delta}$$

$$t = t_0^{-1}\left(\frac{T_{\rm RW} - T}{T_{\rm RW}}\right)$$

scaling fields

$$h = h_0^{-1}\left(\frac{\hat{\mu}_B - i\pi}{i\pi}\right) \qquad \hat{\mu}_B = \mu_B/T$$

$$\hat{\mu}^R_{\rm LY} = \pm\pi\left(\frac{z_0}{|z_c|}\right)^{\beta\delta}\left(\frac{T_{\rm RW} - T}{T_{\rm RW}}\right)^{\beta\delta}$$

$$\hat{\mu}^I_{\rm LY} = \pm\pi,$$

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$T_{\rm RW}$ = 206.7(2.6) MeV

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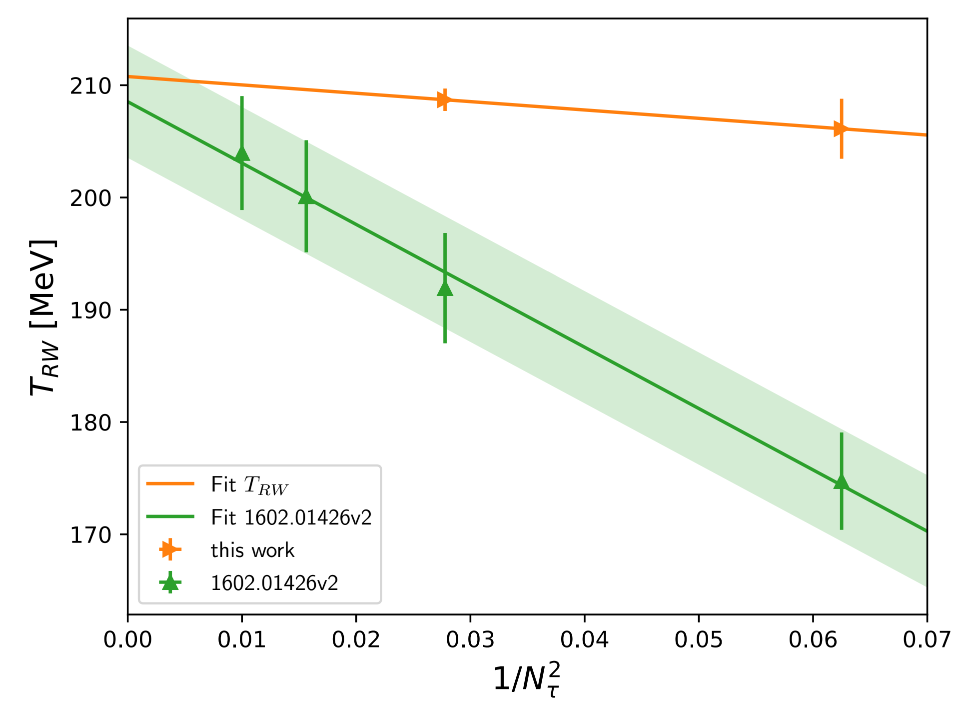
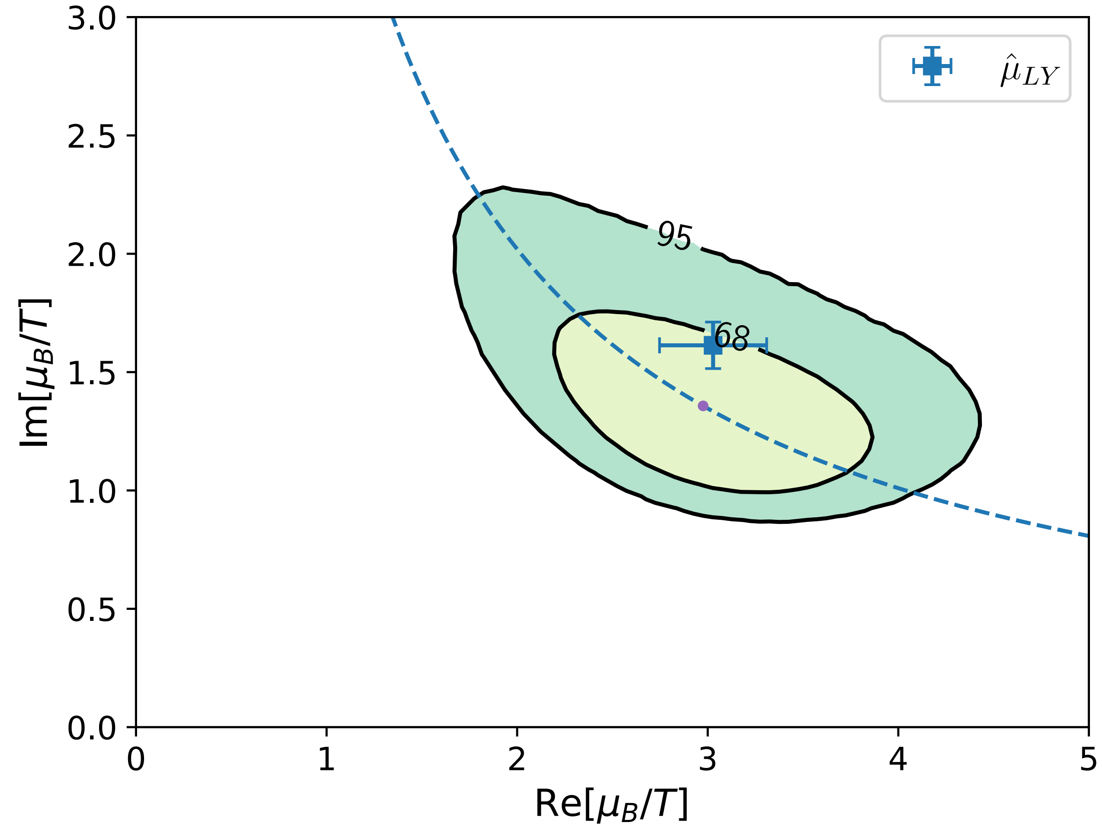
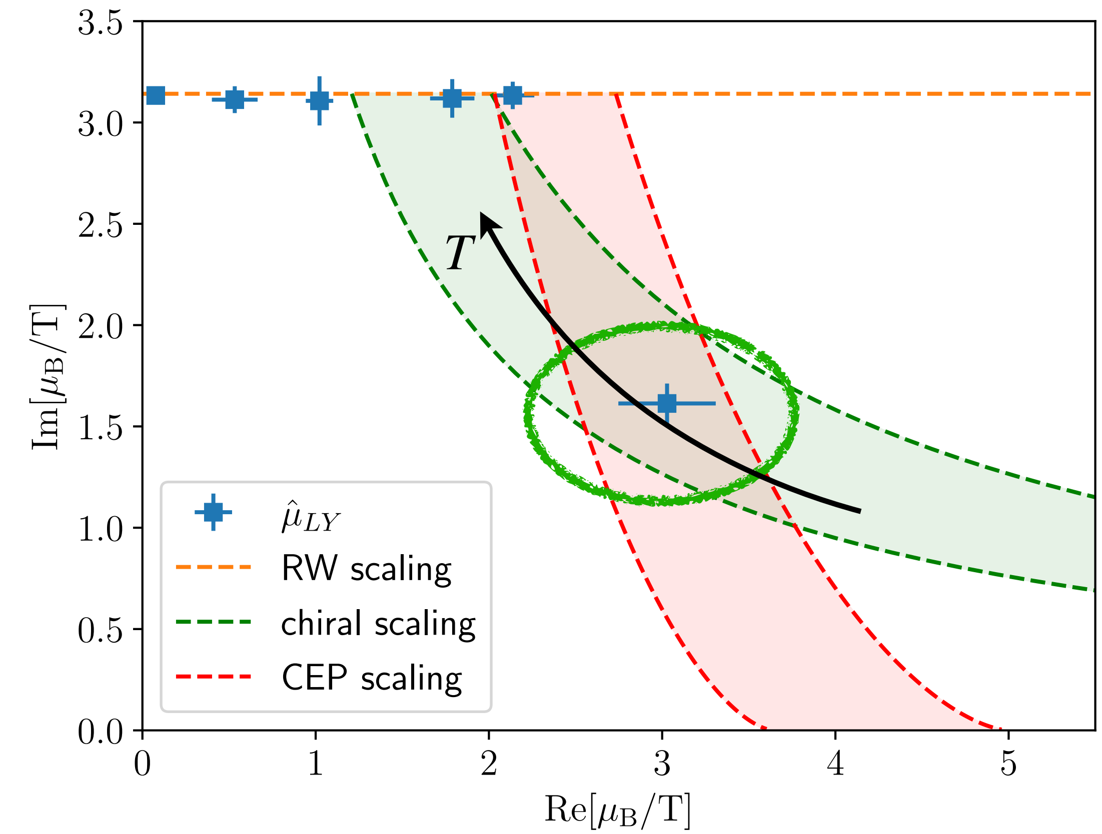


2+1 HISQ, at a lower (145 MeV) temperature, N_t=6

PHYSICAL REVIEW D **105,** 034513 (2022)





Care needed! … but intriguing … what we found is compared with 68% and 95% confidence regions of a theoretical prediction (no fit!)
Our first, preliminary indication of a chiral singularity…

CONCLUSIONS

1. We saw two different examples of studies in the complex plane, ending up with predictions for phase diagrams obtained from (multi-point) Padè analysis.

2. Thimbles + Taylor + Padè can still enable some new progress (avoiding multi-thimble simulations)

3. The program of (multi-point) Padè could provide interesting informations on Lee Yang edge singularities in QCD. RW seems solid, we are trying to better understand chiral transition. The Holy Grail (needless to say) is the critical point…

4. Work is going on: stay tuned!

Critical points pattern for Thirring

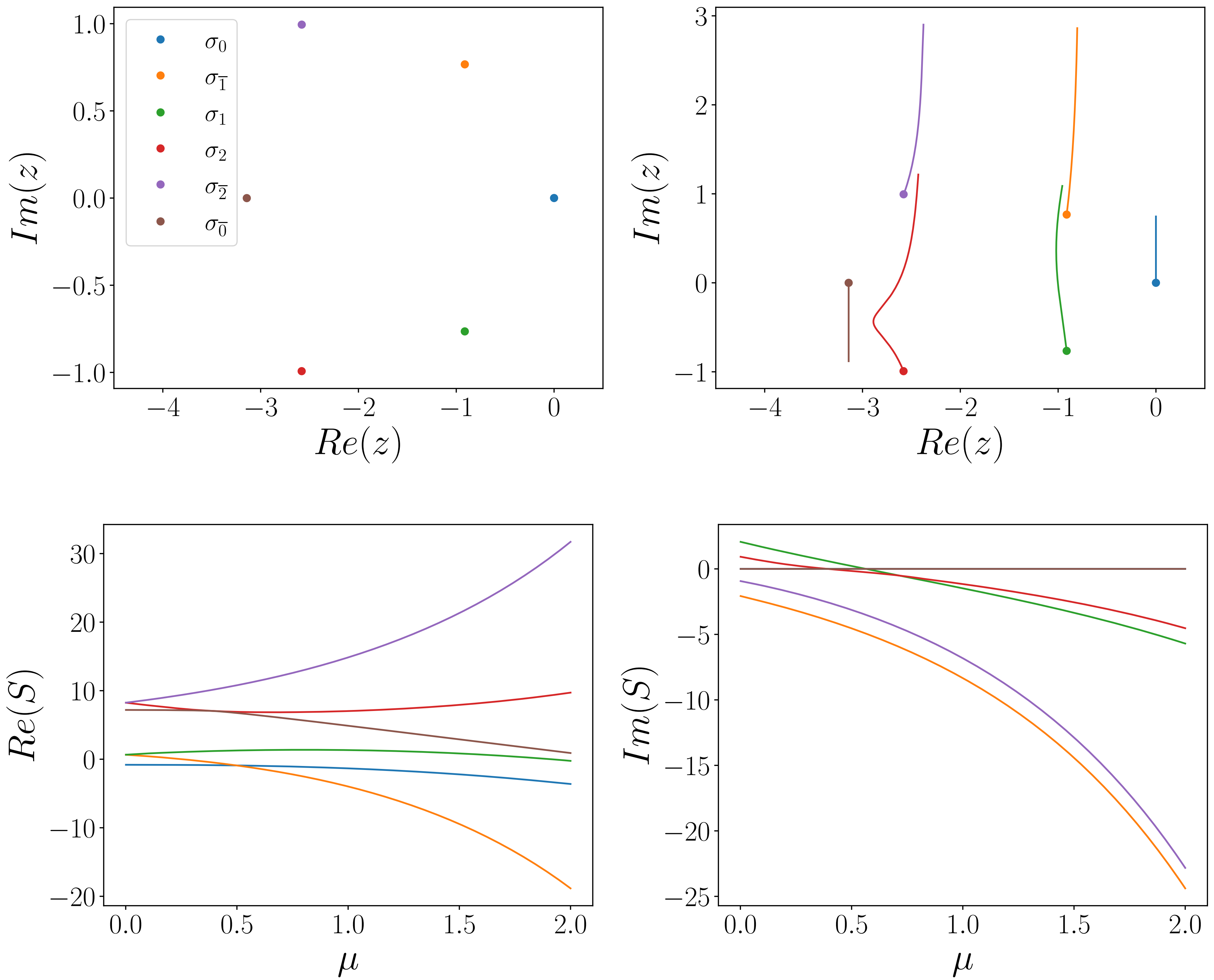


FIG. 1. Critical points for $L = 4$, $\beta = 1$ and $ma = 1$: solutions for $\hat{\mu} = 0$ (top left), solutions for $\hat{\mu} \in [0.0, 2.0]$ (top right), real part of the action as a function of $\hat{\mu}$ (bottom left) and imaginary part of the action as a function of $\hat{\mu}$ (bottom right).

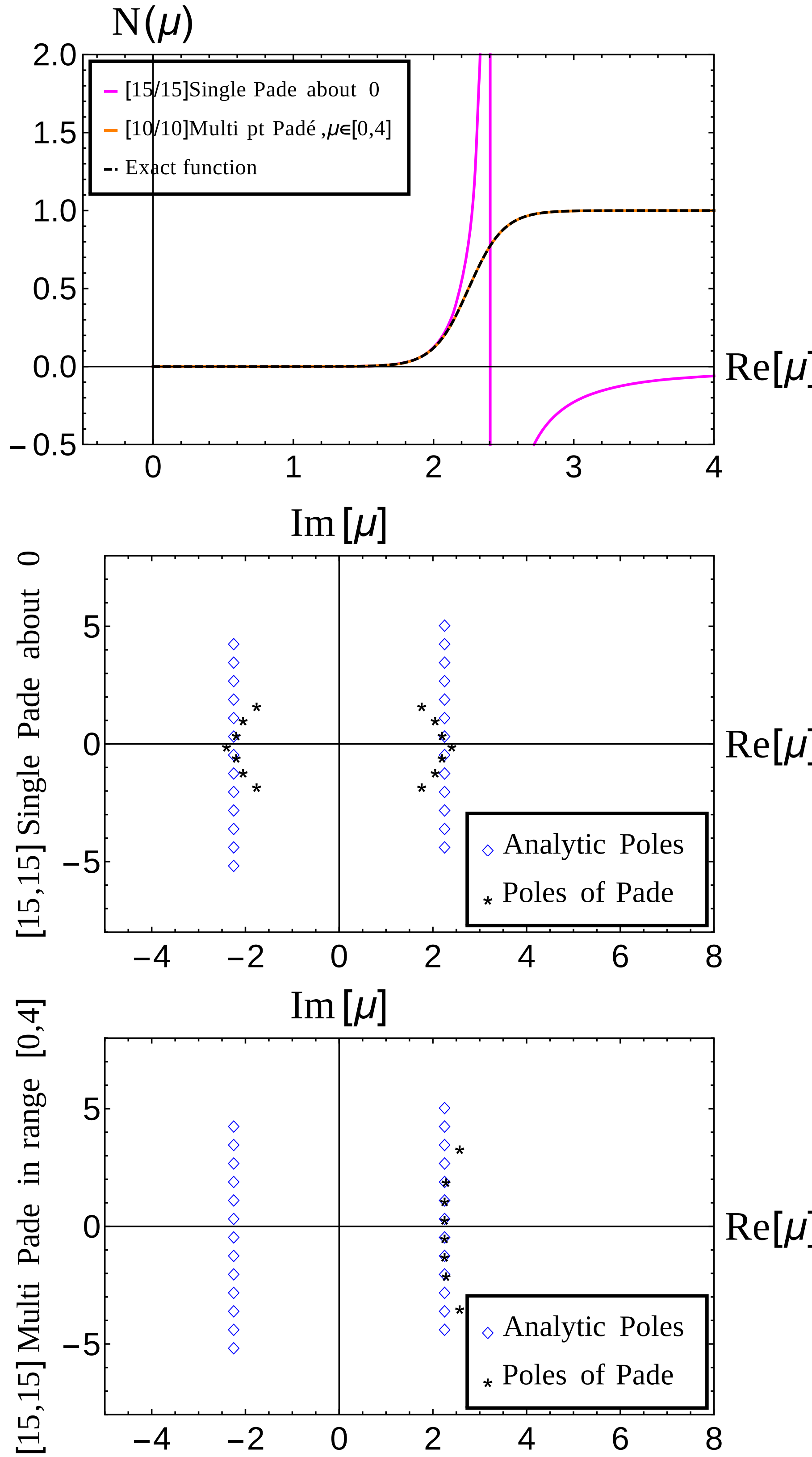


FIG. 11. Thirring 1D. Top: comparison between the approximation of a [15/15] order single-point Padé about 0 and a [10/10] order multipoint Padé constructed in the interval [0,4] with only up to first derivatives. Middle, Bottom: depiction of the poles as seen by the single-point and multipoint Padé, respectively.

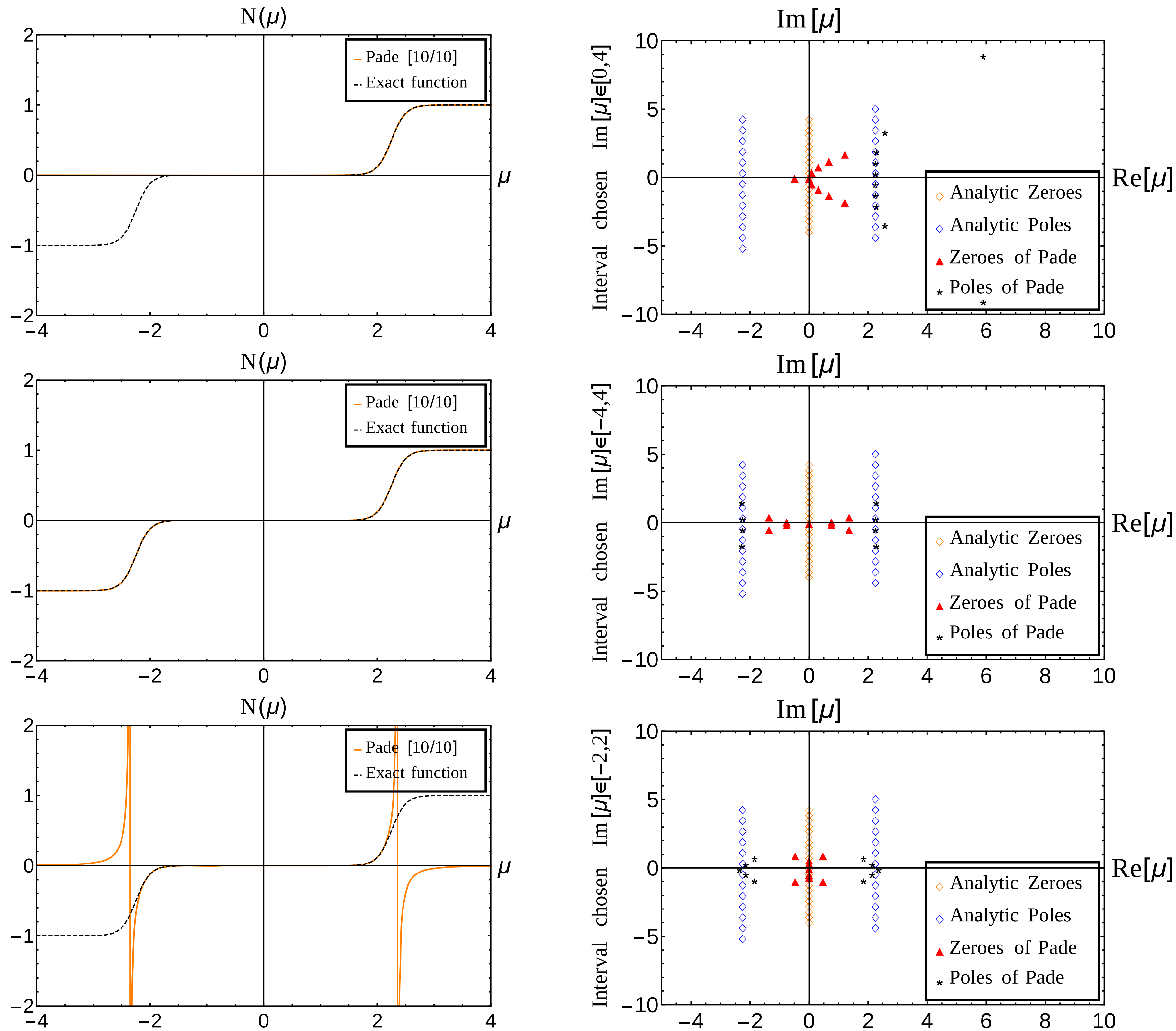


FIG. 14. 1D Thirring model: functional form of the rational approximation (left) and sensitivity to different sets of poles (right) whe sampled in different intervals: [0, 4] (top), [–4, 4] (middle), [–2, 2] (bottom).