Free Quarks and the Roberge-Weiss Transition

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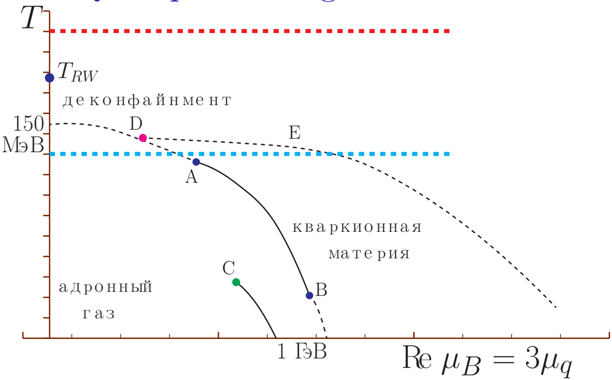
Outline

1. Motivation: probability distribution of fireballs in the net-baryon number
2. Roberge-Weiss periodicity and the concept of triality
3. Problem of negative probabilities in free fermon theory
4. The Lee-Yang approach to phase transitions
5. Patterns of Lee–Yang zeroes at different triality sets

В соавторстве с Н.В.Герасименюком
Вклад Н.В.Герасименюка поддержан грантом РНФ 23-12-00072 «Изучение теории
сильных взаимодействий в экстремальных условиях методами решёточного моделирования»,

The QCD phase diagram



AB - chiral phase transition; DE - deconfinement transition;
We study the net-quark number density at $T > T_c$ and $\mu_B = \imath\mu_I$ as well as the distribution in the quark number **q**.

The grand canonical partition function

$$Z_{GC}(\theta, T, V) = \sum_j \langle j| \exp\left(\frac{-\hat{H} + \mu \hat{\mathbf{q}}}{T} \right) |j\rangle$$

can be expanded in the Laurent series in fugacity $\xi = e^{\theta}$ $(\theta = \mu/T = \theta_R + \imath\theta_I\ )$:

$$Z_{GC}(\theta) \ = \sum_{n=-\infty}^{\infty} Z_C(n) e^{n\theta},$$

$$Z_C(n) = \sum_{j:\hat{\mathbf{q}}|j\rangle = n|j\rangle} \langle j| \exp\left(-\frac{\hat{H}}{T} \right) |j\rangle,$$

Pressure and density of the net-baryon number are given by

$$p(\theta) = \frac{T}{V} \ln Z_{GC}(\theta) \qquad \rho(\theta) = \frac{1}{T}\frac{\partial p}{\partial \theta}$$

The quark(or baryon) density can be evaluated in lattice QCD simulations:

$$\begin{aligned} B(\theta) &= \frac{1}{N_c}\frac{\partial \ \ln Z_{GC}}{\partial \theta} \\ &= \frac{N_f}{N_c Z_{GC}} \int \mathcal{D}U e^{-S_G} [\det \Delta(\theta)]^{N_f} \mathbf{tr} \left[\Delta^{-1} \frac{\partial \Delta}{\partial \theta} \right] , \end{aligned} \qquad (1)$$

$\mathbf{q} = 3B, \theta_q = \frac{1}{3}\theta_B$

$$Z_{GC}(\imath\theta_I) \; = \; \sum_{n=-\infty}^{\infty} Z_C(n) e^{\imath n\theta},$$

$$Z_C(n) = \int_{-\pi}^{\pi} \frac{d\theta_I}{2\pi} e^{-in\theta_I} Z_{GC}(\theta)\Big|_{\theta_R=0} \; ,$$

$\left[\hat{H}, \hat{\mathrm{q}}\right] = 0, n \in \mathbb{Z} \Longrightarrow Z_{GC}(\theta)$ is periodic in θ with the period $2\pi\,\imath$.

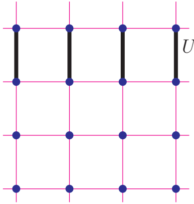
C-parity $\Longrightarrow \quad Z_C(n) = Z_C(-n)$.

At $\theta = 0$, the probability that the quark number equals n has the form

$$\mathbf{P}_n = \frac{Z_C(n)}{Z_{GC}(0)} \, .$$

Roberge-Weiss periodicity

$$\boxed{Z_{GC}(\imath\theta_I) = Z_{GC}\left(\imath\theta_I + \frac{2\pi\imath k}{N_c}\right),\ k \in \mathbb{Z}}$$



$$U_{x,\mu} = \exp\left(\imath g a A_\mu(x)\right)$$

$$\bar\psi_x U_4 e^{\theta} \psi_{x+\hat 4}, \qquad \bar\psi_{x+\hat 4} U_4^\dagger e^{-\theta} \psi_x$$

$$\frac{a^4}{4} F_{\mu\nu}^2 = \frac{2N}{g^2}\left(1 - \frac{1}{N} \mathrm{Re}\, Tr\, U_{x,\mu} U_{x+\hat\mu,\nu} U^\dagger_{x+\hat\nu,\mu} U^\dagger_{x,\nu}\right) + \underline{O}(a^6)$$

Triality

Triality $\Upsilon = \mathbf{q} (mod\ 3)$
Triality is related to the centre of SU(3) ($\Upsilon = \mathbf{0.1.2}$):

$$\exp\left(\frac{2\imath\pi\Upsilon}{3}\right) = \exp\left(\frac{2\imath\pi\Upsilon\lambda_8}{\sqrt{3}}\right)$$

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} e^{2\imath\pi/3} & 0 & 0 \\ 0 & e^{2\imath\pi/3} & 0 \\ 0 & 0 & e^{2\imath\pi/3} \end{pmatrix} \begin{pmatrix} e^{4\imath\pi/3} & 0 & 0 \\ 0 & e^{4\imath\pi/3} & 0 \\ 0 & 0 & e^{4\imath\pi/3} \end{pmatrix}$$

Gauss law for the $\mathbb{Z}_3$ group (SU(3) centre):
triality in a volume V equals central flux through its surface
(central fluxes were used by G.'t Hooft in 1979 to model confinement)

Roberge–Weiss approach

$$Z(T) = \mathrm{Tr}\exp\left(-\frac{\hat{H}}{T}\right)\int_{A(0)=A(1/T)} DA\; e^{-S_E[A]}$$

Temporal static gauge

$$\frac{\partial A_0}{\partial t} = 0, \qquad A_0^a(\vec{x}) = \delta_{a3}\eta_3(\vec{x}) + \delta_{a8}\eta_8(\vec{x})$$

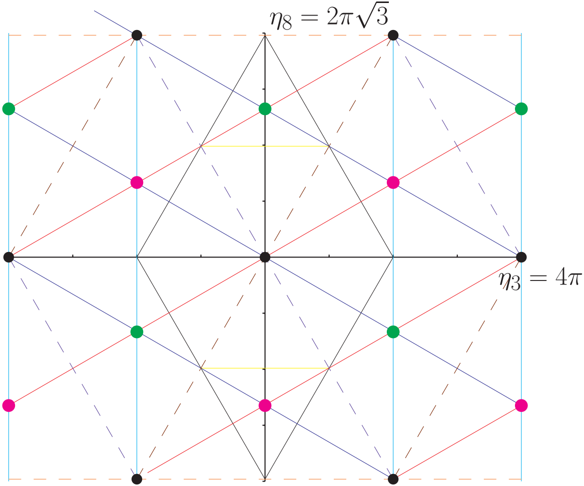
Polyakov loop ($e^{\text{free energy of a quark}}$):

$$P(\vec{x}) \equiv \frac{1}{N_c}\mathrm{Tr\ Pexp}\left(ig\int_0^{1/T} A_0(\vec{x},\tau)\; d\tau\right)$$

.

$$A_0 = \frac{T}{g} \begin{pmatrix} \phi_1 & 0 & 0 \\ 0 & \phi_2 & 0 \\ 0 & 0 & \phi_3 \end{pmatrix}$$

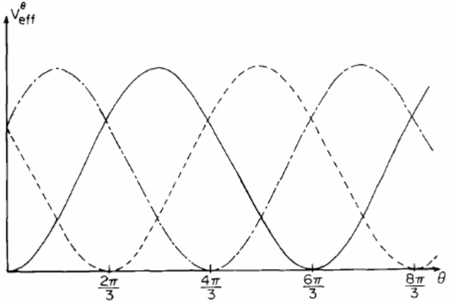
$$\begin{aligned} \phi_1 &= \frac{\theta}{\sqrt{6}} + \frac{\eta_8}{2\sqrt{3}} + \frac{\eta_3}{2} \\ \phi_2 &= \frac{\theta}{\sqrt{6}} + \frac{\eta_8}{2\sqrt{3}} - \frac{\eta_3}{2} \\ \phi_3 &= \frac{\theta}{\sqrt{6}} - \frac{\eta_8}{\sqrt{3}} \end{aligned}$$



Relief of V_{eff} at $\theta = 0$

Colored dots -
are local minima,
black are global minima

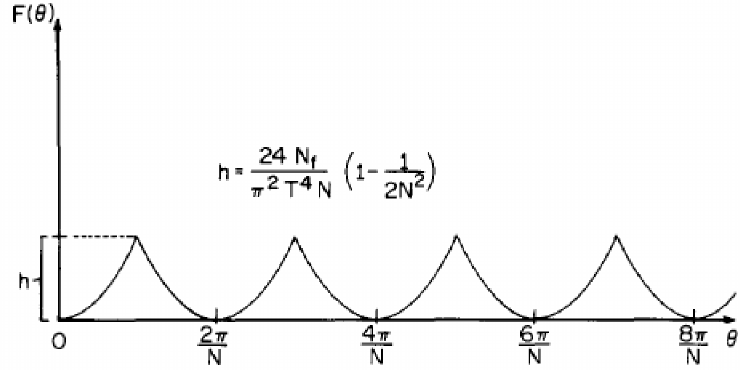
We search for
$V(\theta) =$
$= \min_{\eta_3,\eta_8} V_{eff}(\theta, \eta_3, \eta_8)$



The effective potential as a function of θ at the three Z_3 images of $\phi = 0$, for the group SU(3).

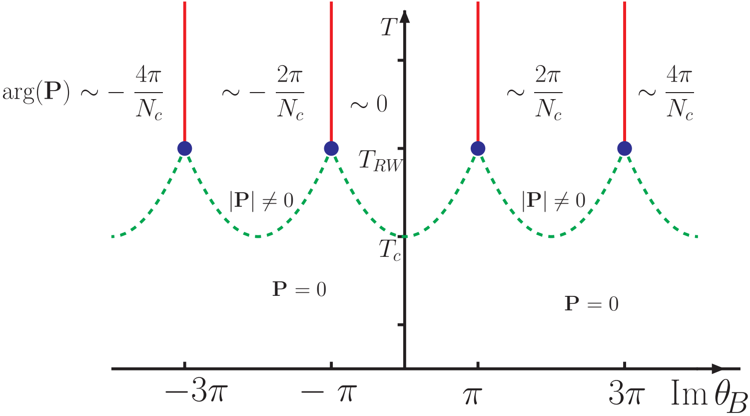
$V(\theta)$ in different minima in η_3, η_8

(Fig. from RW, 1986)

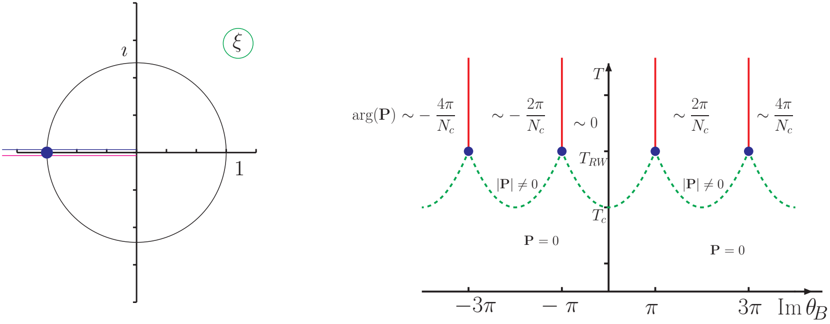


Breaks in the top points of the curve
indicate the first-order phase transition.

(Fig. from RW, 1986)

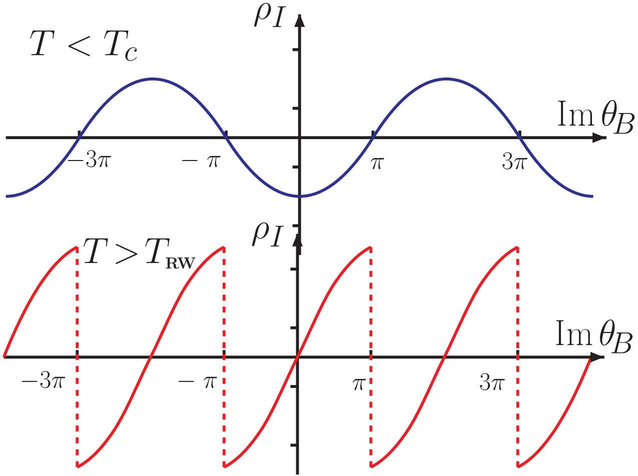


The Roberge-Weiss transition is shown by red lines ($N_c = 3$).
The Polyakov-loop sectors are marked by the values of its phase.



Left panel: The RW transition in the fugacity plane. Blue vertrex at $\xi = -1$ corresponds to the red lines on the right panel.

Lattice results



$T < T_{RW}$ — HRG; $T > T_{RW}$ - gas of free massless fermions

- We study gas of free fermions at $\Upsilon = 0$.
- We are interested in differences between the cases $\Upsilon = 0$ and "arbitrary Υ".
- We begin with a detailed analysis of the convensional gas of free fermions.

Partition function of free-fermion gas at temperature T in a box of volume $V = L^3$:

$$Z_{GC}(\theta) = \prod_{\mathbf{k}} \left(1 + e^{\theta} w(\mathbf{k})\right)^{2N_C N_F} \left(1 + e^{-\theta} w(\mathbf{k})\right)^{2N_C N_F} , \qquad (2)$$

$$\mathbf{k}_i = 2\pi n_i / L, \qquad n_i \in \mathbb{Z}$$

$$w(\mathbf{k}) = \exp\left(- \frac{E_{\mathbf{k}}}{T} \right),$$

The energy has the form

$$E_{\mathbf{k}} = \frac{2\pi |\mathbf{k}|}{L}, \qquad \text{и} \qquad \frac{E_{\mathbf{k}}}{T} = \frac{2\pi |\mathbf{k}|}{\sqrt[3]{\nu}};$$

Textbook formula for the gas of free massless fermions:

$$\ln Z_{GC}(\theta) = \nu \hat{p} = \frac{\nu g}{12}\left(\frac{7\pi^2}{30} + \theta^2 + \frac{\theta^4}{2\pi^2}\right) , \quad g = N_F N_C N_s ,$$

$\nu = VT^3$ - is the dimensionless parameter. We obtain

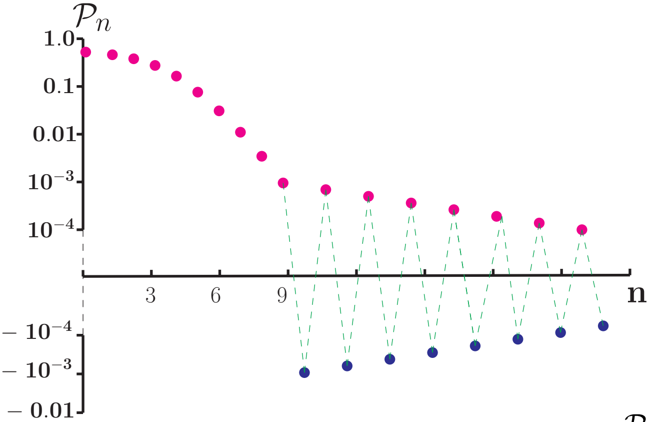
$$B(\theta) = \frac{\partial \ \ln Z_{GC}}{\partial \theta} \implies Z_{GC}(\theta_I)|_{\theta_R=0} = \exp\left(\int_0^{\theta_I} B(x)\, dx\right)$$

and then the canonical partition functions

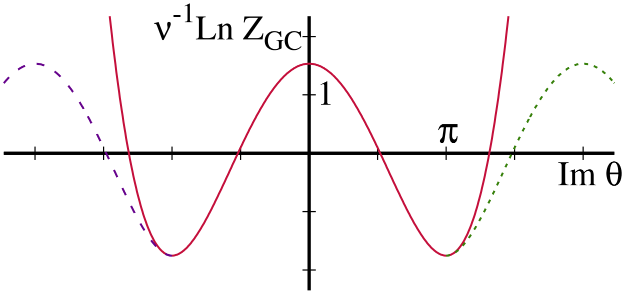
$$Z_C\,(n) = \int_{-\pi}^{\pi} \frac{d\theta_I}{2\pi} e^{-in\theta_I} Z_{GC}(\theta_I) ,$$

Evaluating this numerically (with the 6000 digit precision), we arrive at **confusion**.

The problem of negative probabilities emerges...



$$\mathcal{P}_n = \frac{Z_C(n)}{Z_{GC}(0)}$$



Periodic continuation of the pressure from the segment $\pi \leq \theta_I \leq \pi$, where it has the form

$$\hat{p}(\theta_I) = C - \frac{(\theta_I)^2}{6} + \frac{(\theta_I)^4}{12\pi^2}\,, \qquad N_s = 2, N_C = N_F = 1$$

to the entire imaginary axis results in discontinuities of its third derivative with respect to θ:

$$\hat{p}'''(\pi + 0) - \hat{p}'''(\pi - 0) = \frac{4}{\pi}$$

Thus the Fourier expansion of the pressure takes the form

$$\hat{p}(\theta_I) = \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^4} \Big(1 - \cos(n\theta_I) \Big),$$

giving rise to alternating sign of the canonical partition functions

$$Z_C^{\infty}(n) = \frac{2\nu}{\pi^2} \exp\left(- \frac{2\pi^2 \nu}{45} \right) \frac{(-1)^{n+1}}{n^4} + \underline{O}\left(\frac{1}{n^6} \right) ,$$

- Negative probabilities appear: $\mathcal{P}_{2n+1} < 0$ if $n > 1.6\nu$
- The rate of decrease of $Z_C(n)$ leads to divergence of the fugacity expansion in $\xi = e^{\theta}$ at $|\xi| \neq 1$
- $\nu = VT^3$ - $(2\pi)^3 \times$ the number of excited modes in volume V at temperature T

To exclude negative probabilities

One can either evaluate the integral

$$Z_C(n) = \int_{-\pi}^{\pi} \frac{d\theta_I}{2\pi} e^{-in\theta_I} Z_{GC}(\theta_I) \ ,$$

in the saddle-point approximation, using the Laplace asymptotic formula

or compute the partition function

$$Z_{GC}(\theta) = \prod_{\mathbf{k}\in\mathbb{Z}^3} \left(1 + e^{\theta} w(\mathbf{k})\right)^{2N_C N_F} \left(1 + e^{-\theta} w(\mathbf{k})\right)^{2N_C N_F} \ ,$$

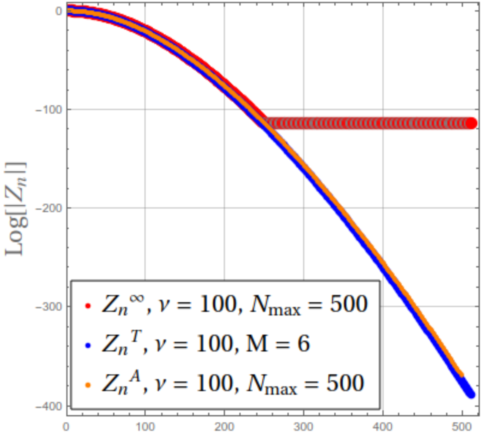
$$w(\mathbf{k}) = \exp\left(- \frac{2\pi|\mathbf{k}|}{\sqrt[3]{\nu}} \right), \qquad \mathbf{k}_i = 2\pi n_i/L, \qquad n_i \in \mathbb{Z}$$

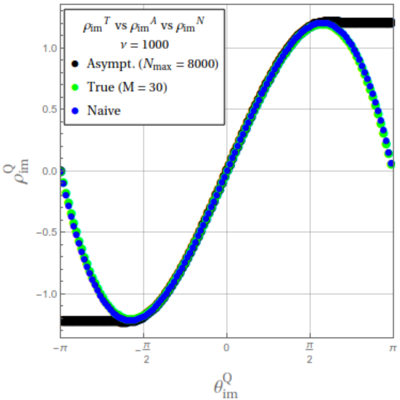
without integration with respect to $\mathbf{k}$

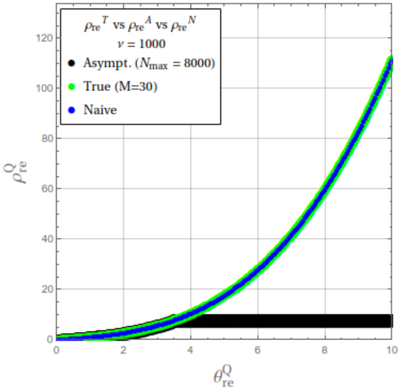
The asymptotic formula gives physically meaningful result

$$\mathbf{P}_n \sim \exp\left(-\frac{3}{4}\sqrt[3]{\frac{3\pi^2}{\nu}}\, n^{4/3} + \ldots \right) > 0 \qquad \text{при} \quad n \gg \nu$$

However, we are not sure that this is true!







Net-quark number probability distribution $Z_C^A(n)$
obtained by the asymptotic formula
does not reproduce the quark density
at imaginary chemical potentials

Lee–Yang approach

$$Z_{GC}(\theta) = \prod_{\mathbf{k}} \left(1 + e^{\theta} w(\mathbf{k})\right)^{2N_C N_F} \left(1 + e^{-\theta} w(\mathbf{k})\right)^{2N_C N_F}$$

- The grand canonical partition function can be approximated by a polynomial:

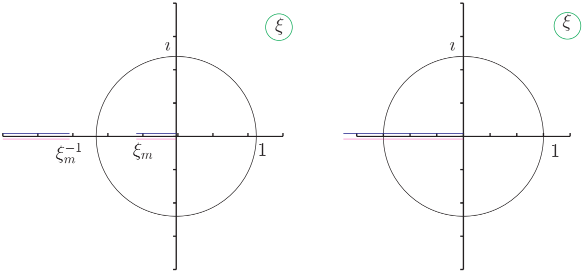
$$e^{N\theta} Z_{GC}(\theta) \; \approx \; Z_{PLY}(\xi) = \sum_{n=0}^{2N} Z_C(n-N)\xi^n, \qquad \xi = e^{\theta}$$

- Roots of this polynomial line up along some curve in the ξ plane
- A phase transition – nonanalyticity in $\ln Z_{GC}(\theta)$ –

  emerges in the limit $V \to \infty$,

  in which lines of zeroes $\{\xi_i : Z_{PLY}(\xi_i) = 0\}$
  turn into branch cuts of $\ln Z_{GC}(\theta)$

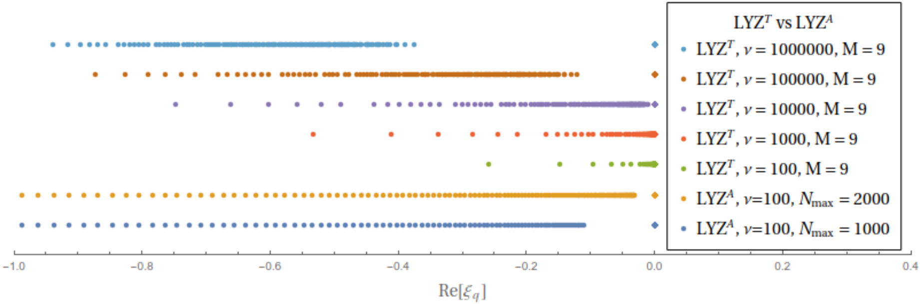
Line density of Lee–Yang zeroes is proportional to the jump of the quark density at the discontinuity!

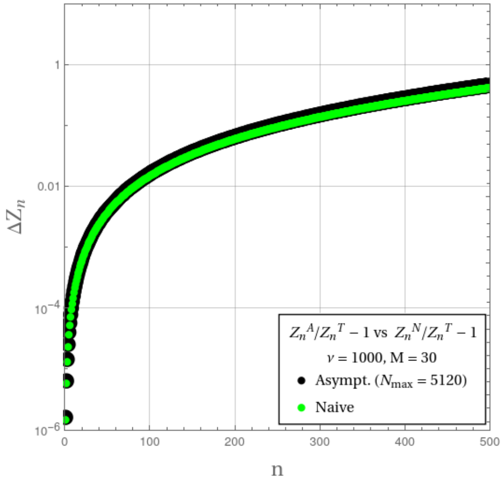


The Lee-Yang zeroes (all trialities) $\xi_{\mathbf{k}} = w^{\pm 1}(\mathbf{k})$ are located at the real negative semiaxis. Each of them is related to the energy level.

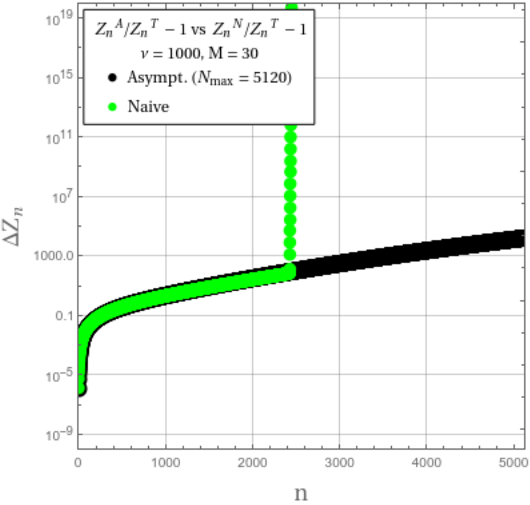
Left: $\xi_m = - \exp\left(-\frac{m}{T}\right)$ Right: $m = 0$

$$\nu \to \infty : \quad p \to \frac{N_f}{6N_c}\left(\ln^2\xi + \frac{\ln^4\xi}{2N_c^2\pi^2}\right)$$



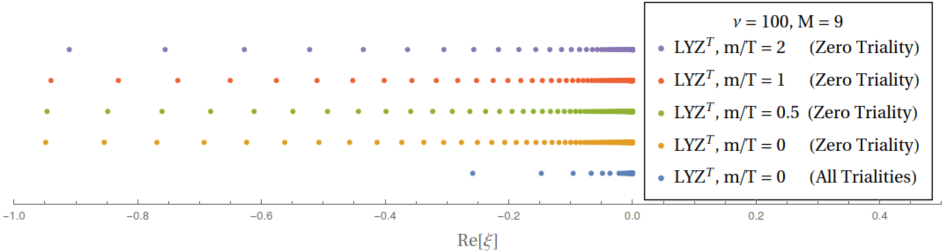


Relative deviations of Naive and Asymptotic probabilities from their true values (at small n).



Relative deviations of Naive and Asymptotic probabilities from their true values (at large n).

The main result of our study



Patterns of the Lee–Yang zeroes along the segment $-1 < \xi_B < 0$ at zero triality.

Note enhanced (as compared with the last line) density of zeroes neat $\xi_B = -1$. It is temptful to interprete each zero as the baryon-like state at high temperature.

Conclusions:

- We have carefully estimated the infinite-volume limit for a free quark gas in a box at finite T and μ to avoid negative probabilities that follow from the textbook formulas.
- At $V \to \infty$, free quark gas of arbitrary triality undergoes the 1st-order Roberge-Weiss transition at

$$\theta_q = \theta_{qR} \pm \imath\pi, \quad \theta_R > \frac{m}{T}\,;$$

  at $m = 0$ and $\theta_{qR} = 0$ it is of the 3rd order
- At $V \to \infty$ and $\Upsilon = 0$ the free quark gas undergoes the 1st-order Roberge-Weiss transition at $\theta_B = \theta_{BR} \pm \imath\pi$ at arbitrary θ_{BR}.
- Zero-triality free quark gas is statistically equivalent to a system with incredibly high denstity of low-lying levels, associated with a unit net-baryon number

Thank you for attention!