Complex Lagevin and QCD Thermodynamics

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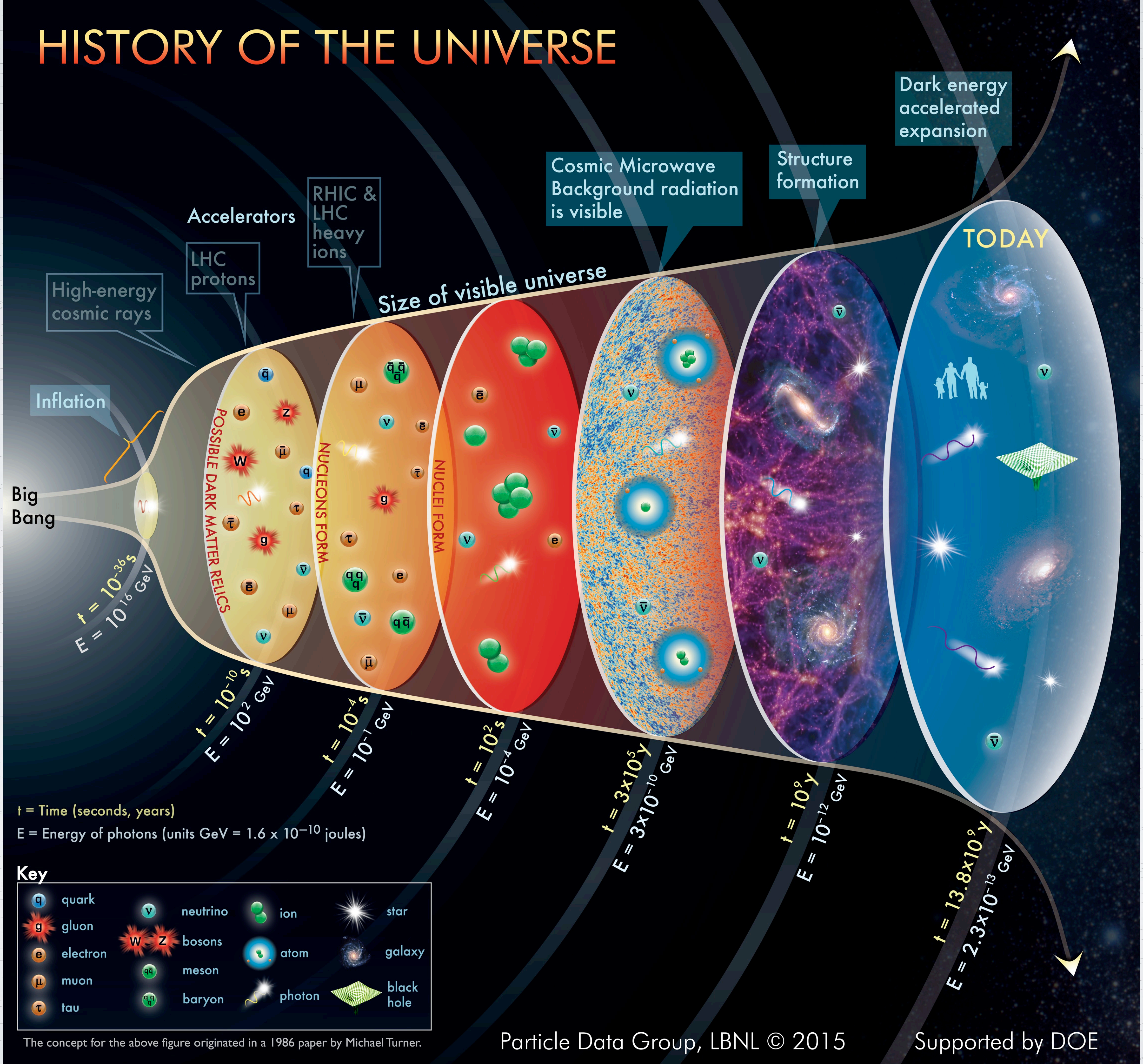
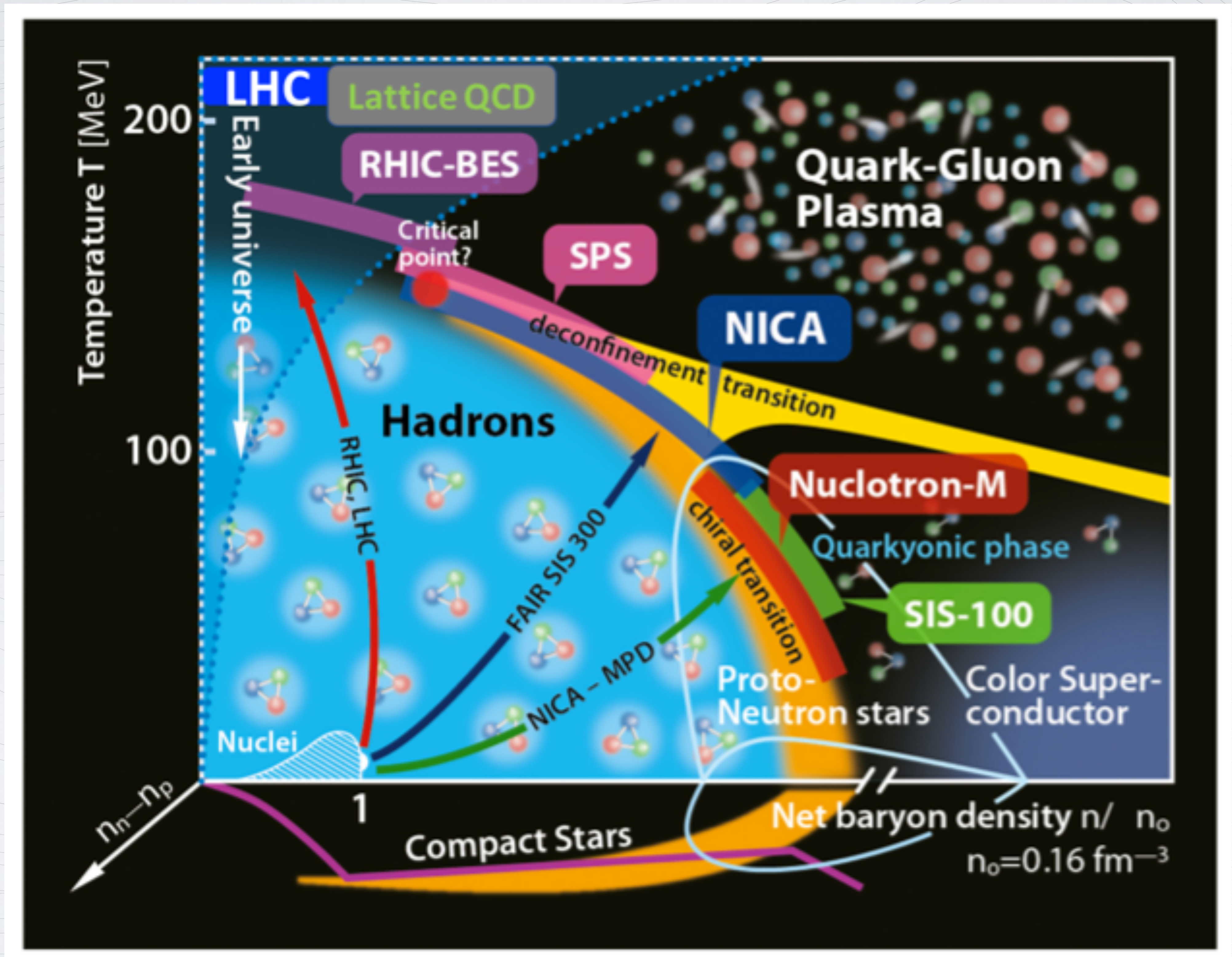
QUANTUM THEORY CENTER

D·IAS

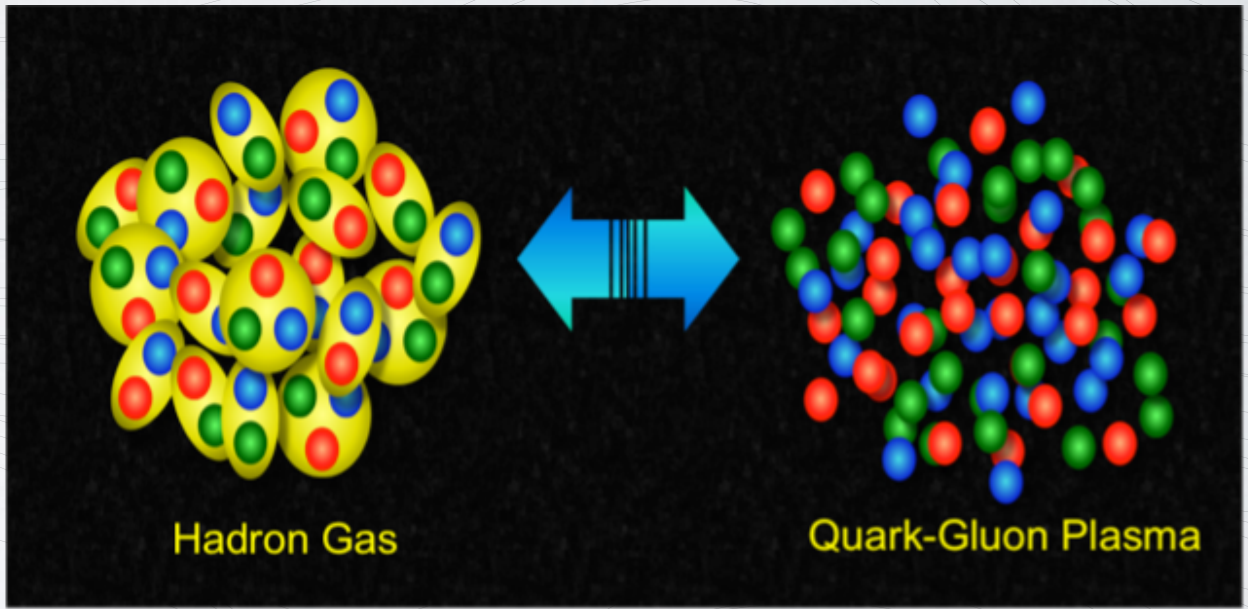

HISTORY OF THE UNIVERSE
Dark energy accelerated expansion
Structure formation
Cosmic Microwave Background radiation is visible
RHIC & LHC heavy ions
Accelerators
LHC protons
High-energy cosmic rays
Size of visible universe
TODAY
Inflation
Big Bang
POSSIBLE DARK MATTER RELICS
NUCLEONS FORM
NUCLEI FORM
t = 10^-36 s
E = 10^16 GeV
t = 10^-10 s
E = 10^2 GeV
t = 10^-4 s
E = 10^-1 GeV
t = 10^2 s
E = 10^-4 GeV
t = 3x10^5 y
E = 3x10^-10 GeV
t = 10^9 y
E = 10^-12 GeV
t = 13.8x10^9 y
E = 2.3x10^-13 GeV
t = Time (seconds, years)
E = Energy of photons (units GeV = 1.6 x 10^-10 joules)
Key
quark
gluon
electron
muon
tau
neutrino
bosons
meson
baryon
ion
atom
photon
star
galaxy
black hole
The concept for the above figure originated in a 1986 paper by Michael Turner.
Particle Data Group, LBNL © 2015
Supported by DOE

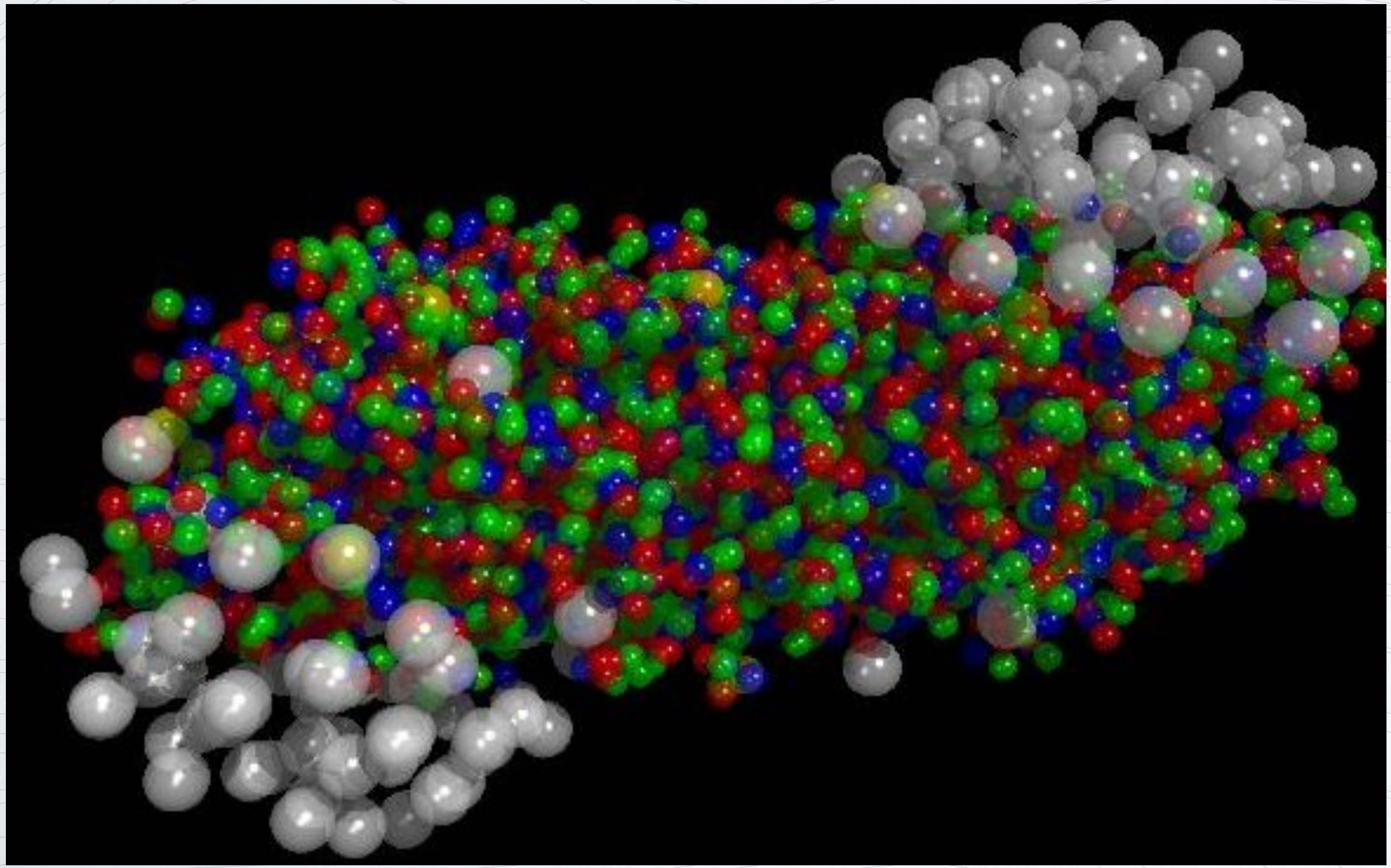
QCD Thermodynamics



QCD Thermodynamics

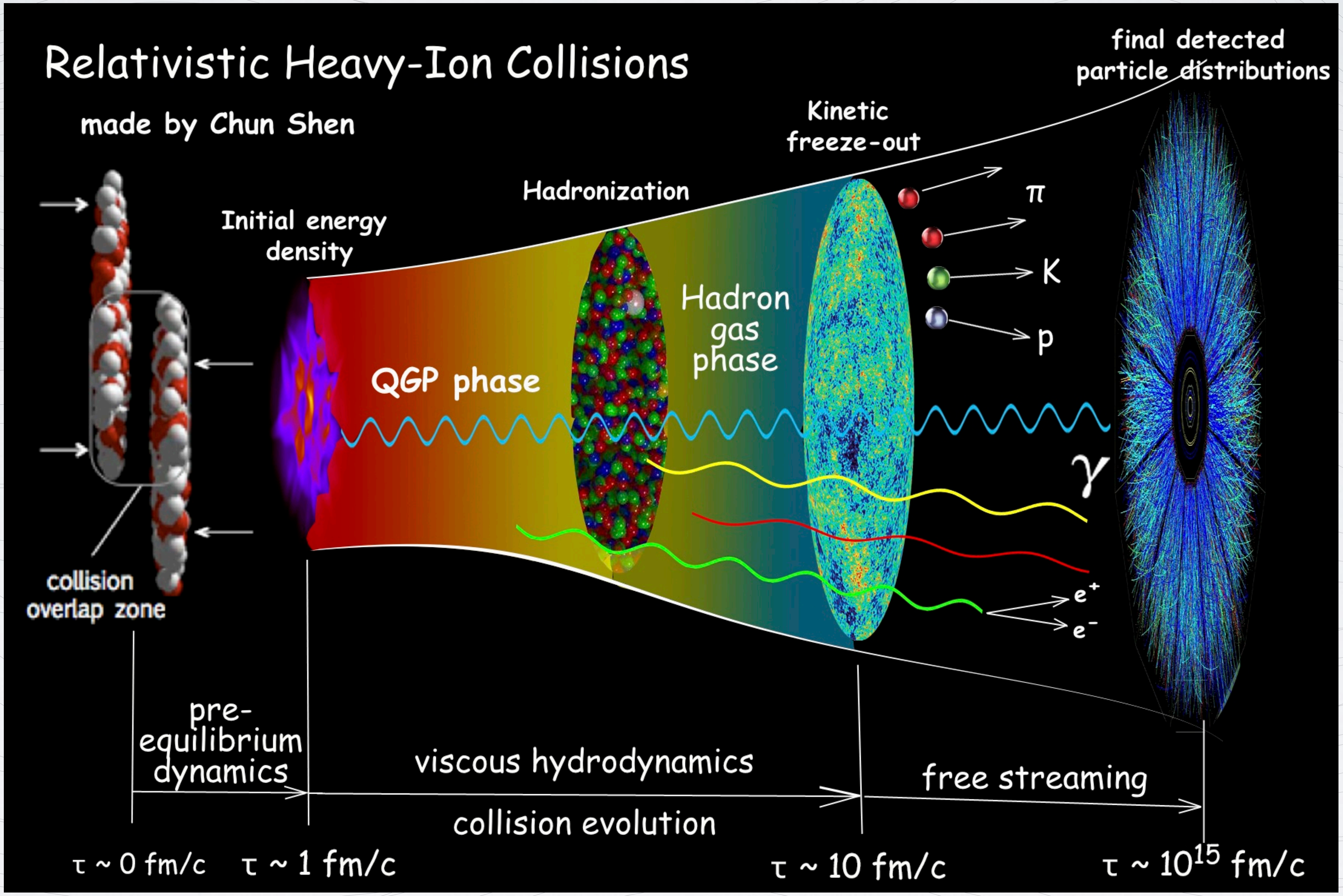
Understand the transition



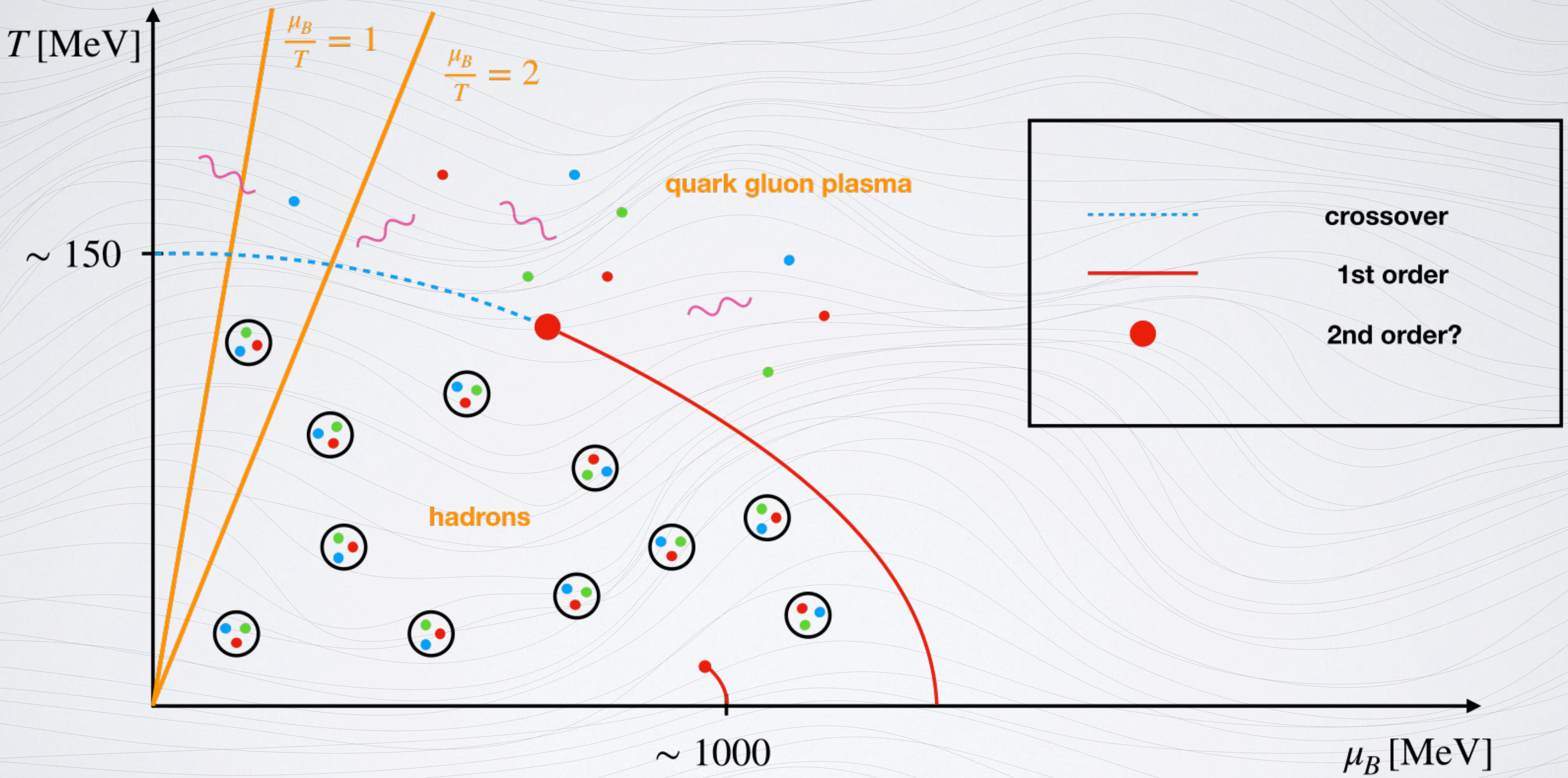


Heavy-Ion
Collision
Experiments

Heavy-Ion Collision Experiments

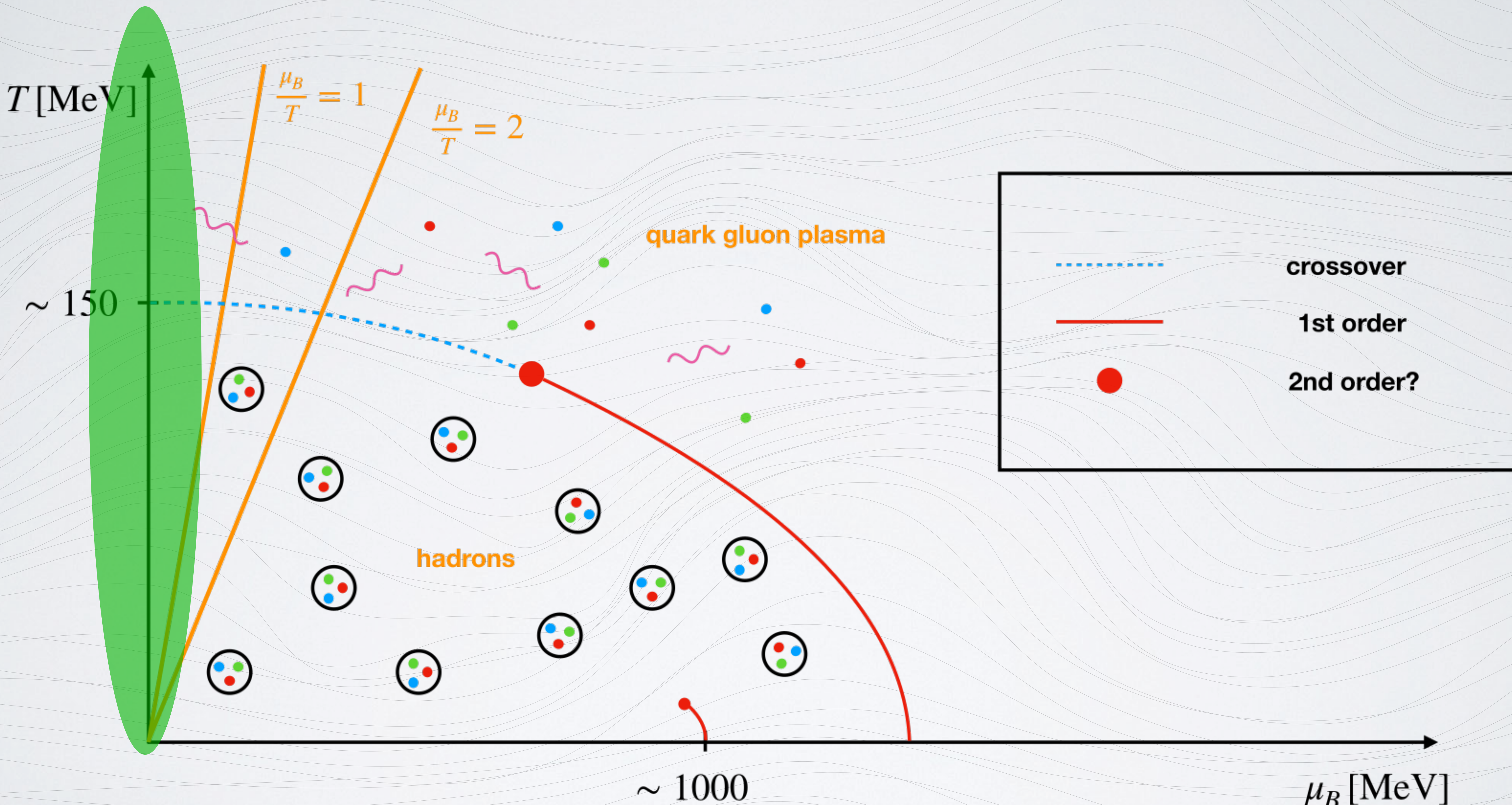


QCD phase diagram



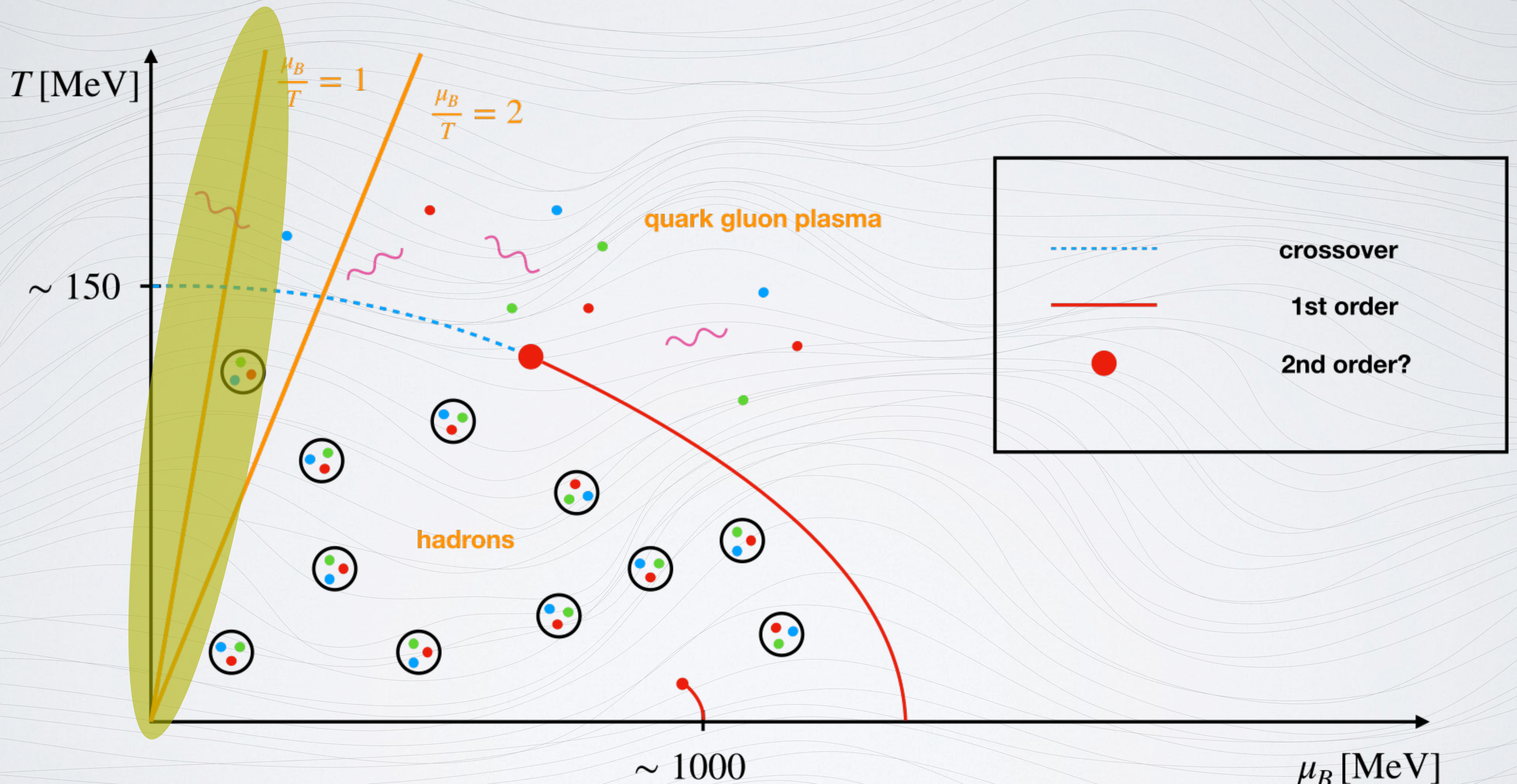
Here: Focus on QCD phase diagram with complex Langevin

QCD phase diagram



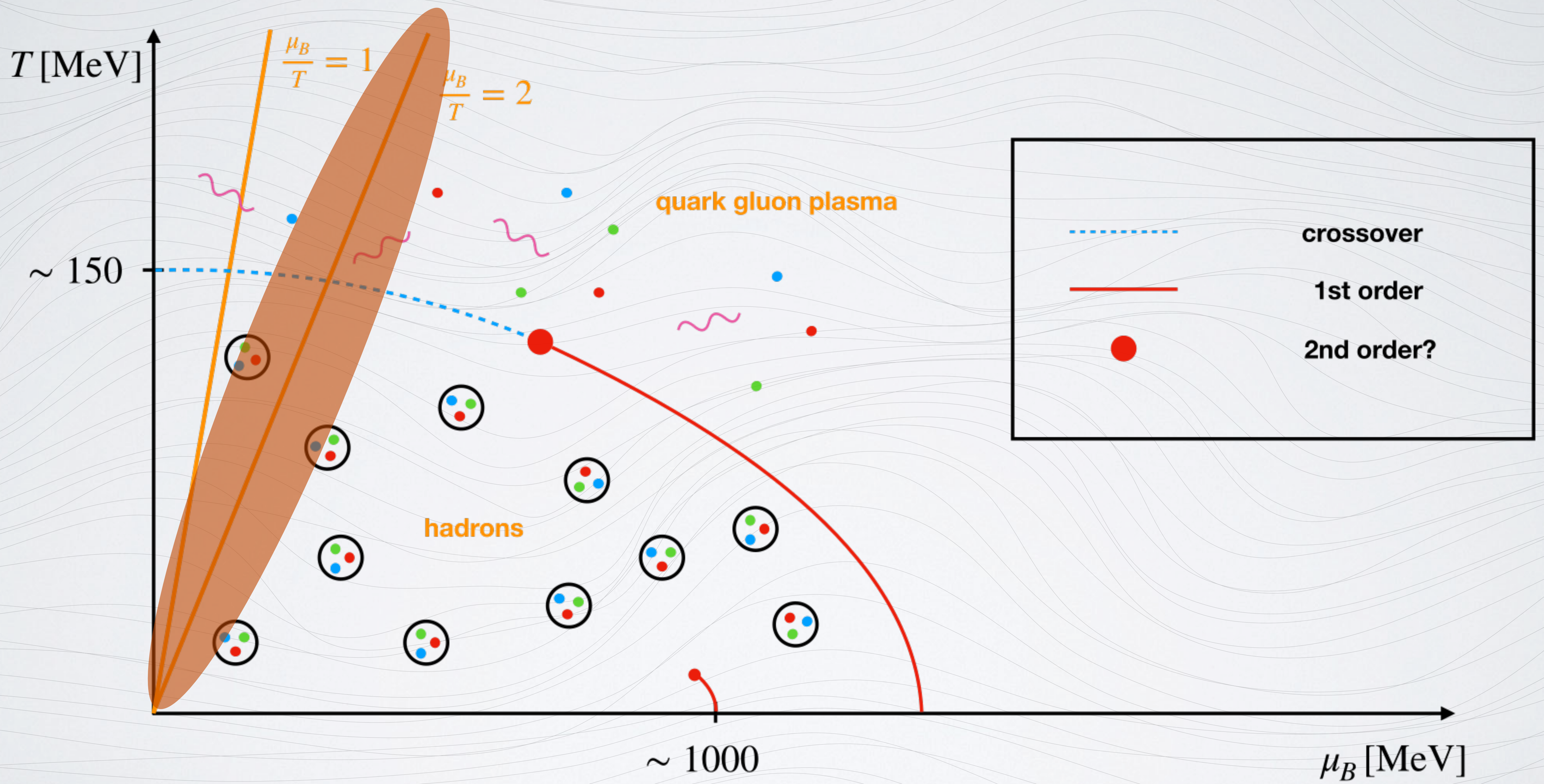
Thermodynamics ($\mu = 0$) - Easy

QCD phase diagram



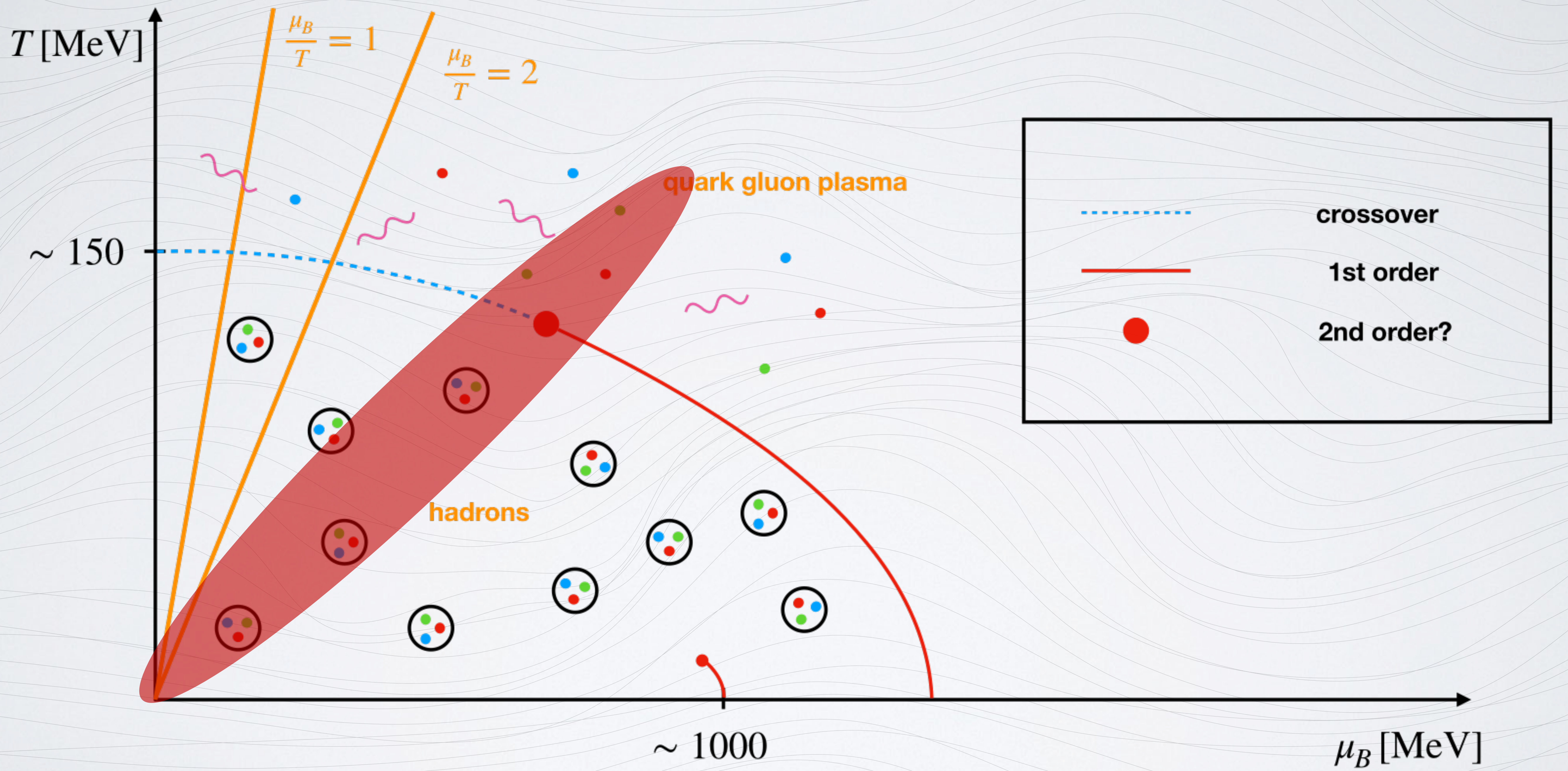
Small expansions - Medium

QCD phase diagram



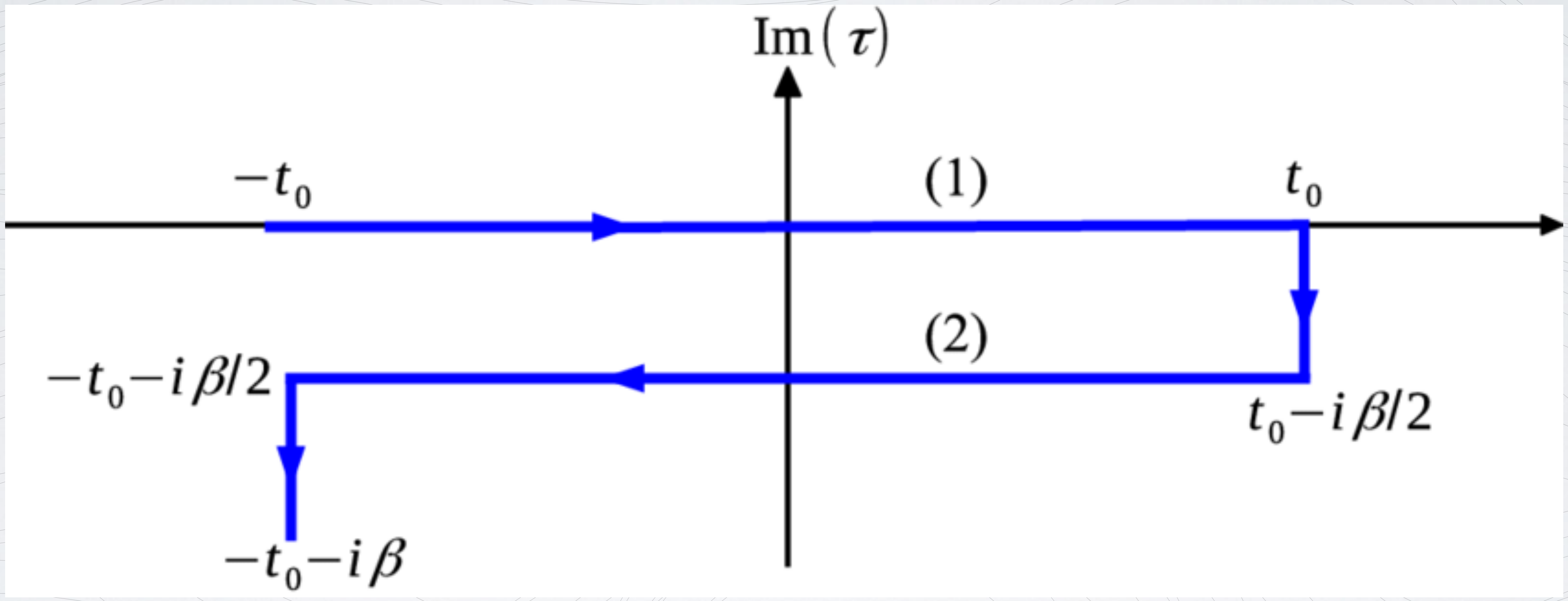
Larger expansions - Hard

QCD phase diagram



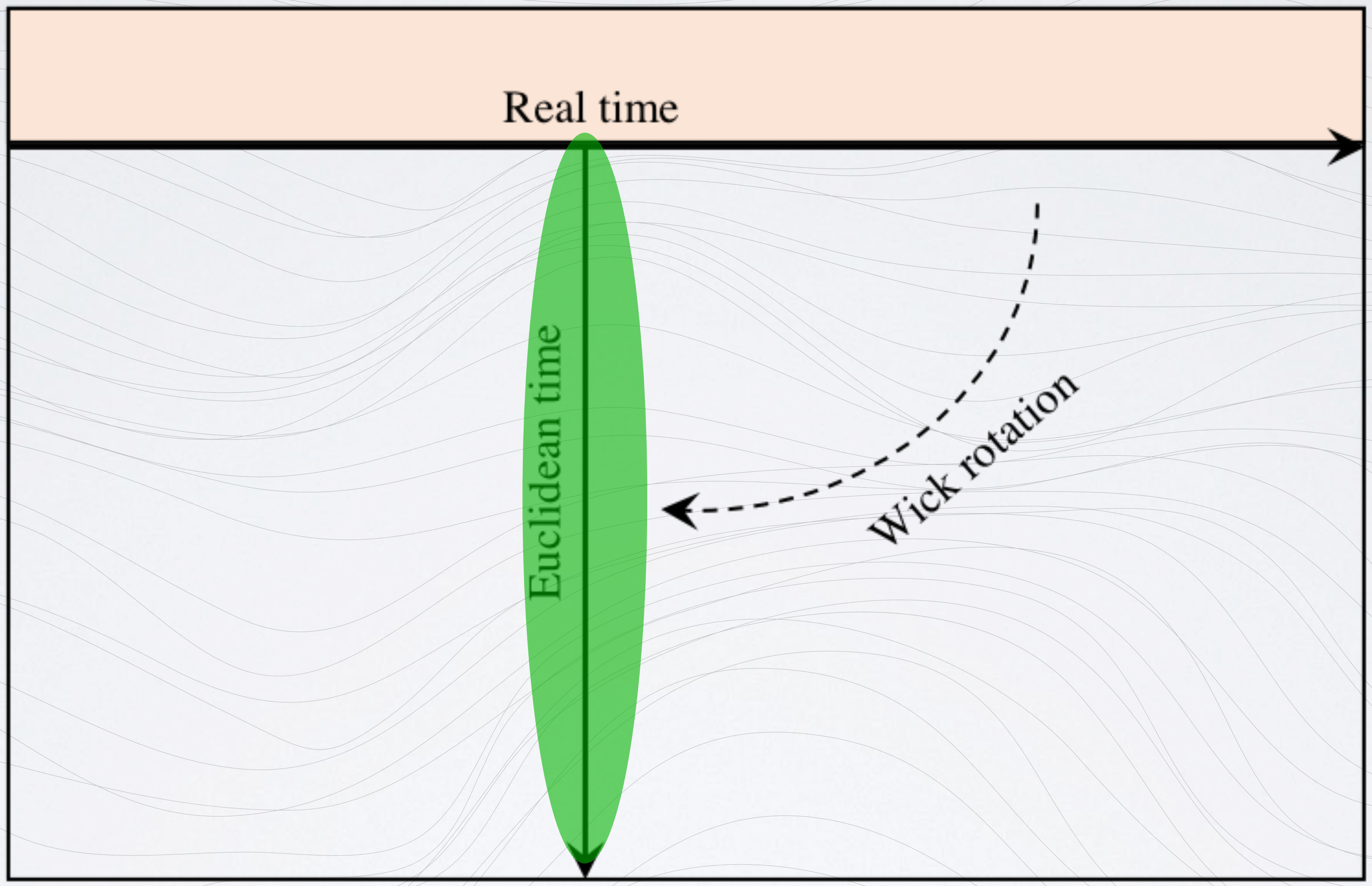
Finite μ - Very hard (exponential in volume)

Real-time QCD



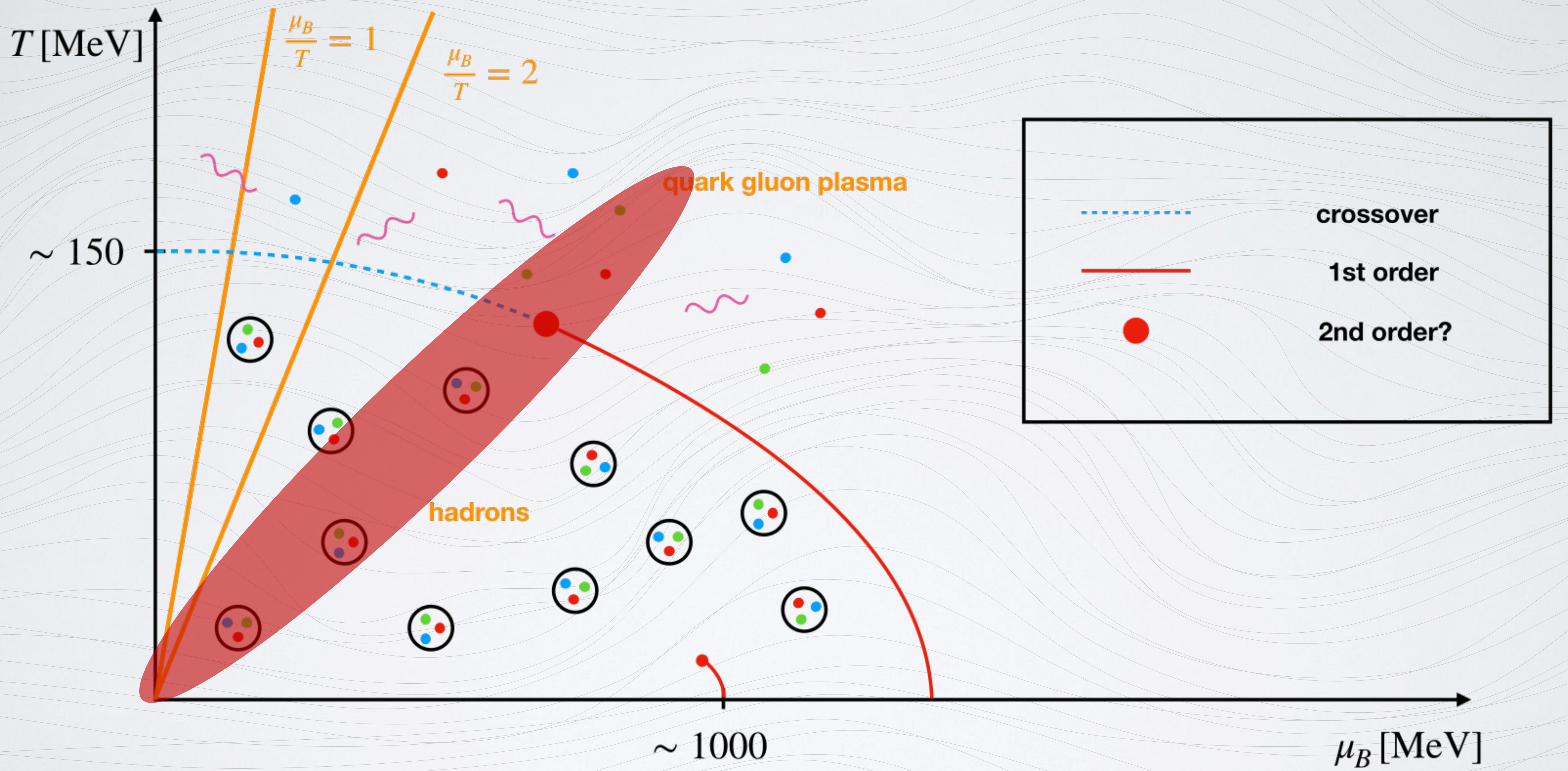
Schwinger-Keldysh contour - Extremely hard

In Minkowski space-time



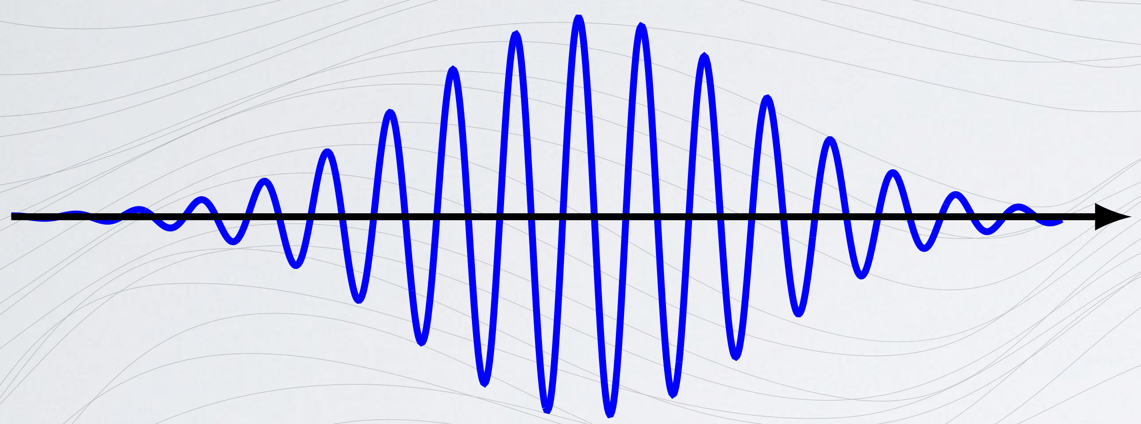
In Minkowski space-time - Currently impossible

Back to QCD phase diagram



Finite μ - Very hard (exponential in volume)

Sign Problem



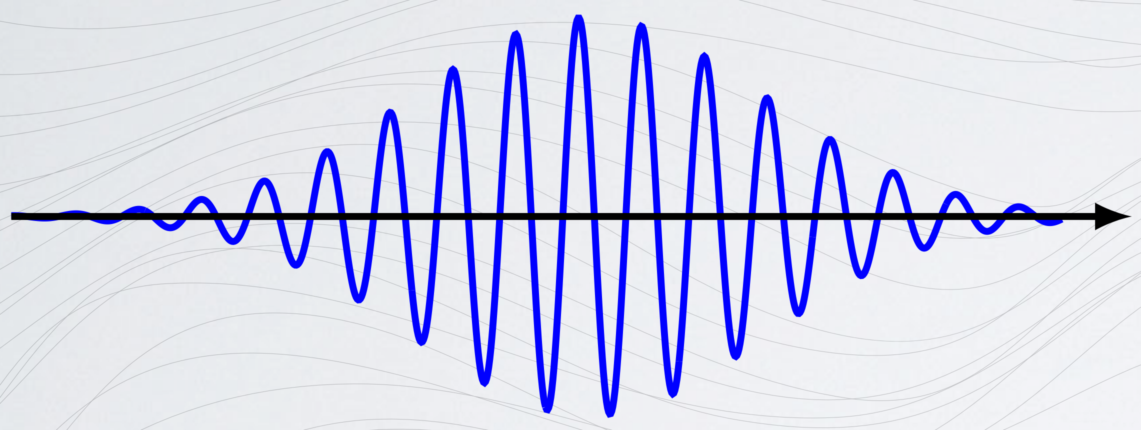
Sign Problem

- With $\mu_B \neq 0$ the path integral becomes complex
- Reason: $\det(D) \in \mathbb{C}$

$$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}[U]\, O(U)\, |\det D|\, \mathrm{e}^{i\phi}\, \mathrm{e}^{-S_G(U)}$$

- Importance Sampling Monte Carlo not applicable :(

Sign Problem



Example

- Simple one-dim. integral

$$Z = \int \mathrm{d}x \, e^{-x^2 + i\lambda x}$$

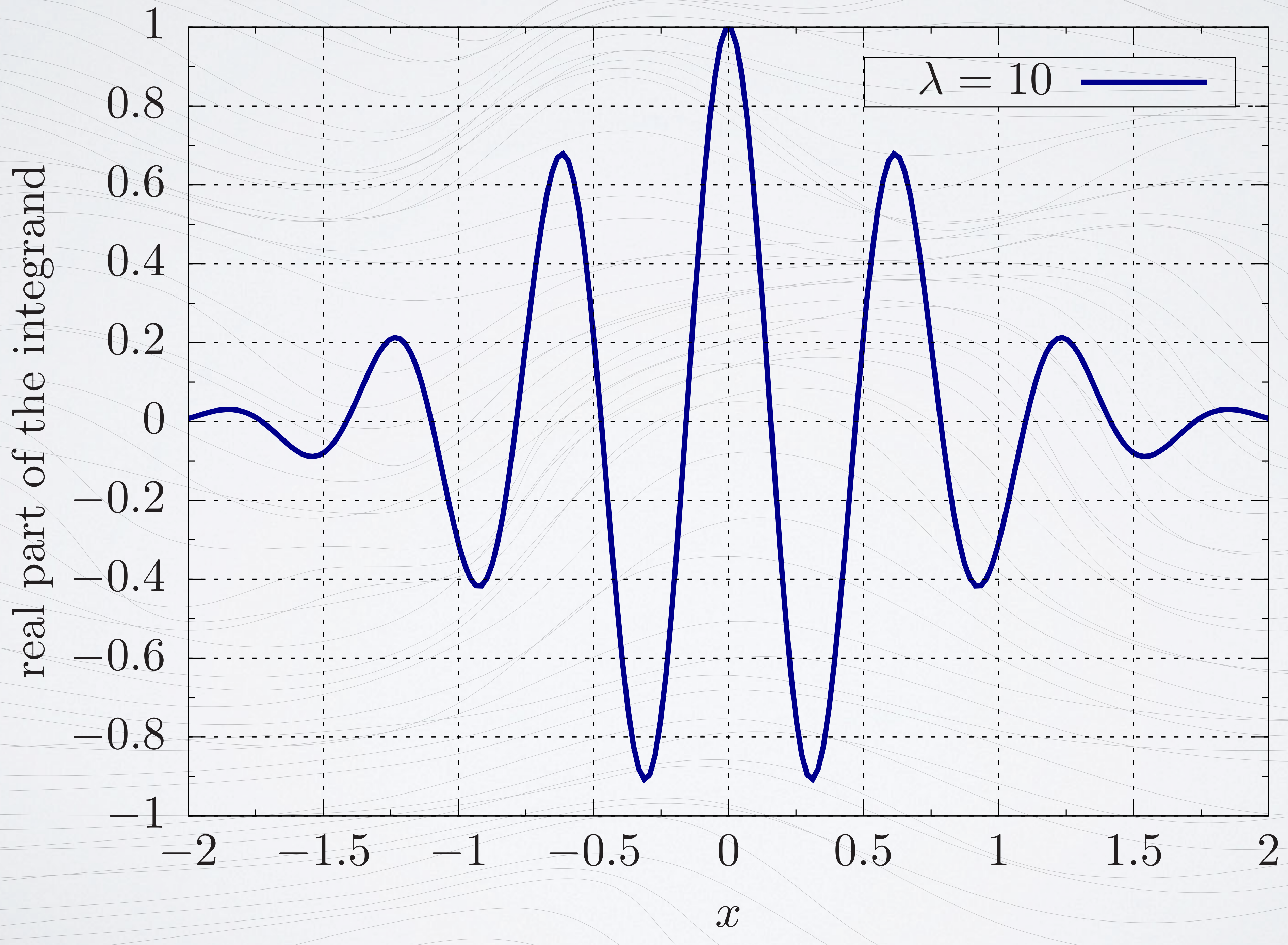
- Exact integration: $Z = \sqrt{\pi}\, e^{-\lambda^2/4}$

$$\Re(Z) = \int \mathrm{d}x \, exp(-x^2)\, \cos(\lambda x)$$

Sign Problem

Example ($\lambda = 10$)

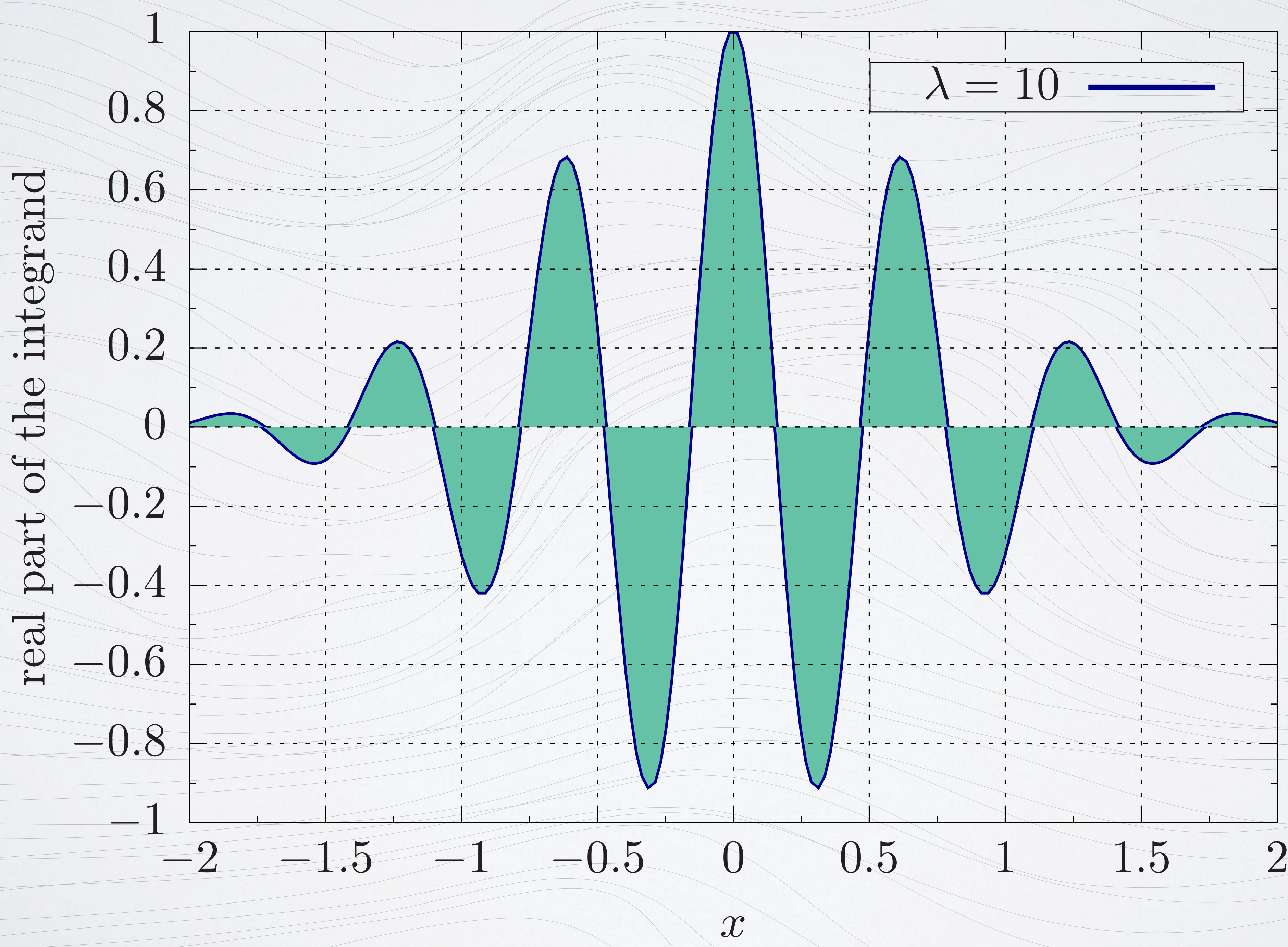
$$Z = \int \mathrm{d}x \, e^{-x^2 + i\,\lambda\,x}$$



Sign Problem

Example ($\lambda = 10$)

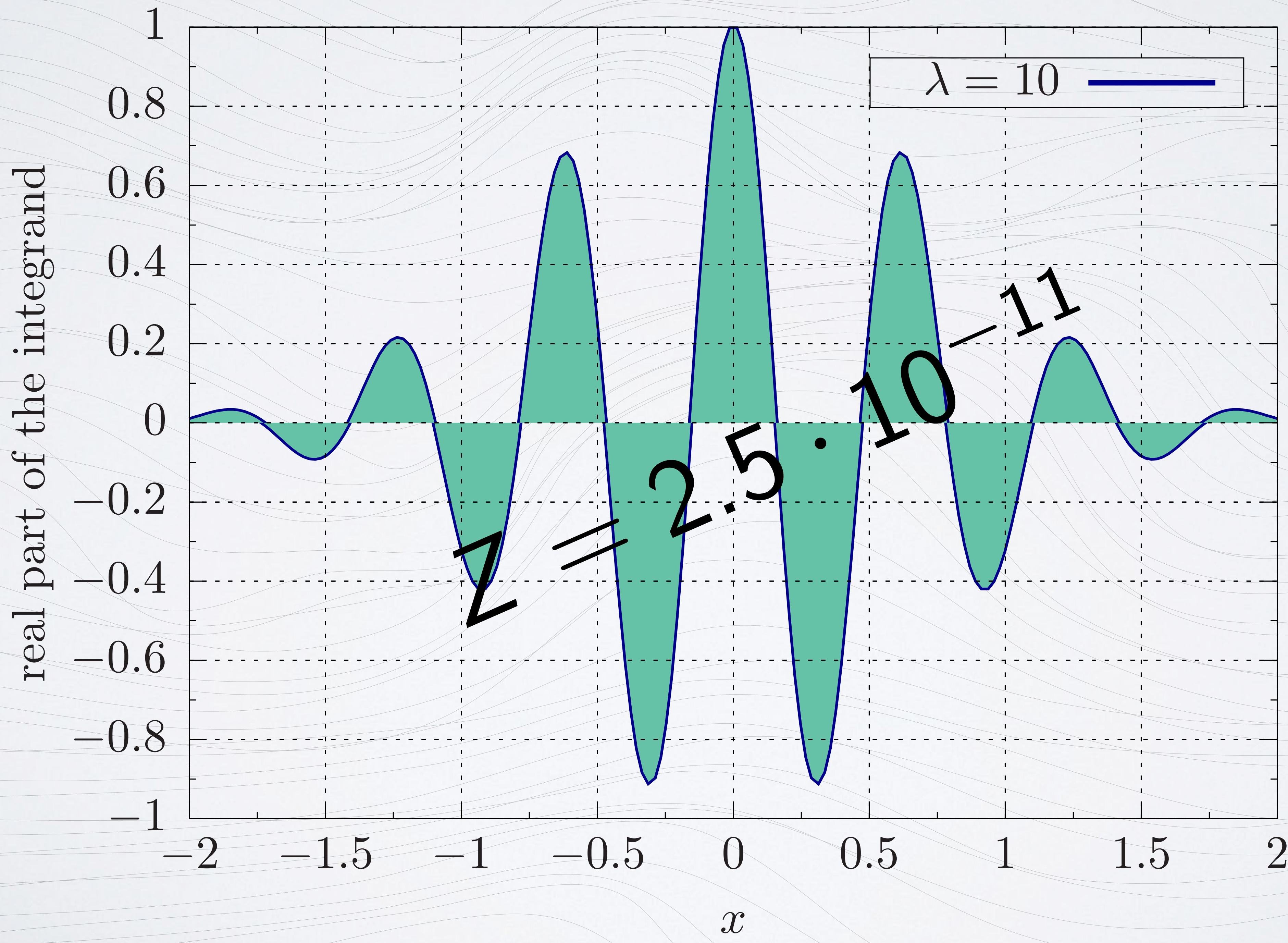
$$Z = \int \mathrm{d}x \, e^{-x^2 + i\lambda x}$$



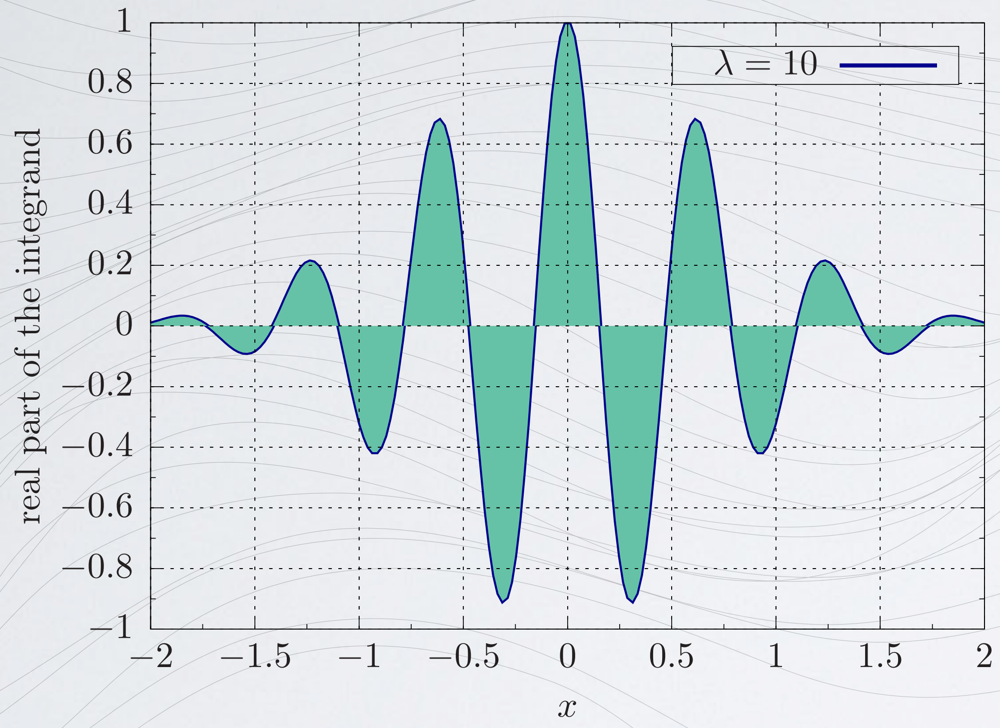
Sign Problem

Example ($\lambda = 10$)

$$Z = \int dx \, e^{-x^2 + i\lambda x}$$



Sign Problem



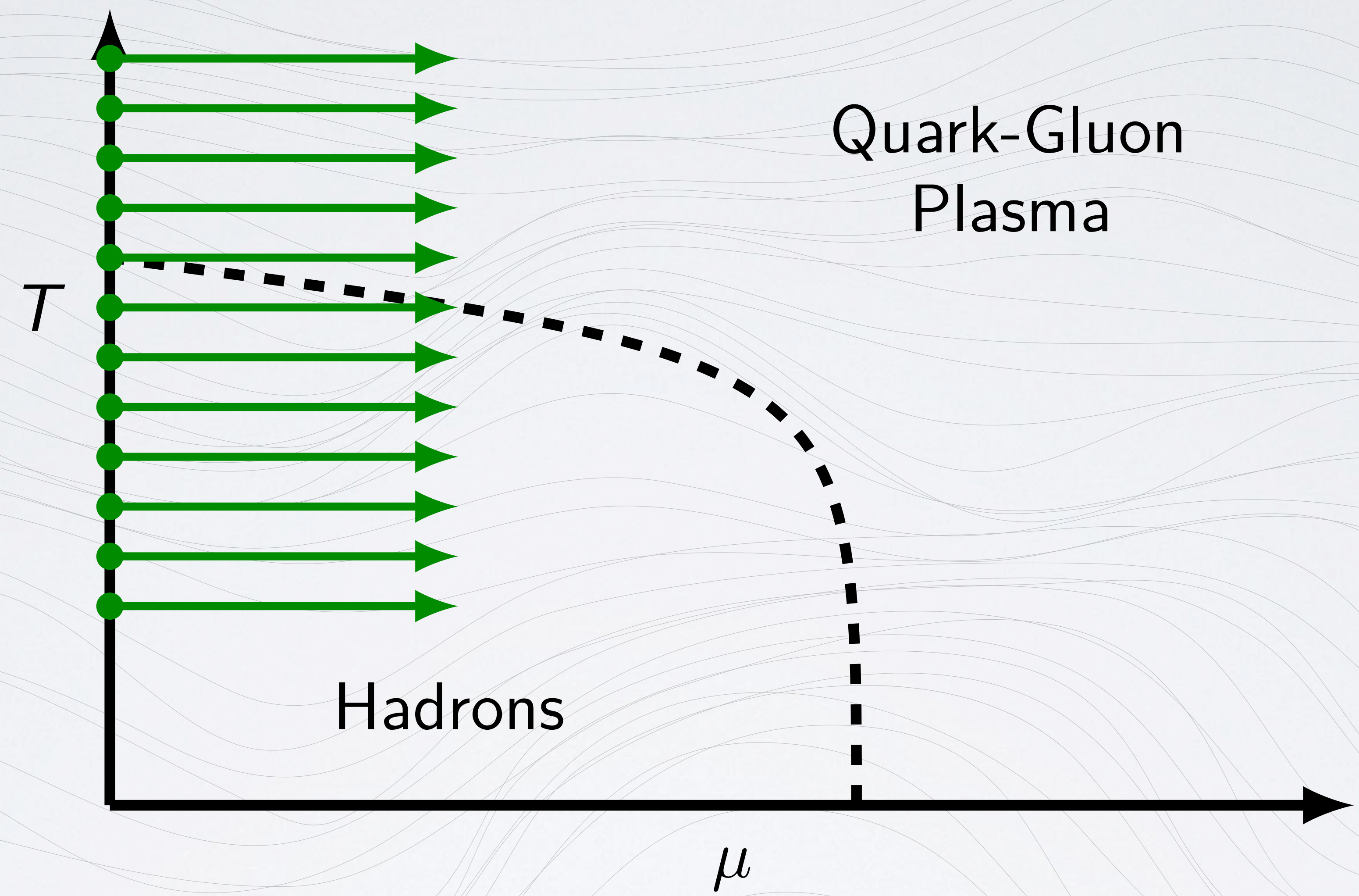
Sign Problem

- Relies on precise cancelations
- Numerical very challenging
- For QCD:

$$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}[U]\, O(U)\, |\det D|\, e^{i\phi}\, e^{-S_G(U)}$$

- New methods needed and developed:
  - Taylor Expansion, Imaginary μ, Deforming the contour, …
  - Focus here: Complex Langevin

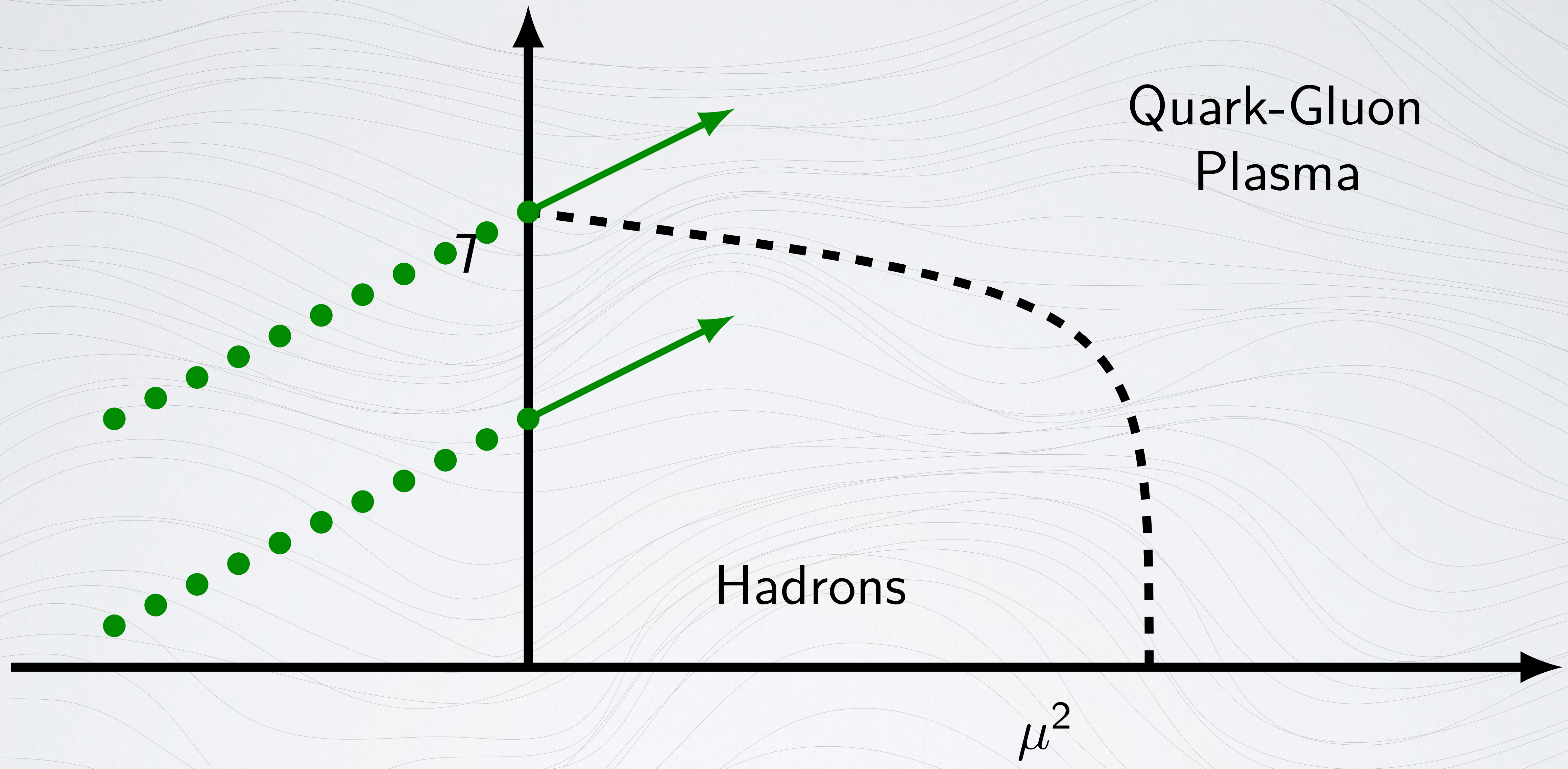
Taylor Expansion



- Simulate at zero chemical potential and expand

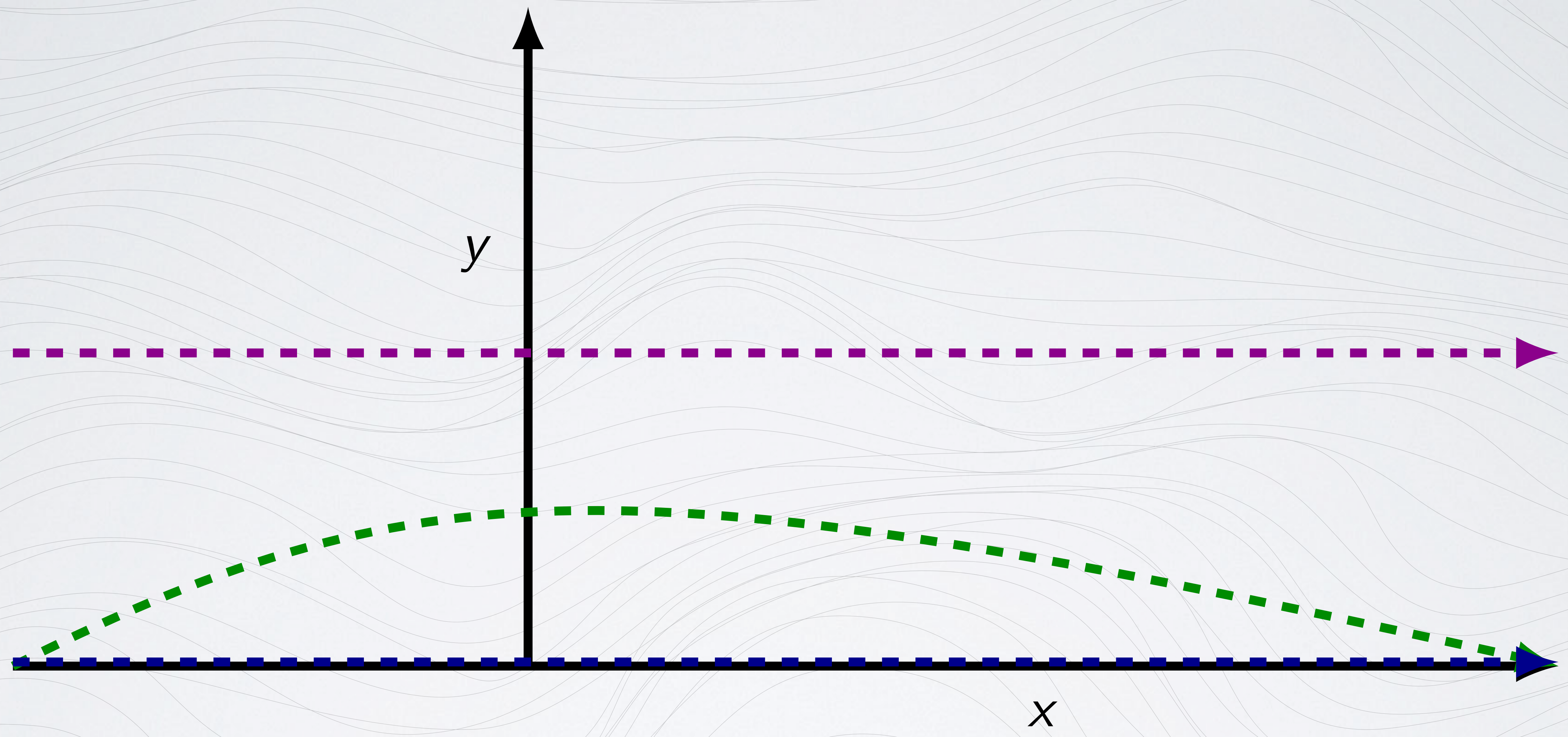
$$\frac{p}{T^4} = \sum_k c_k(T) \left(\frac{\mu}{T}\right)^k, \quad k = 0, 2, \ldots$$

Imaginary μ



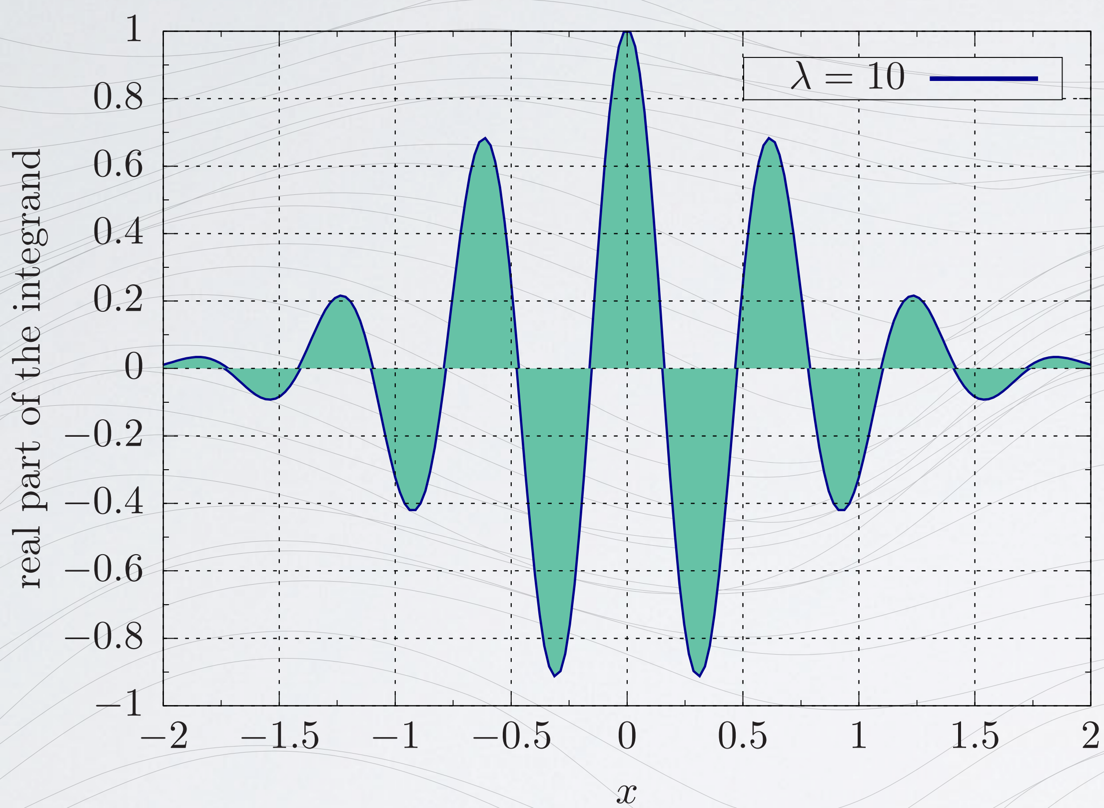
- Simulate at imaginary chemical potential and extrapolate to the QCD phase diagram

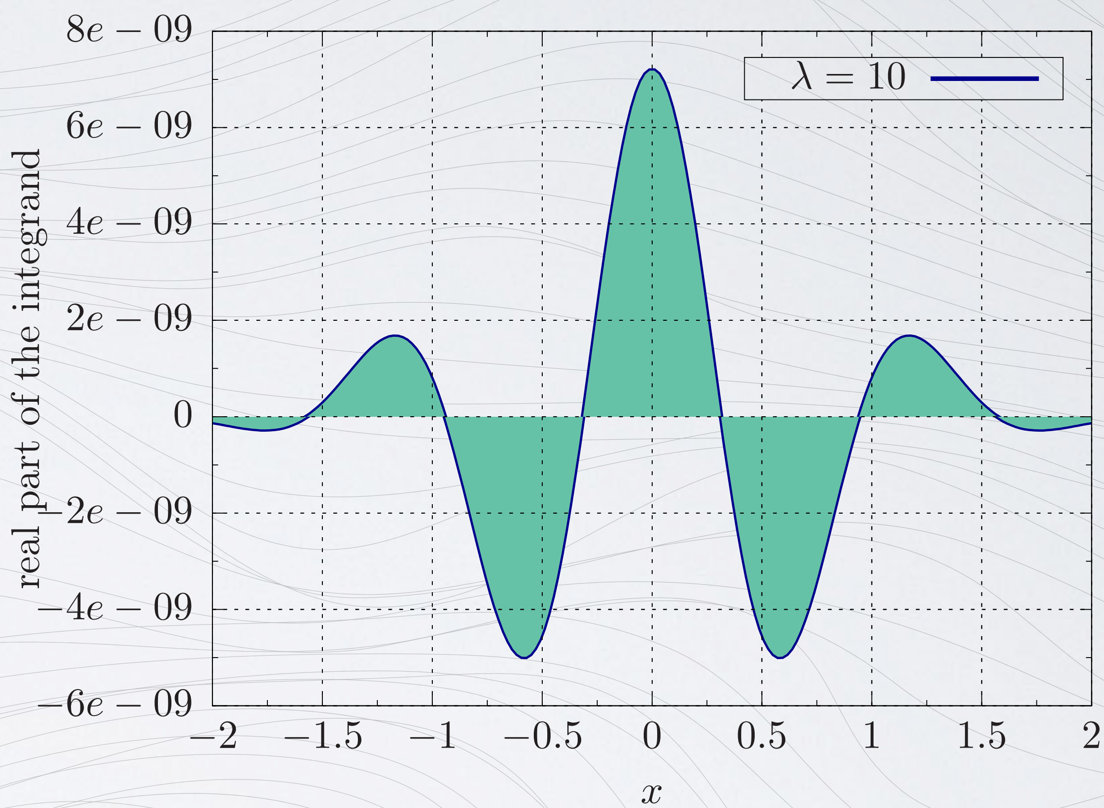
Complex Deformation



- **Go complex!**
- Deform the integration contour to reduce sign problem

Complex Deformation



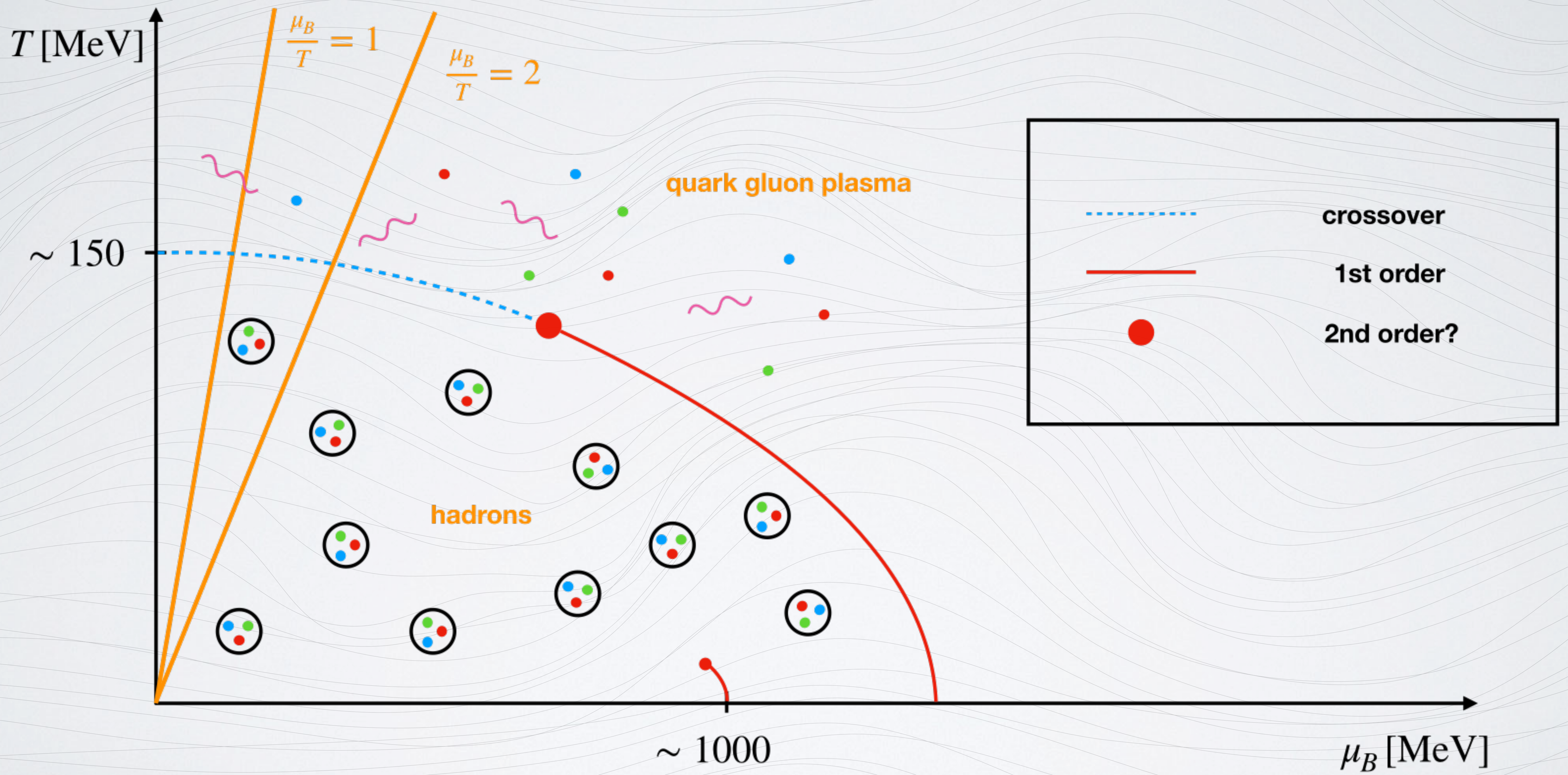


$$z = x - \frac{1}{4}\, i\,\lambda$$

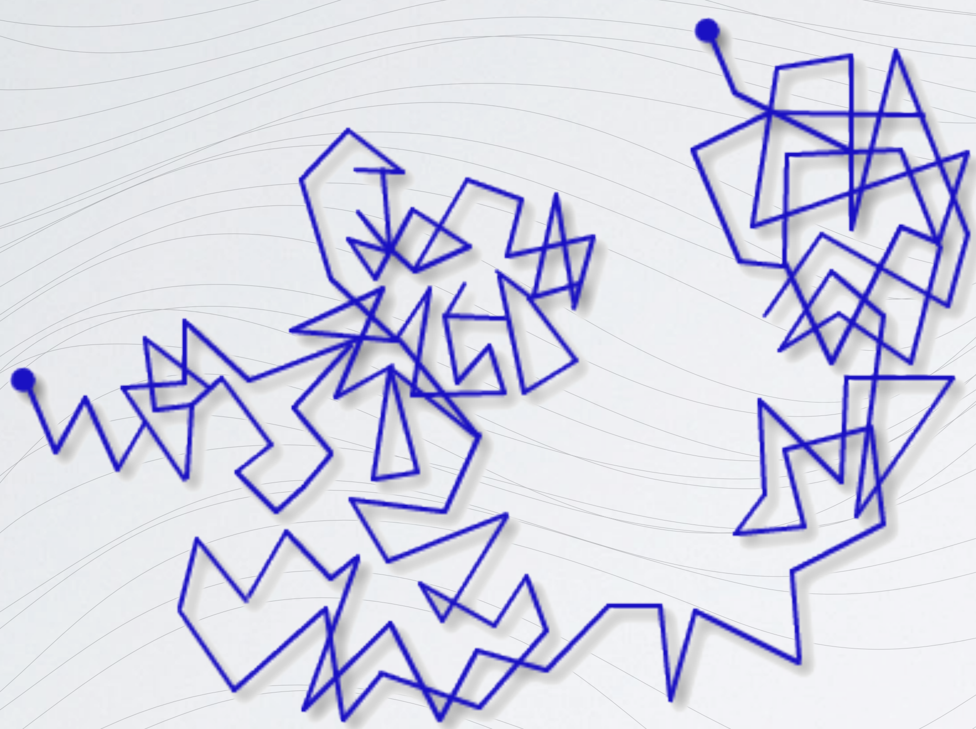
$$Z = \int \mathrm{d}x\, e^{-x^2 + i\,\lambda\, x} \qquad Z = \int \mathrm{d}z\, e^{-z^2 + i\,\lambda\, z}$$

- Previous example: Deform contour

QCD phase diagram



Complex Langevin



- Complexify degrees of freedom

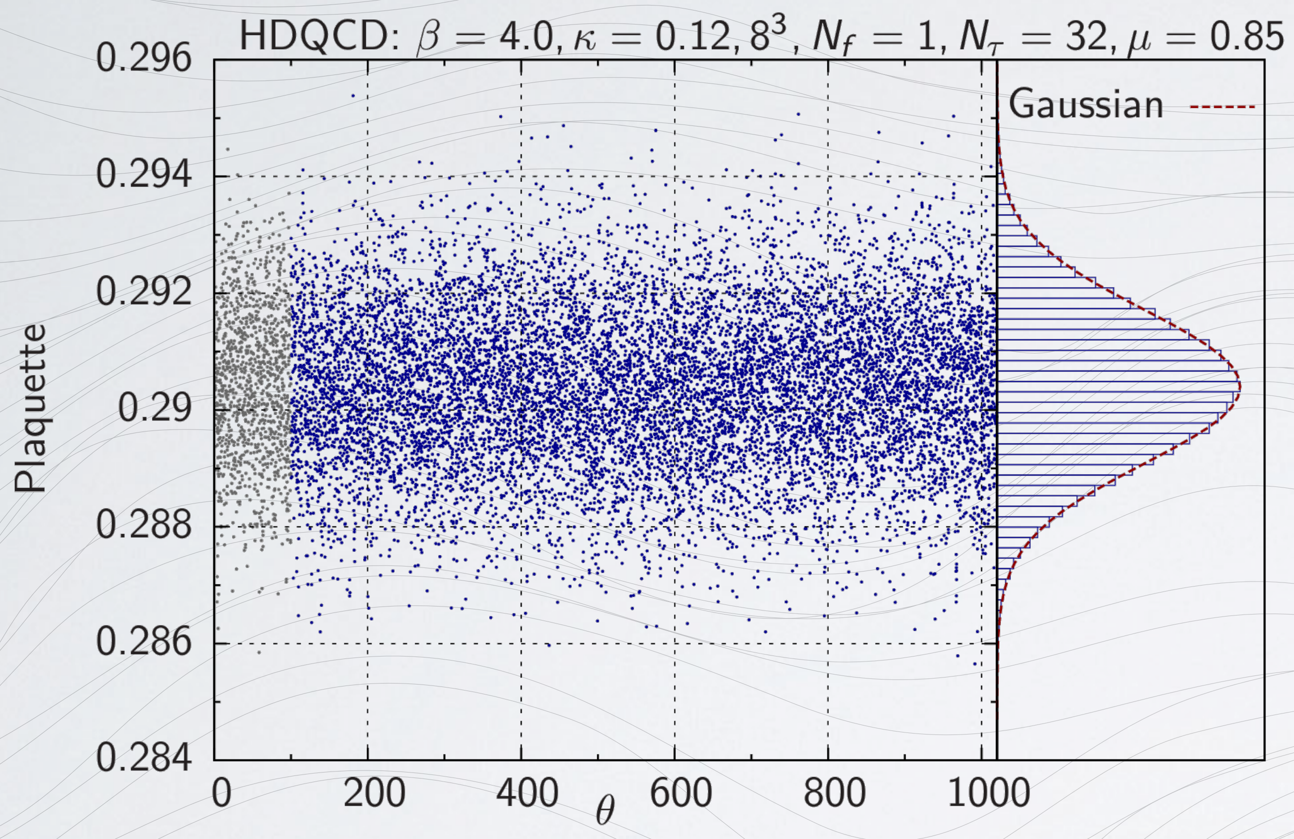
$$x \to z = x + \mathrm{i}\, y$$

- Stochastic Quantization:
  Langevin Eq:

$$\frac{\partial z}{\partial \theta} = \frac{\partial S}{\partial z} + \eta(\theta)$$

- Sign problem can be circumvented, even if it is severe! :)
- However, convergence only when:
  - Action and observables are holomorphic
  - Extension into the non-SU(3) manifold is compact

Complex Langevin



- Gauge theories (QCD)

$$\mathrm{SU}(3) \to \mathrm{SL}(3, \mathbb{C})$$

- Non-compact gauge group

$$U_{x,\mu} = \exp\left[\mathrm{i}\, a\, \lambda_c \left(A^c_{x,\mu} + \mathrm{i} B^c_{x,\mu}\right)\right]$$

- Update scheme (First order discretisation)

$$U_{x,\mu}(\theta + \epsilon) = \exp\left[\mathrm{i}\, a\, \lambda_c \left(-\epsilon\, D^c_{x,\mu} S + \sqrt{\epsilon}\, \eta^c_{x,\mu}\right)\right] U_{x,\mu}(\theta)$$

- Accept-reject step not possible, but extrapolation $\epsilon \to 0$

Foundation

- Complex Langevin ↔ Fokker-Plank equation
  - Stationary solution of FP is equilibrium solution e^{-S}
- Mathematical foundations ↔ Criteria of correctness
  - Aarts & Stamatescu, JHEP 09 (2008) 018
  - Seiler et.al., Phys. Lett. B723 (2013)
  - Nishimura et.al., Phys. Rev. D 92 (2015)
  - Scherzer et. al., Phys. Rev. D 101 (2020)
- More work on the foundation needed, but getting there :)
- Criteria more or less known, but can only be checked afterwards …

Stablising complex Langevin

- Complexification creates enlarged space, i.e. $\mathrm{SL}(3,\mathbb{C})$ - Doubling of degrees of freedom

- Keep simulations close to $\mathrm{SU}(3)$ with small excursions

- Potential issues (seen in models and simulations):
  - Runaway trajectories observed (exploring all of $\mathrm{SL}(3,\mathbb{C})$)
  - Convergence to wrong result (stable)
  - $\log \det M$ has multiple branch cuts (non-holomorphic)
  - Extrapolation in step-size ϵ needed
  - For large μ condition number of M explodes
  - …

Stablising complex Langevin

- Methods (actively developed):
  - Adaptive step - small steps for large forces — Aarts et. al., Eur. Phys. J. A 49 (2013)
  - Gauge cooling - use gauge transformations — Seiler et. al., Phys. Lett. B 723 (2013)
  - Dynamic stablization - add force to get closer to $\mathrm{SU}(3)$, unfortunately non-holomorphic, but $a \to 0$ — Attanasio & Jäger, Eur. Phys. J. C 79 (2019)
  - Implicit solvers - needed for stiff SDE — Alvestad, Larsen & Rothkopf *JHEP* 08 (2021) 138
  - Kernelled complex Langevin - use a symmetry of Fokker-Plank equation, add a kernel in the CL eq. — Alvestad, Larsen & Rothkopf *JHEP* 04 (2023) 057

Computations: Forces

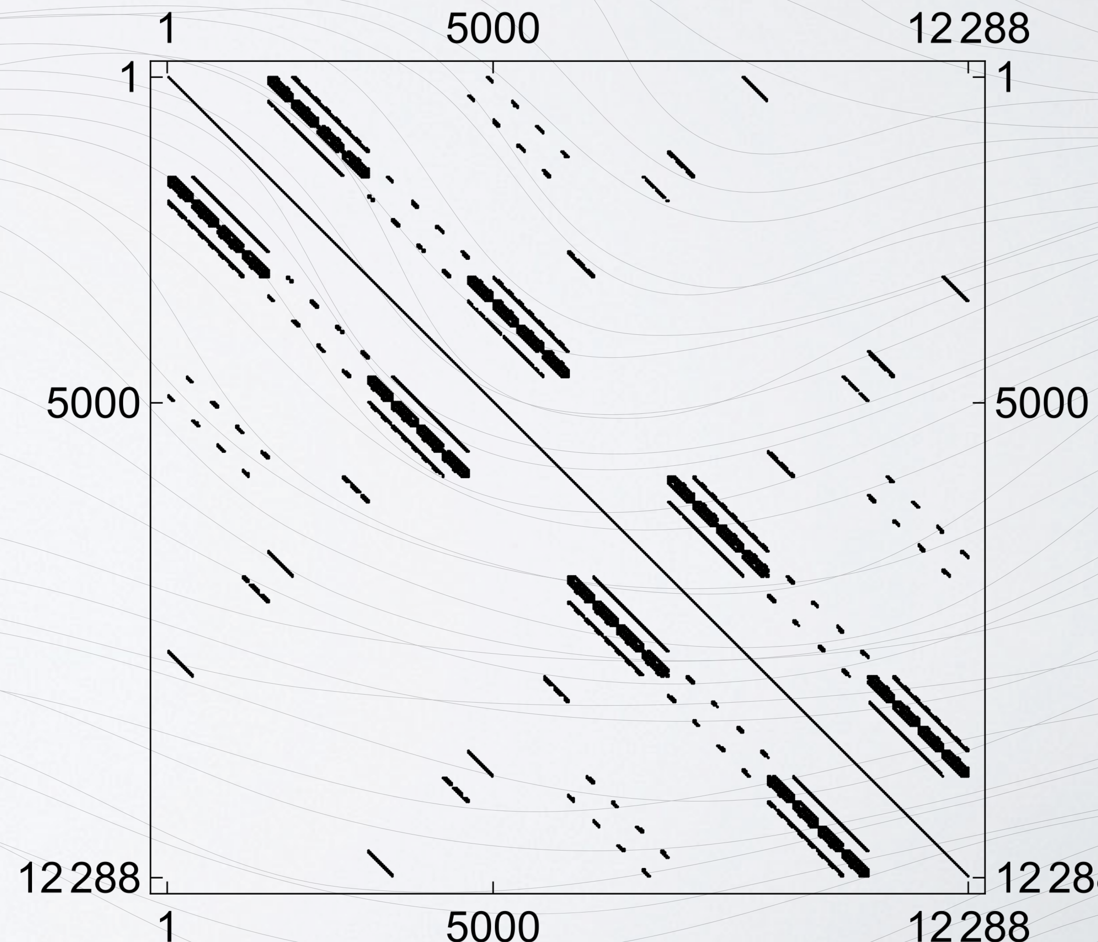
- Gauge drift (straightforward)

  $-D^a_{x,\mu} S_G$ combination of plaquettes with derivatives

- Fermionic drift
  - Bilinear noise scheme (not exact)

  $$-D^a_{x,\mu} S_F = N_f \,\mathrm{Tr}\left[M^{-1} D^a_{x,\mu} M\right]$$

D. Sexty Phys.Lett.B 729 (2014)



- Update scheme
  - Update gauge more frequently
  - Fermion inversion costly
  - Fermions inversion becomes very expensive (cond. number)

Some QCD Success stories :)

- **Heavy-Dense approximation of QCD**
  - Quarks very heavy → Quarks only move in time
  - Full Wilson gauge action
  - Phase Diagram known (Good check)
  - Simpler theory, but still has phase structure

Aarts, Attanasio, Jäger & Sexty, JHEP 09, 087 (2016)

- **Full QCD in a small box & small μ**
  - Staggered quarks
  - Expected plateaus from quark numbers
  - Individual quarks

Ito et. al., JHEP 10, 144, (2020)

Some QCD Success stories :)

- **Full QCD at small chemical potential**
  - Quarks still heavy ($m_\pi \sim 1400 MeV$)
  - Comparison to Taylor expansion
  - Improved action
  - Effects of smearing studied

D. Sexty,
Phys. Rev. D100, 074503 (2019)

- **Full QCD at moderate T and higher densities**
  - Lighter quarks ($m_\pi \sim 480 MeV$)
  - Wilson gauge action and fine lattices ($a \sim 0.06 fm$)
  - Naive Wilson fermions
  - More later!

Attanasio, Jäger & Ziegler,
2203.13144

Real-time QCD Success stories :)

- **Kernelled complex Langevin**
  - Strongly coupled quantum anharmonic oscillator
  - Introduction of kernels to Langevin
  - Machine Learning to optimise kernels
  - More later

Alvestad, Larsen & Rothkopf, JHEP 04, 057 (2023)

- **Anisotropic kernel for SU(2) YM**
  - Using anisotropic kernel
  - SU(2) Yang-Mills in 3+1 dimensions
  - Large time extents possible

Boguslavski, Hotzy and Müller, JHEP 06, 011 (2023)

Non-QCD success stories…

Attanasio & Drut,
Phys. Rev. A 101 (2020)

- **Ultra-cold atoms**
  - Spin-Orbit coupling
  - Bosons with quartic interaction
  - Lattice formulation leads to non-abelian background
  - Time derivative makes action complex

- **Polymers and Complex Fluids**
  - Mixtures require non-equilibrium processing
  - Hamiltonian complex for their model
  - Complex Langevin used to study the model

Fredrickson, Ganesan, & Drolet,
Macromolecules, *35*, 2002.

Some of our recent results

F. Attanasio, **B. Jäger** and F. Ziegler

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Lattice Setup

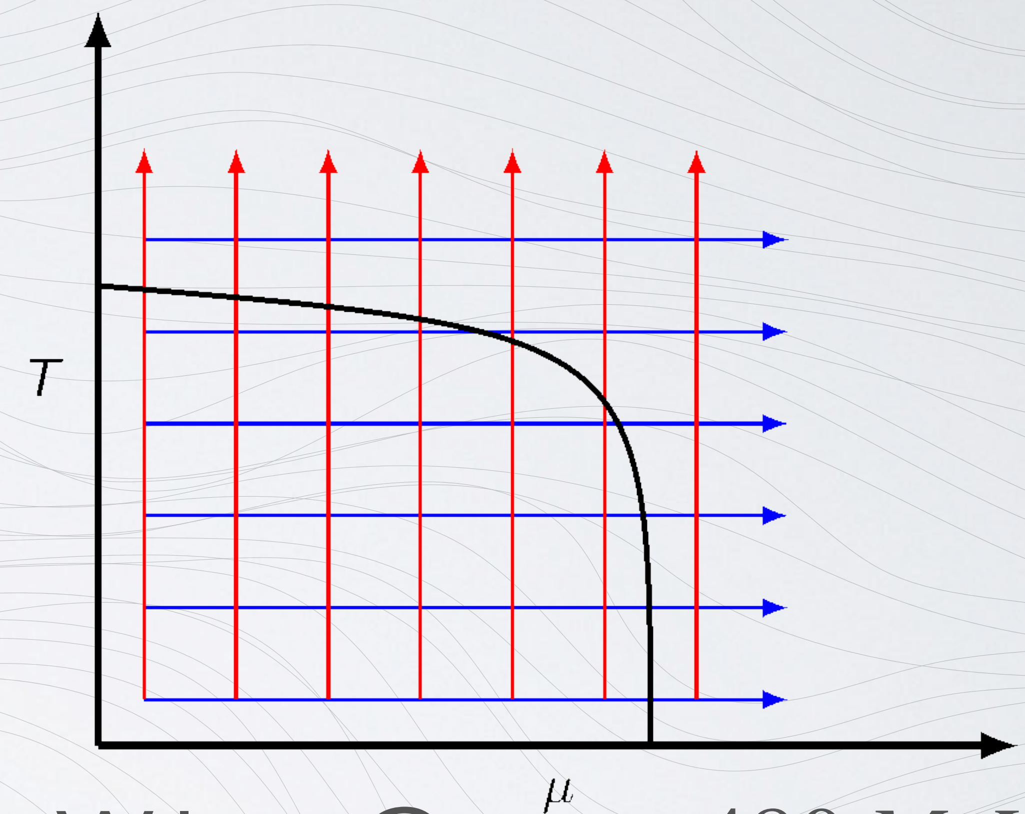
- **Lattice setup**
  - Wilson plaquette action $\beta = 5.8 \leftrightarrow a = 0.06\, fm$
  - Two-flavour dynamical fermions Wilson Fermions $(c_{sw} = 0)$
  - Pion mass $\kappa = 0.1544 \leftrightarrow m_\pi \sim 480\, MeV, m_N = 1.3\, GeV$
  - Volume $V = 24^3 \leftrightarrow m_\pi L = 3.5$

parameters based on
hep-lat:0512021

- **Phase diagram scan**
  - Temperature $N_\tau = 4 - 128 \leftrightarrow 25 - 800\, MeV$
  - Chemical potential $a\mu = 0 - 2 \leftrightarrow \mu = 0 - 6500\, MeV$
  - Gauge Cooling, Adaptive Stepsize & Dynamic Stabilisation

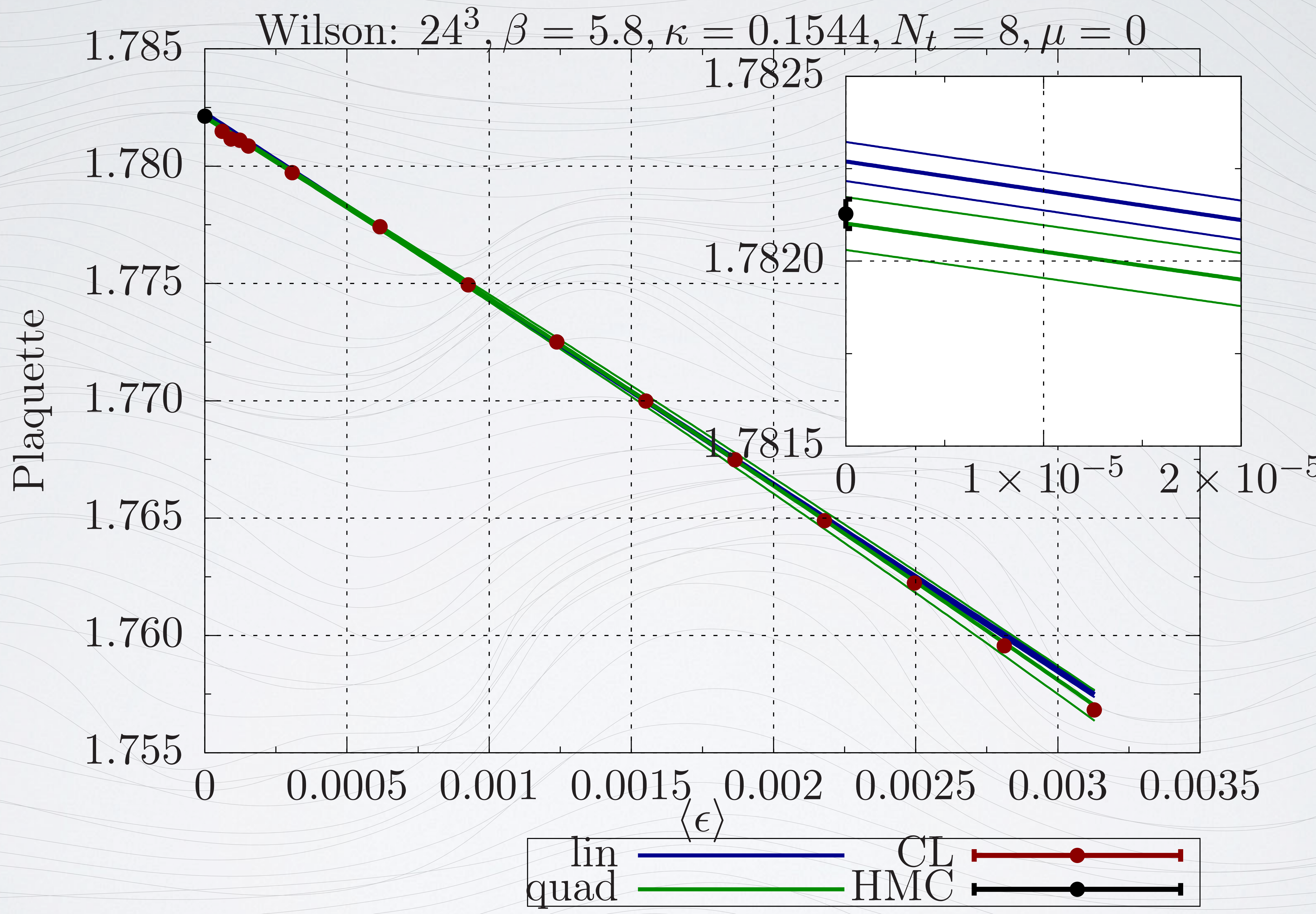
Results

- **Consistency checks @** $\mu = 0$
  - HMC vs. CL
- Histograms
- Observables
  - Fermion density
  - Polyakov loop
- Numerics / Stability
  - Unitarity norm (distance to SU(3))
  - Iterations (Conjugate Gradient)
- Equation of state



Wilson @ $m_\pi \sim 480\, MeV$

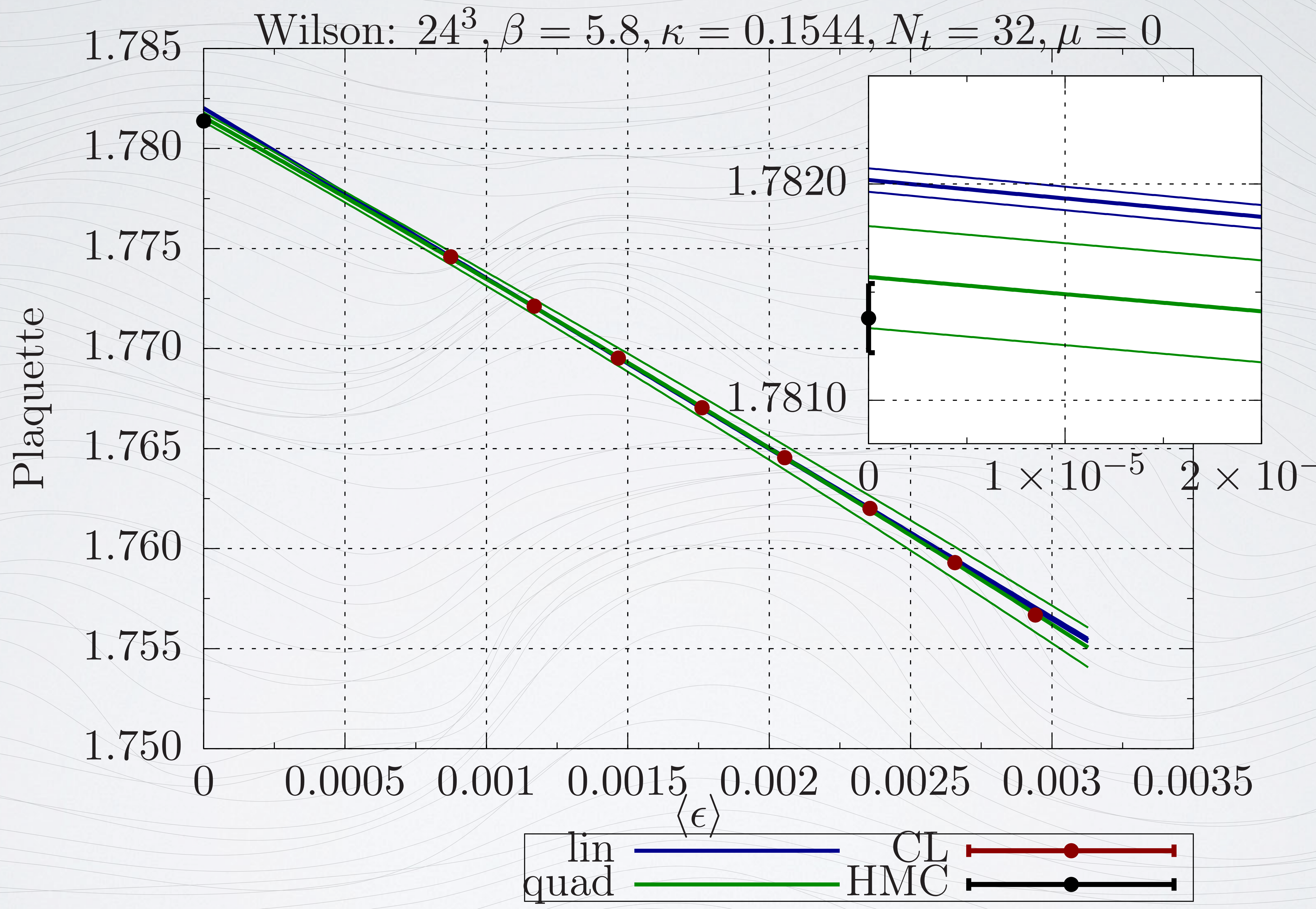
HMC vs CL - deconfined phase



@ $\mu = 0$

$N_t = 8 \leftrightarrow T = 400\ MeV$

HMC vs CL - confined phase



@ $\mu = 0$

$N_t = 32 \leftrightarrow T = 100\ MeV$

Results

- Consistency checks @ $\mu = 0$
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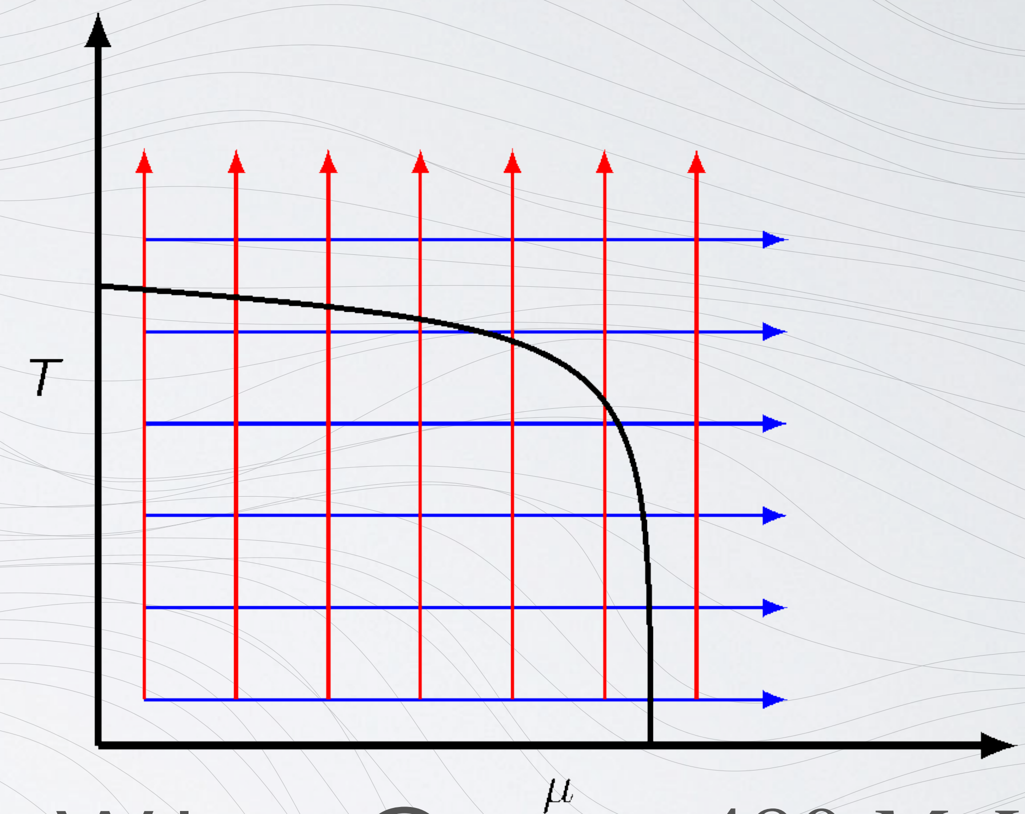
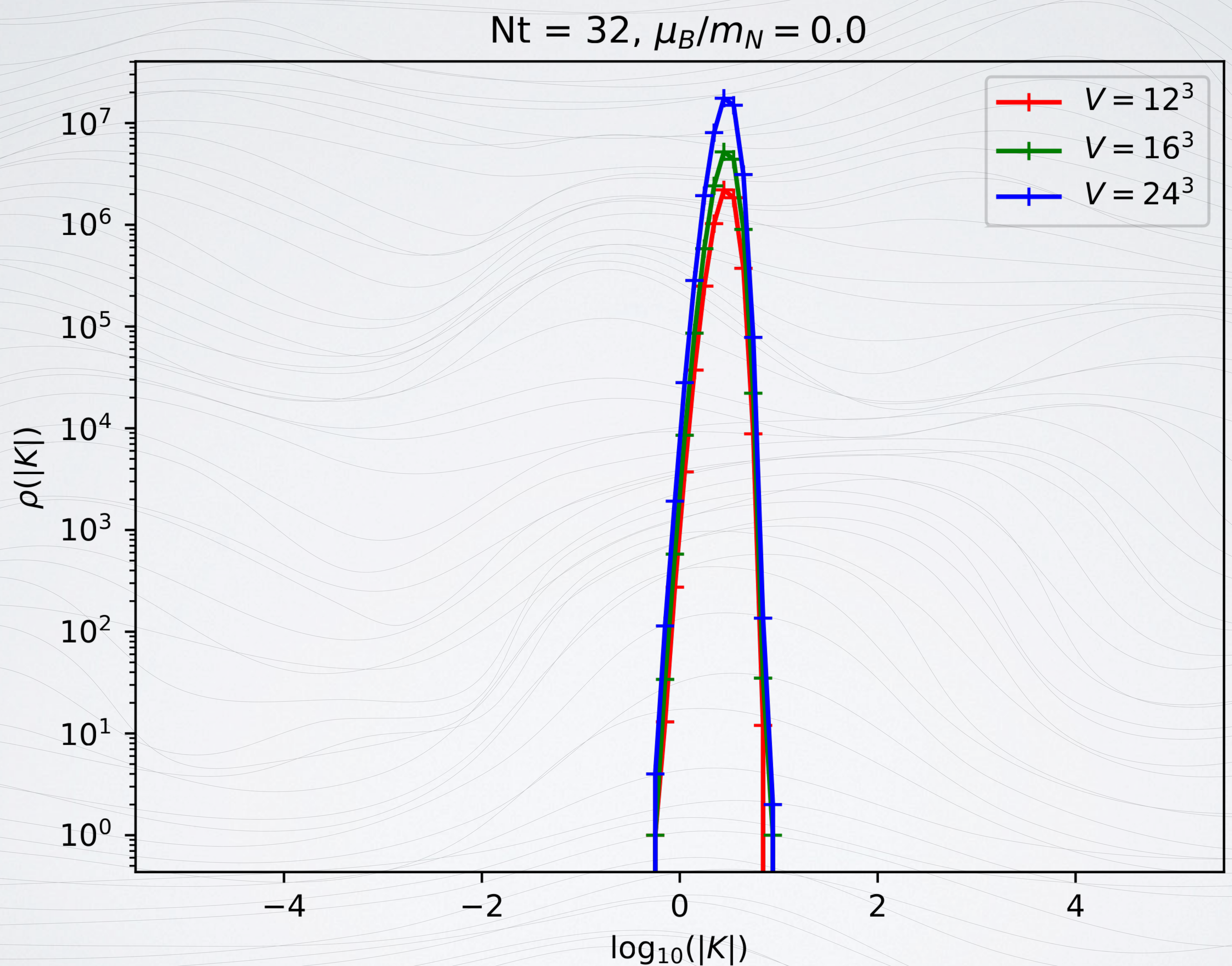
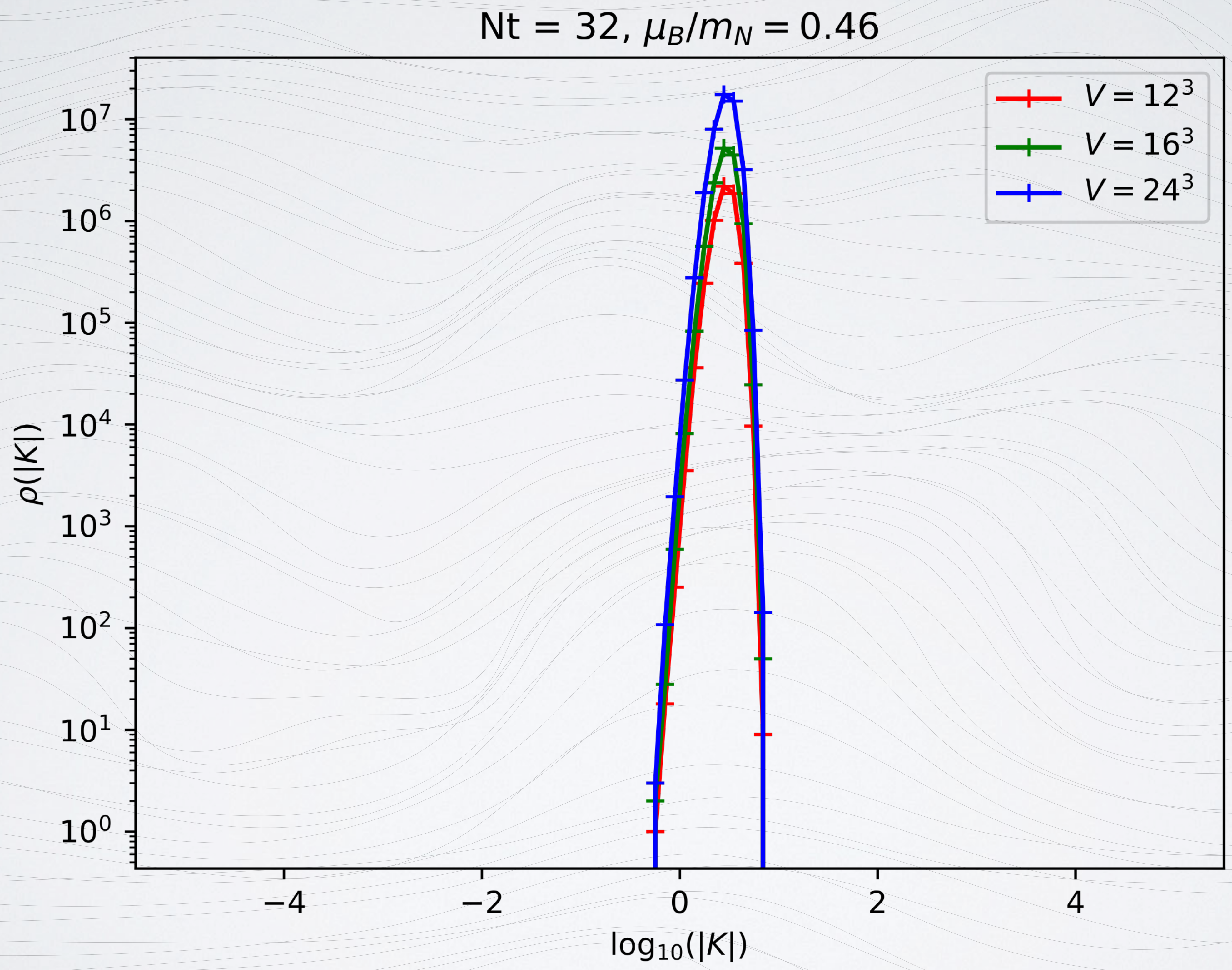


Wilson @ $m_\pi \sim 480\,MeV$

Histograms

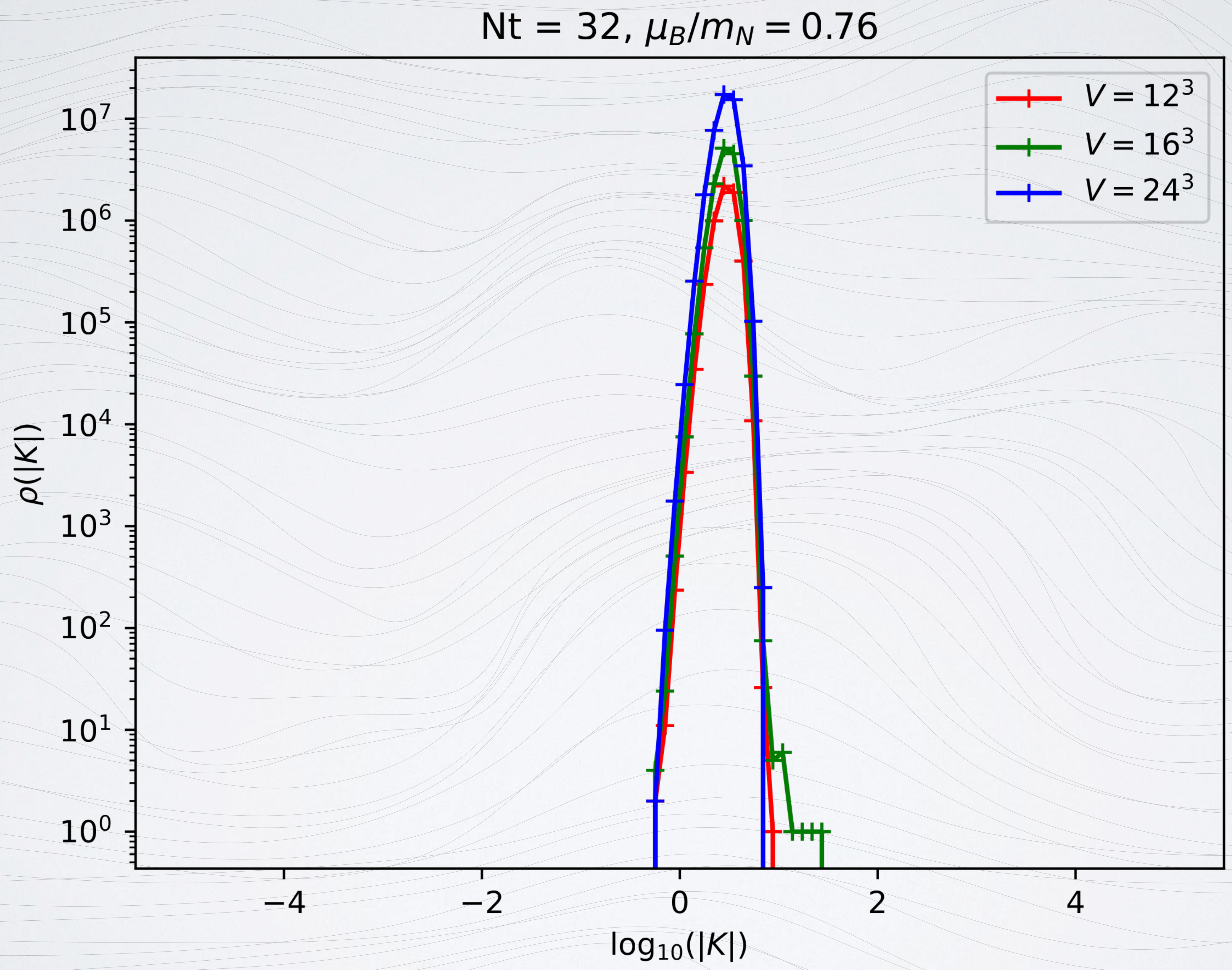

Nt = 32, $\mu_B/m_N = 0.0$
$V = 12^3$
$V = 16^3$
$V = 24^3$
$\rho(|K|)$
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7
−4
−2
0
2
4
$\log_{10}(|K|)$

Histograms



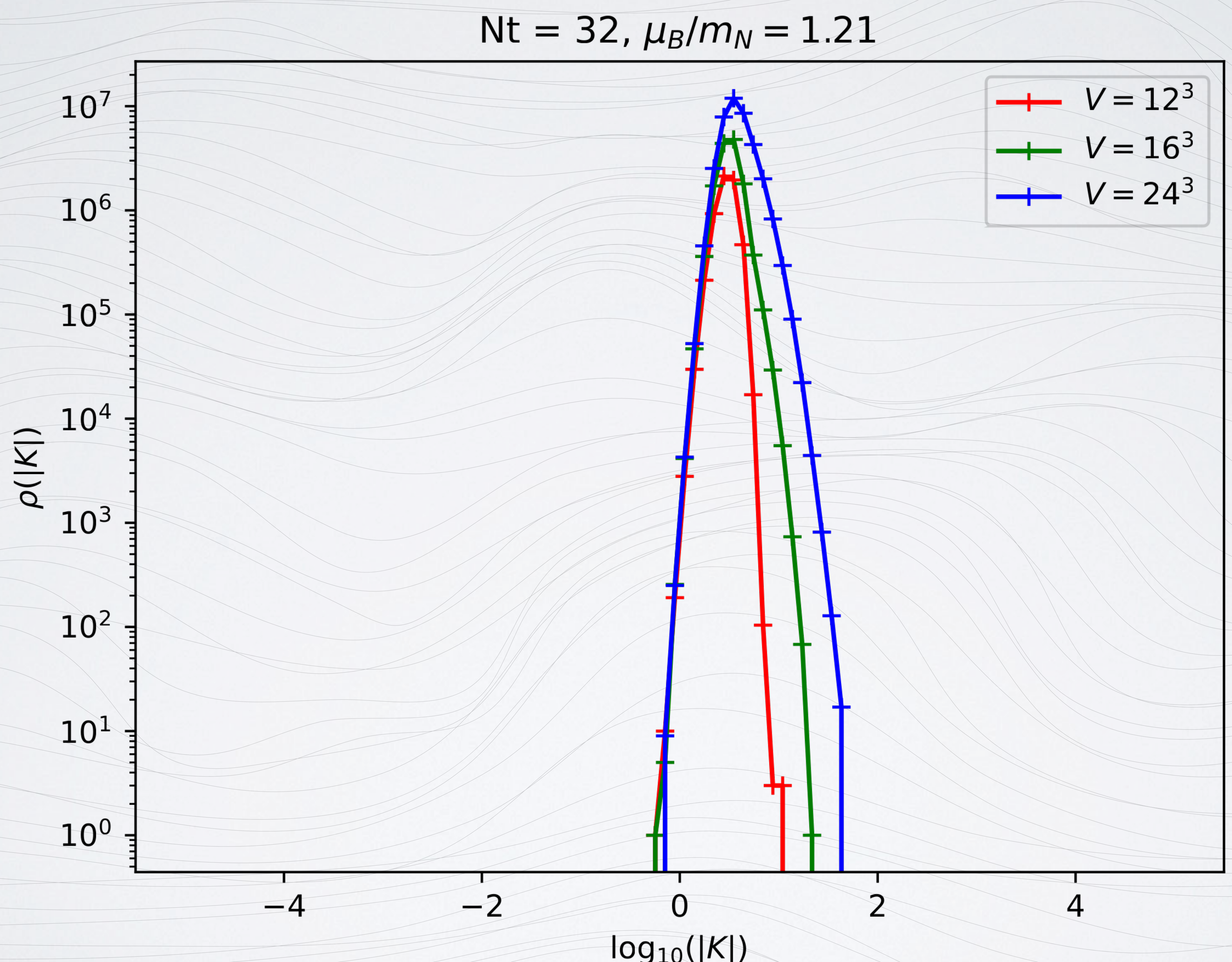
Nt = 32, $\mu_B/m_N = 0.46$
$V = 12^3$
$V = 16^3$
$V = 24^3$
10^7
10^6
10^5
10^4
10^3
10^2
10^1
10^0
$\rho(|K|)$
−4
−2
0
2
4
$\log_{10}(|K|)$

Histograms



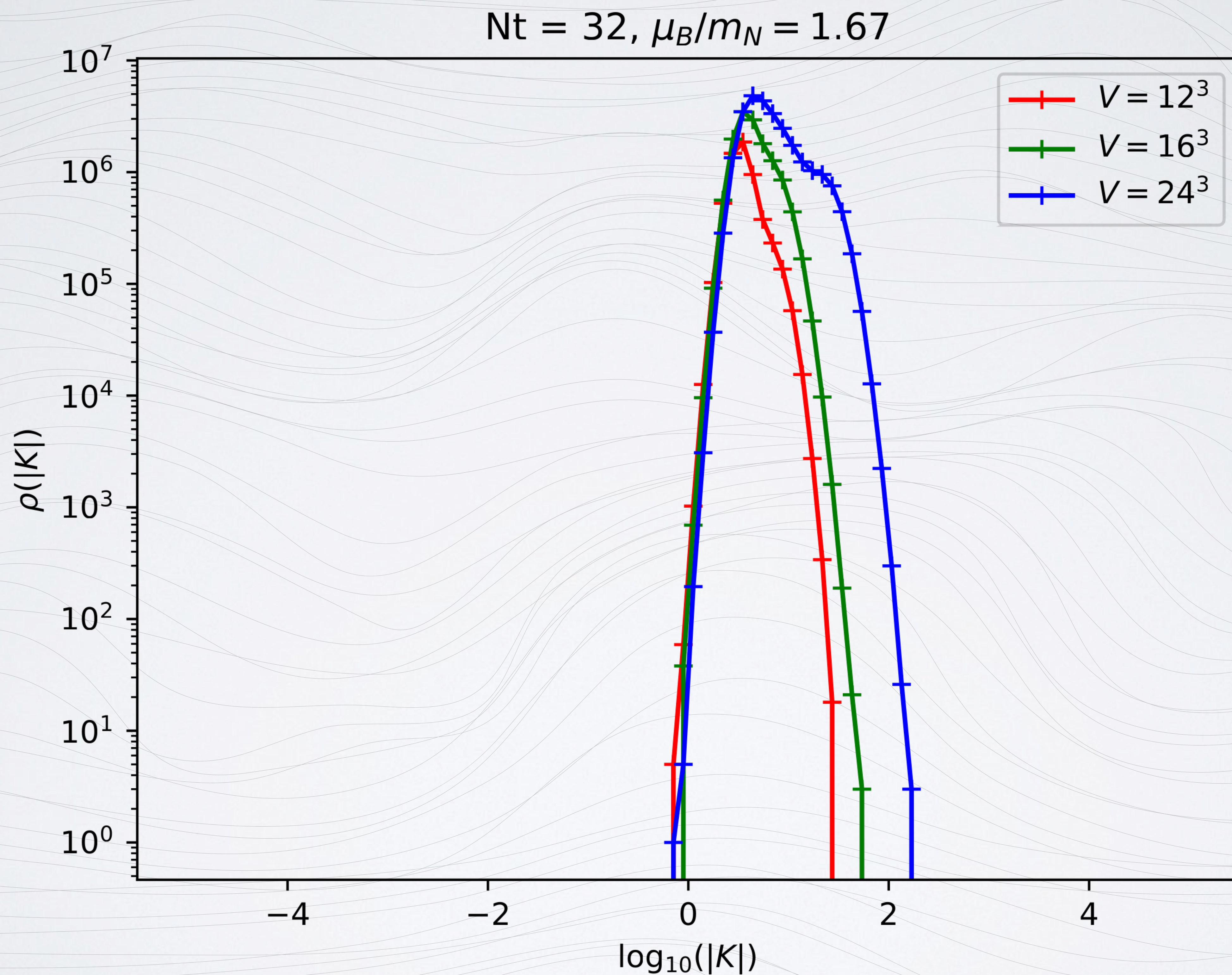
Nt = 32, $\mu_B/m_N = 0.76$
$V = 12^3$
$V = 16^3$
$V = 24^3$
10^7
10^6
10^5
10^4
10^3
10^2
10^1
10^0
$\rho(|K|)$
−4
−2
0
2
4
$\log_{10}(|K|)$

Histograms



Nt = 32, $\mu_B/m_N = 1.21$
$V = 12^3$
$V = 16^3$
$V = 24^3$
$\rho(|K|)$
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7
−4
−2
0
2
4
$\log_{10}(|K|)$

Histograms



Nt = 32, $\mu_B/m_N = 1.67$
$V = 12^3$
$V = 16^3$
$V = 24^3$
$\rho(|K|)$
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7
−4
−2
0
2
4
$\log_{10}(|K|)$

Results

- Consistency checks @ $\mu = 0$
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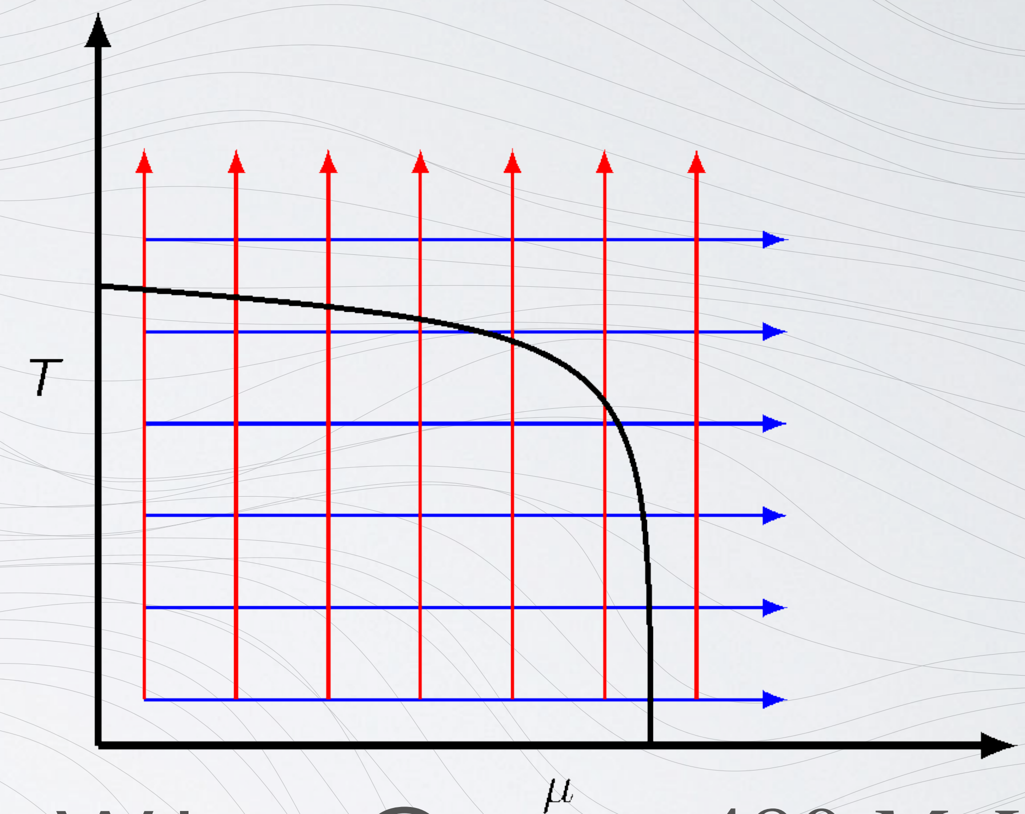
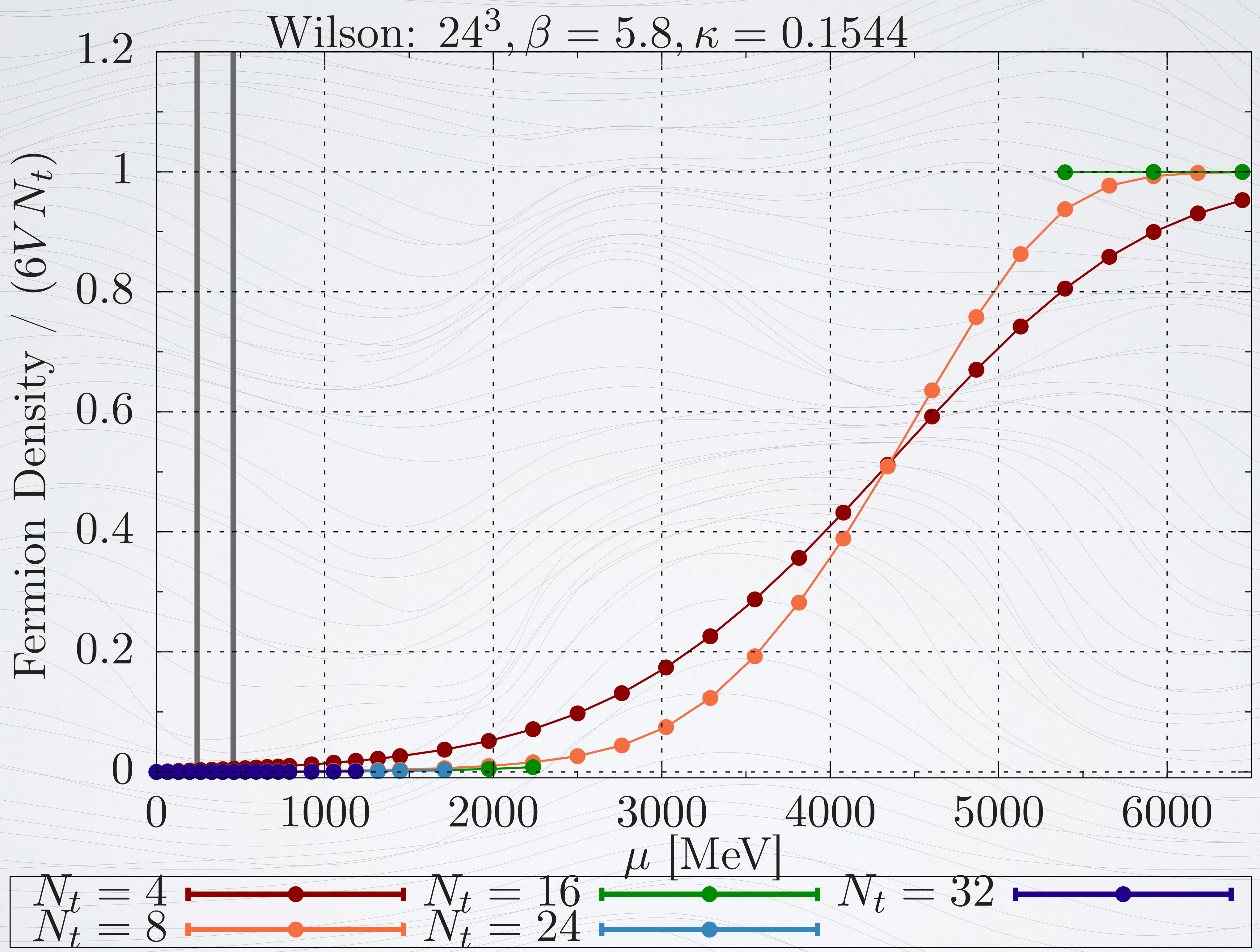
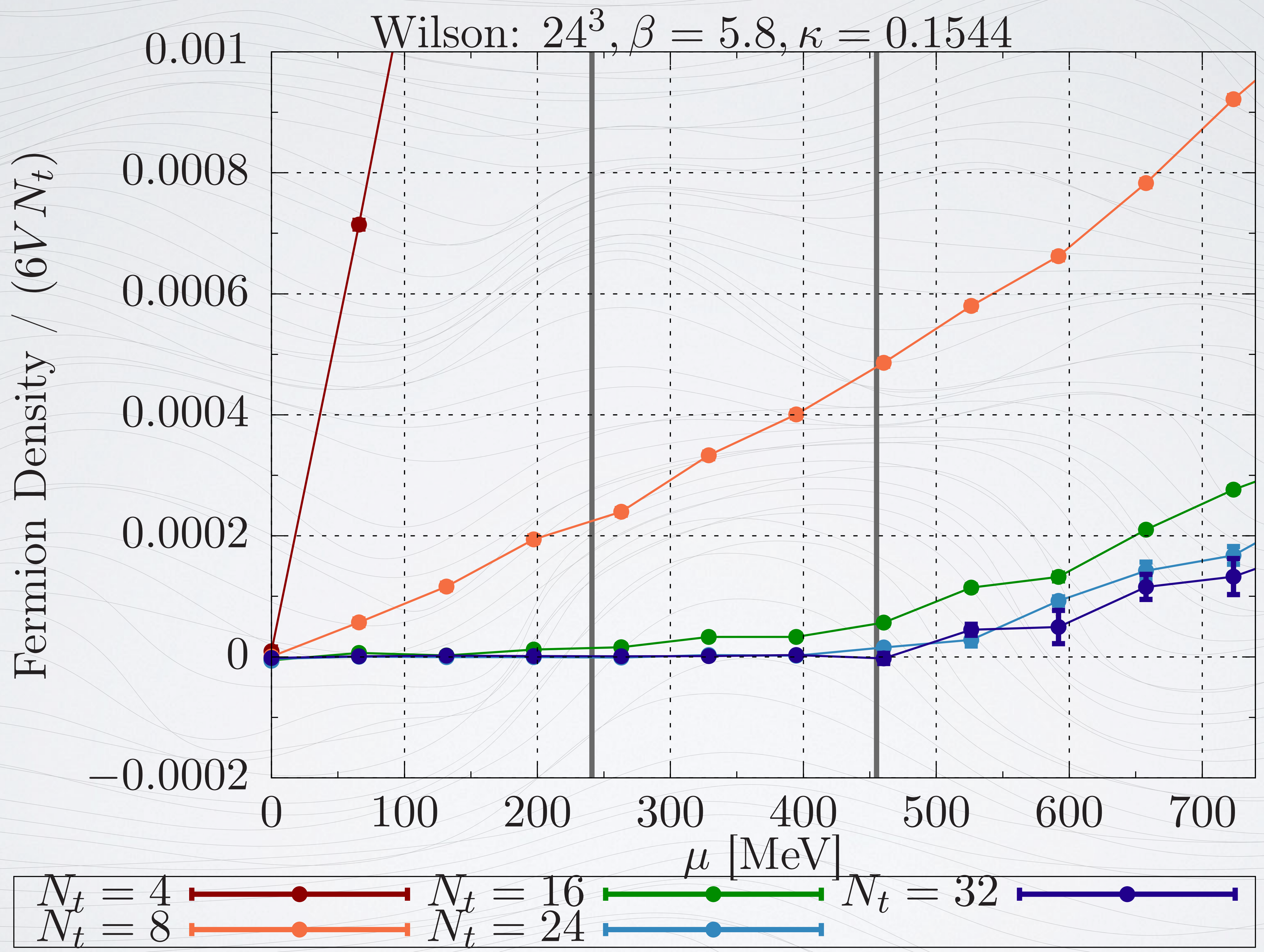


Wilson @ $m_\pi \sim 480\,MeV$

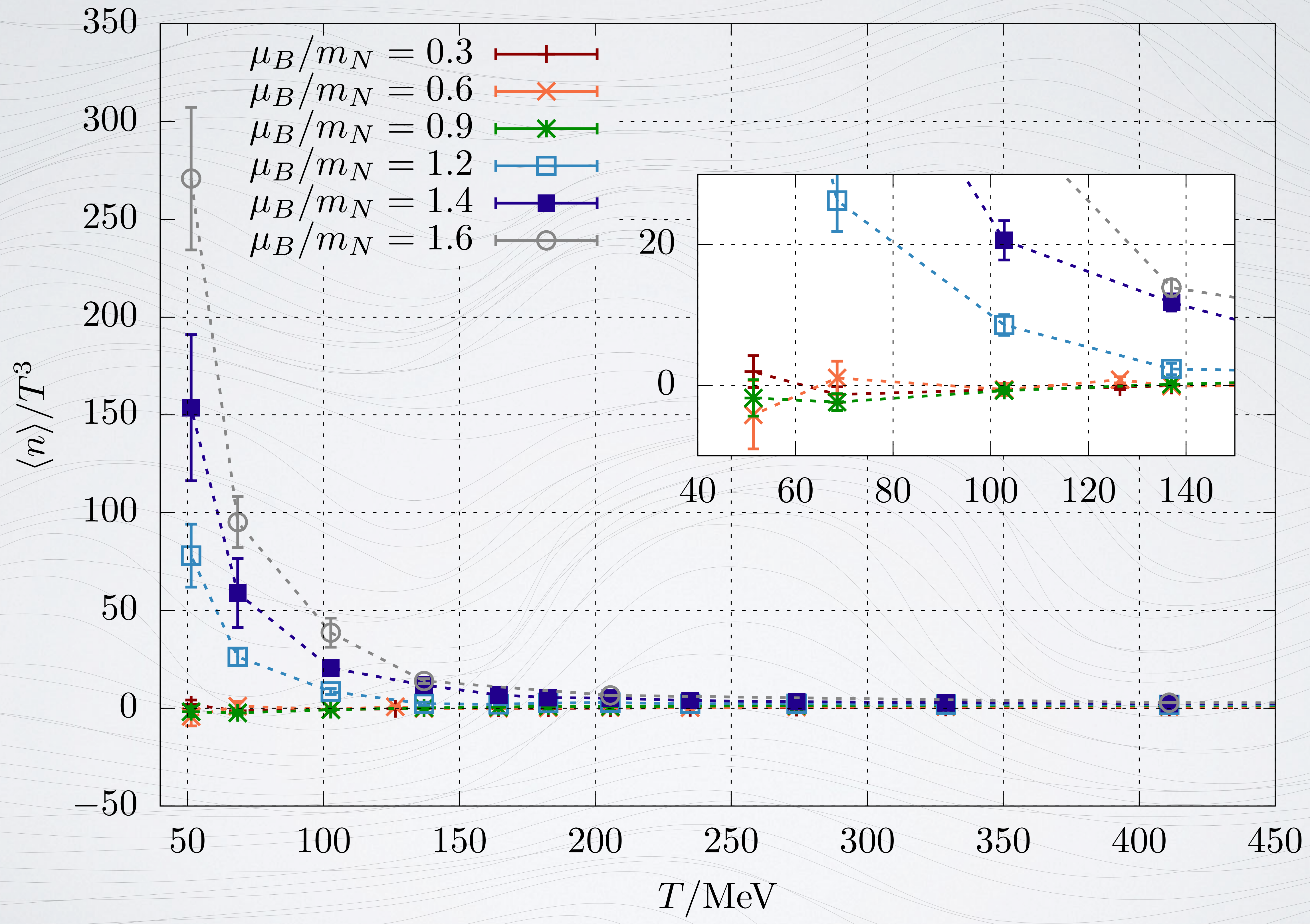
Fermion Density



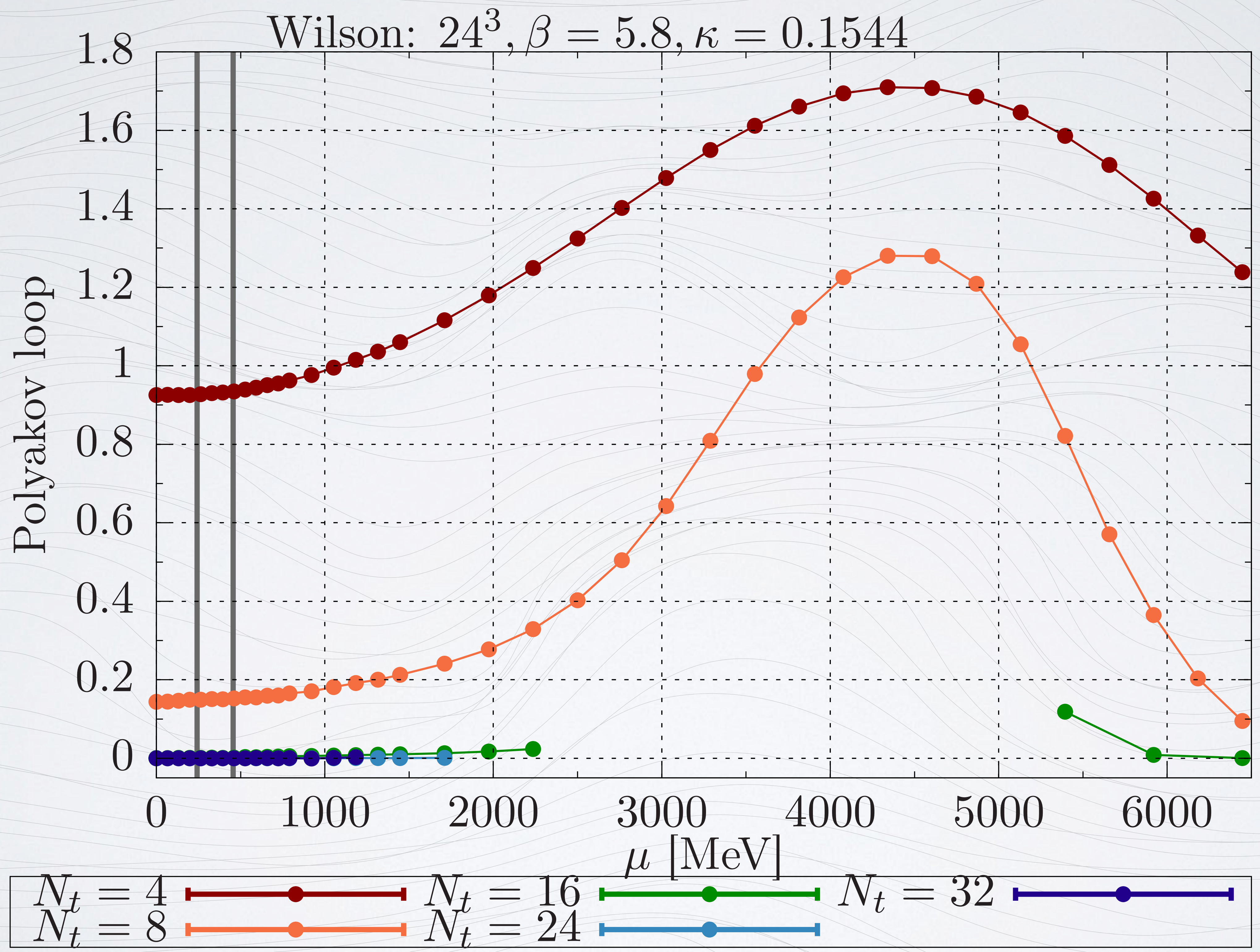
Fermion Density



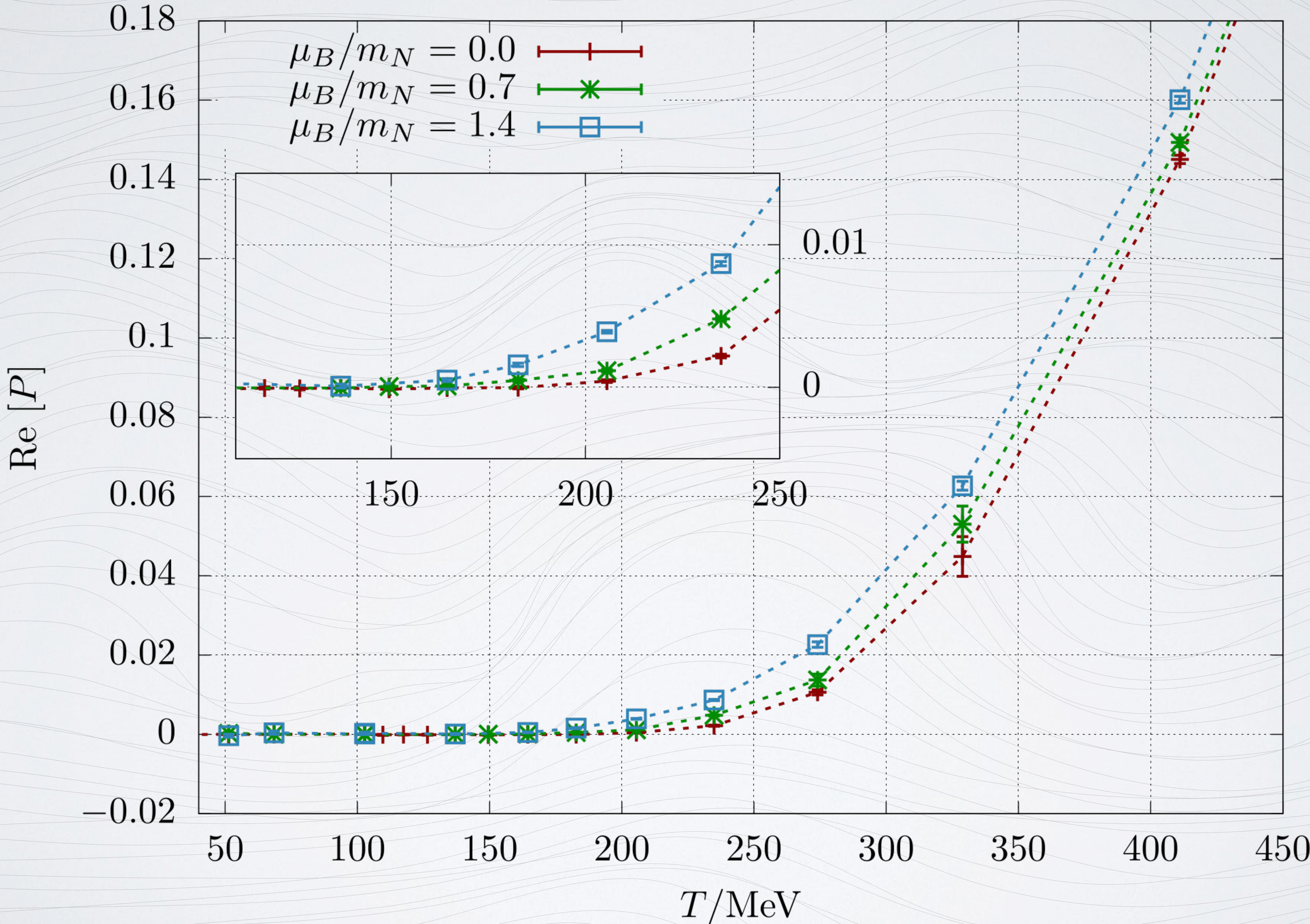
Fermion Density



Polyakov Loop

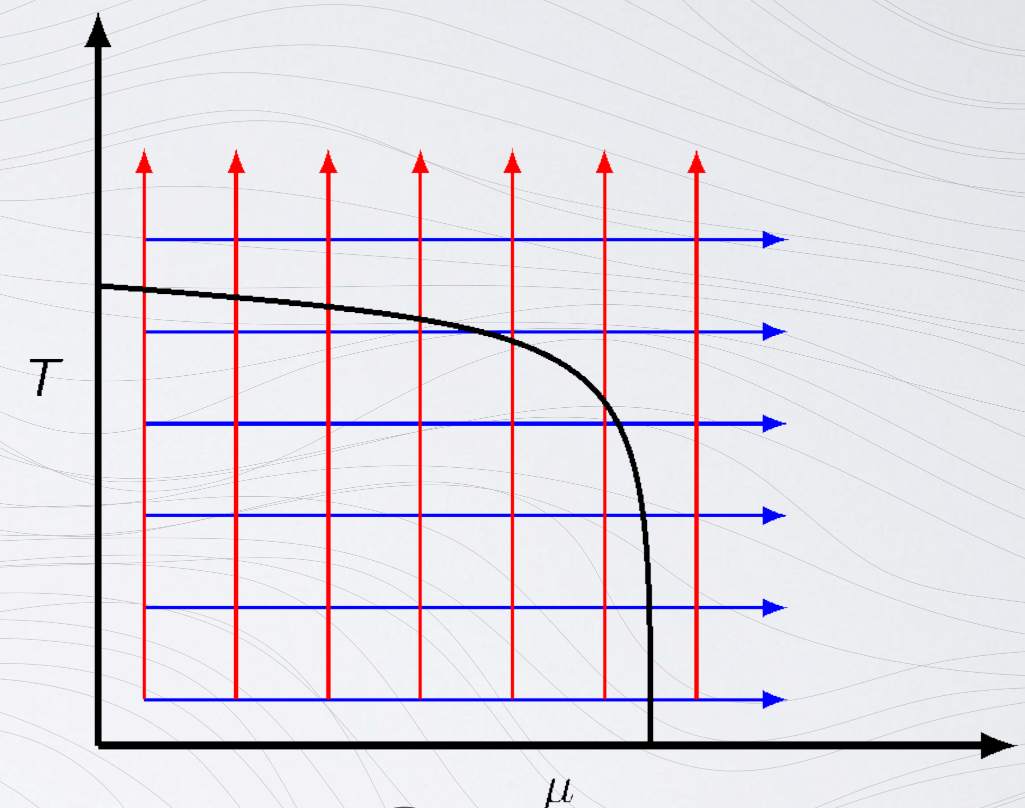


Polyakov Loop



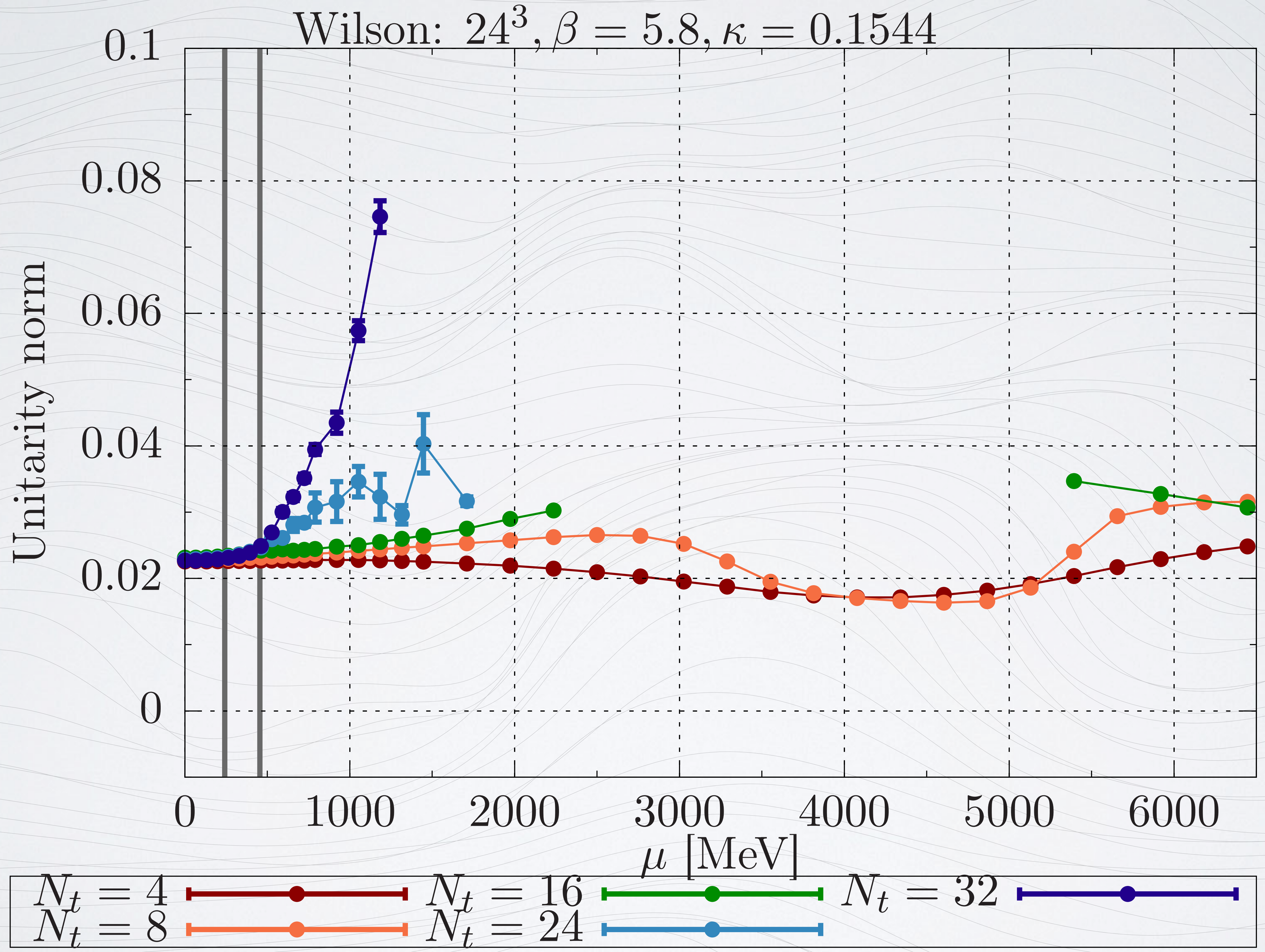
Results

- Consistency checks @ $\mu = 0$
  - HMC vs. CL
- Histograms
- Observables
  - Fermion density
  - Polyakov loop
- **Numerics / Stability**
  - Unitarity norm (distance to SU(3))
  - Iterations (Conjugate Gradient)
- Equation of state

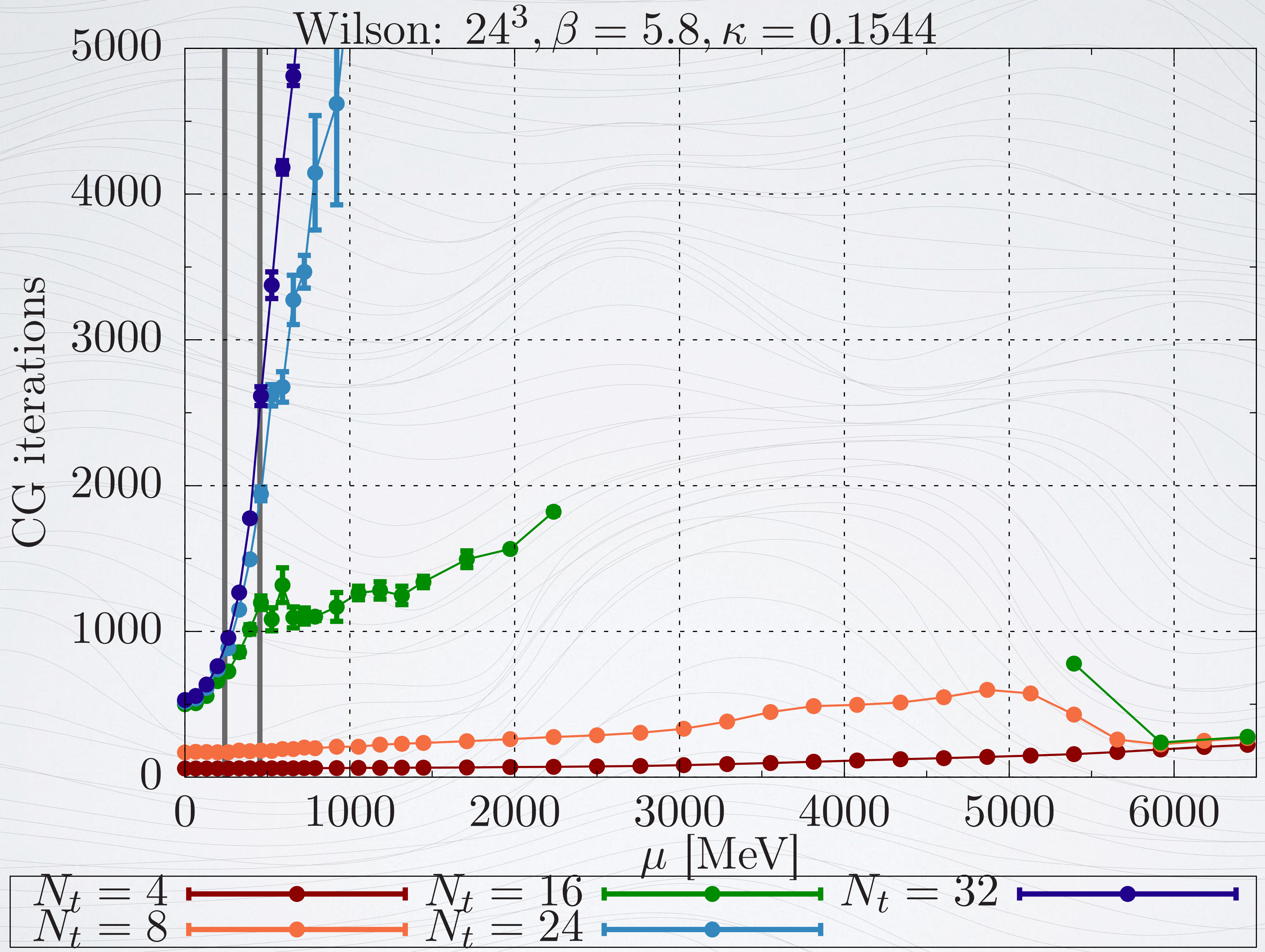


Wilson @ $m_\pi \sim 480\,MeV$

Unitarity Norm

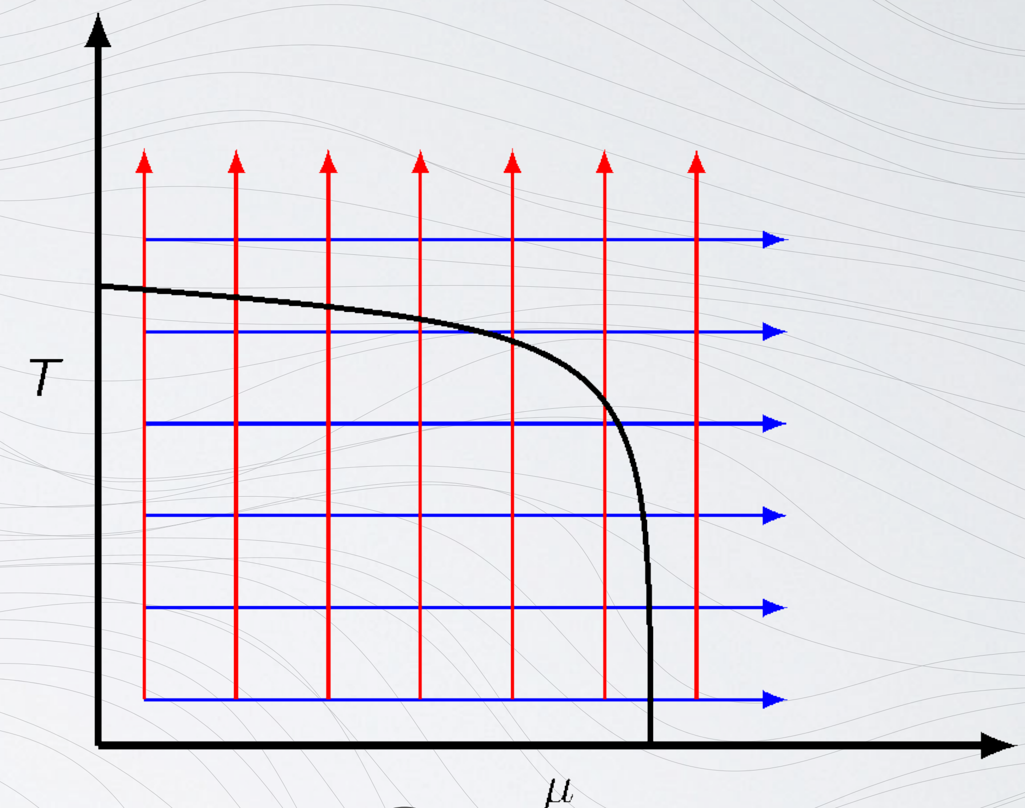


CG Iterations



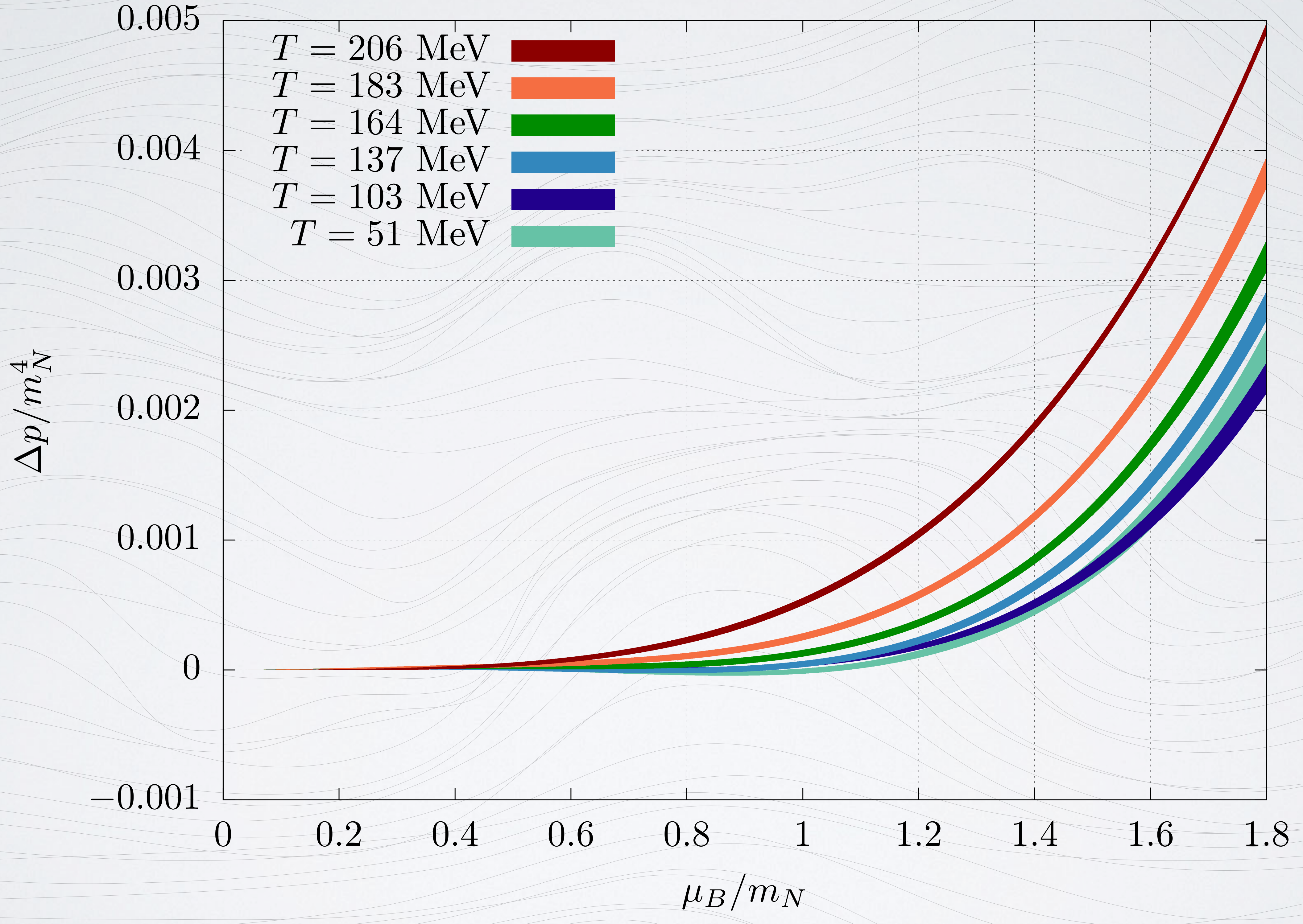
Results

- Consistency checks @ $\mu = 0$
  - HMC vs. CL
- Histograms
- Observables
  - Fermion density
  - Polyakov loop
- Numerics / Stability
  - Unitarity norm (distance to SU(3))
  - Iterations (Conjugate Gradient)
- **Equation of state**

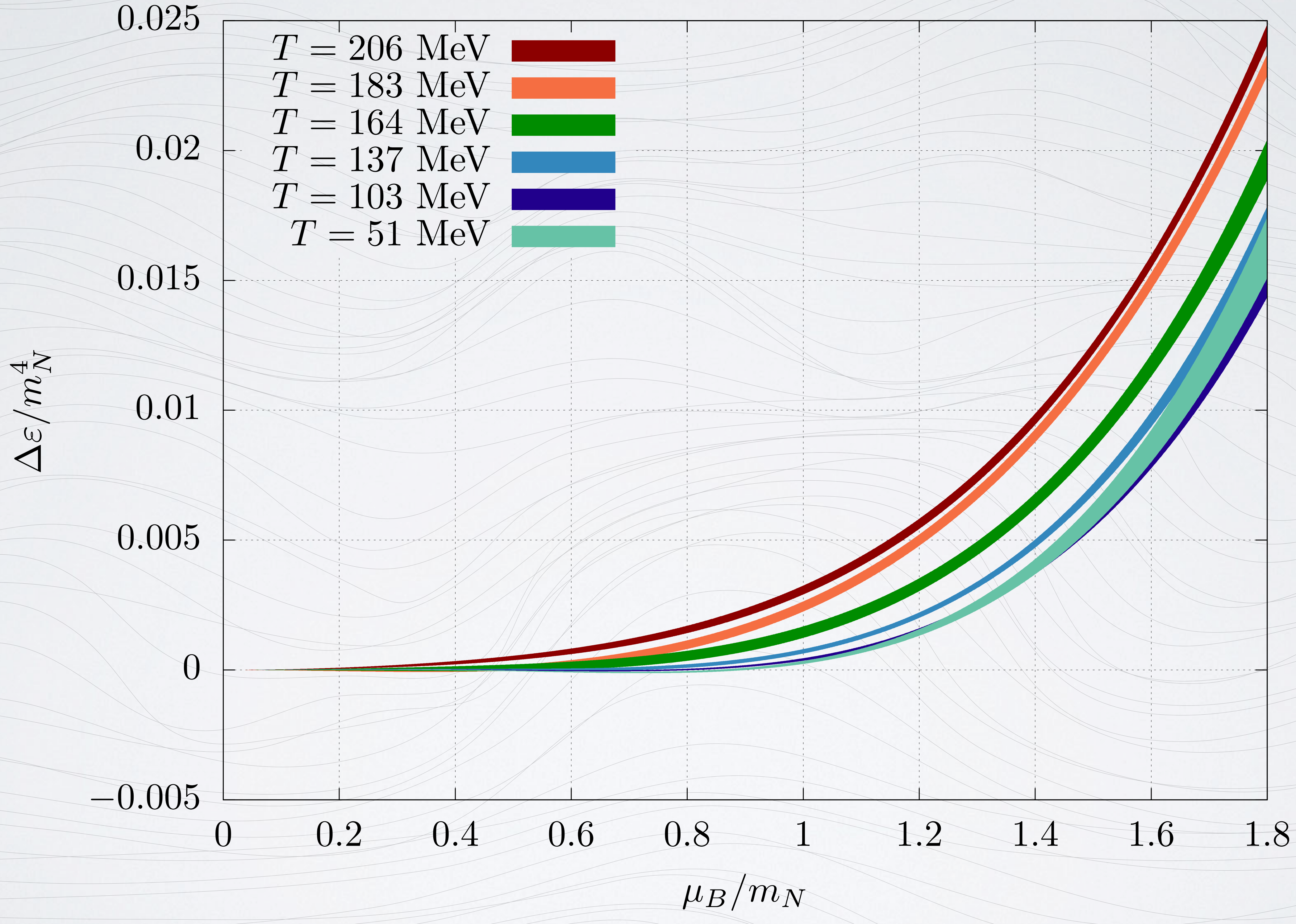


Wilson @ $m_\pi \sim 480\, MeV$

Equation of State - Pressure

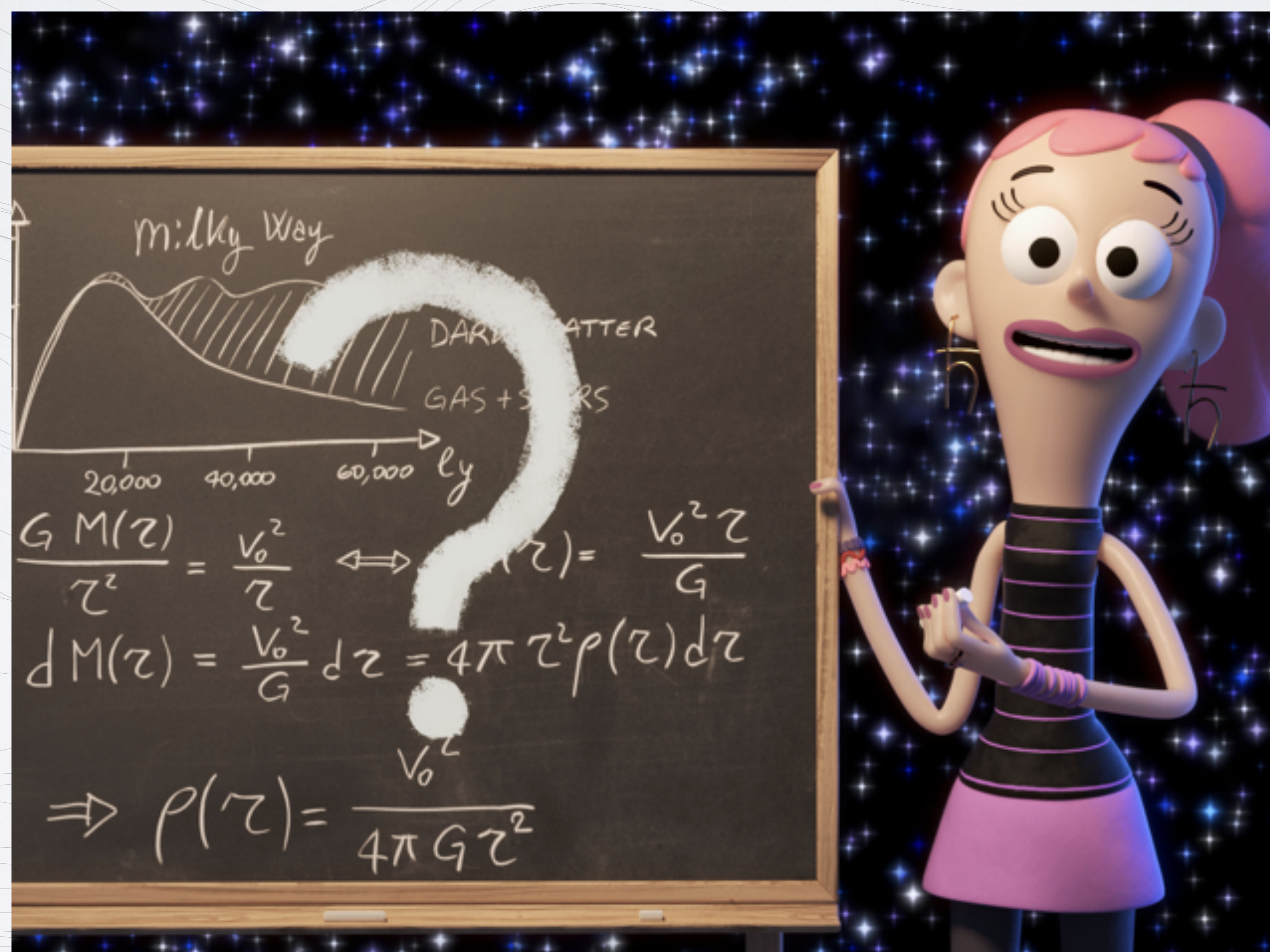


Equation of State - Energy density



Questions?

Thank you for your attention!



Quantum Kate (orig. Kvante Karina): CP3 Outreach http://www.kvantebanditter.dk/en