# QCD under extreme conditions -

## A Lattice View


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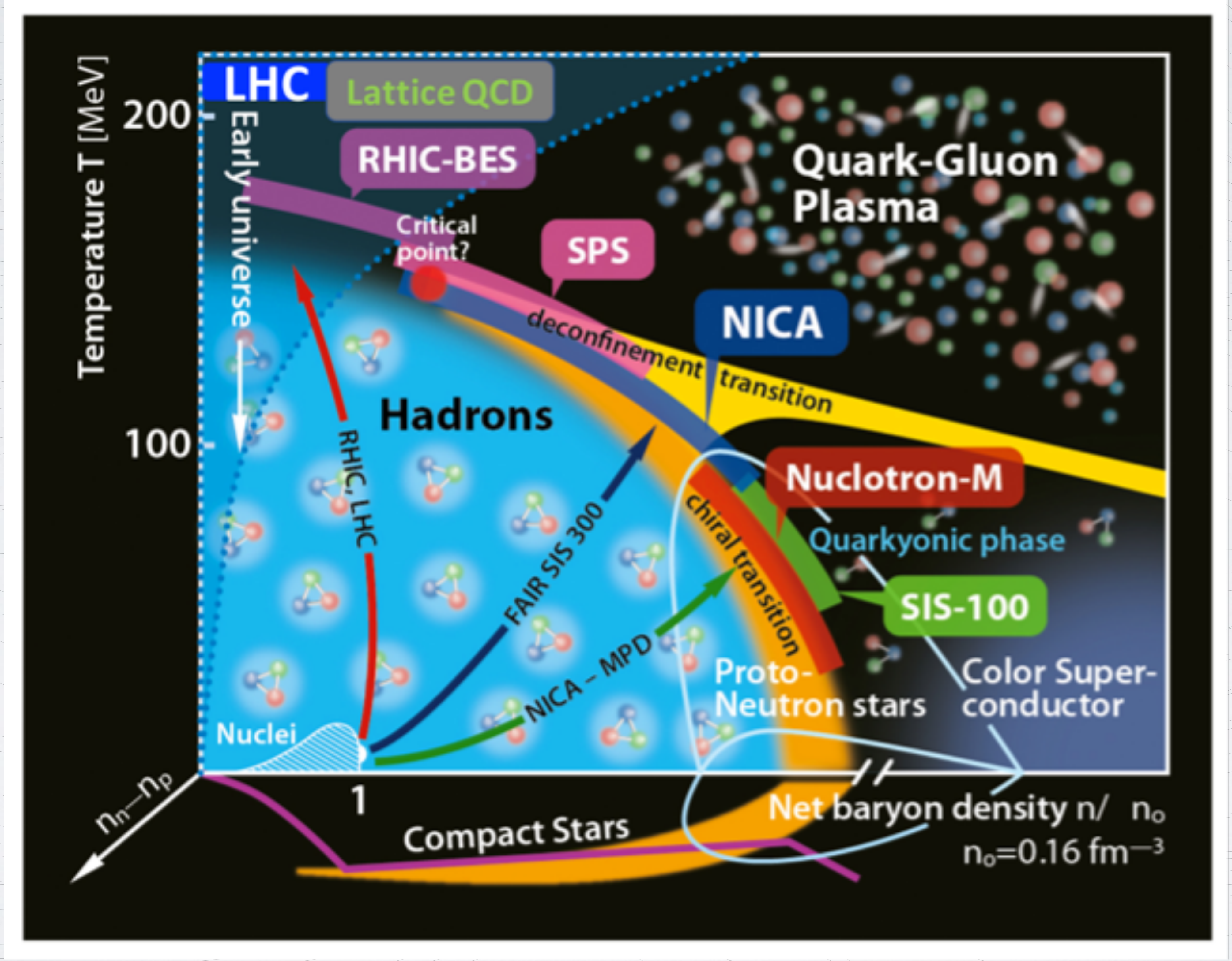
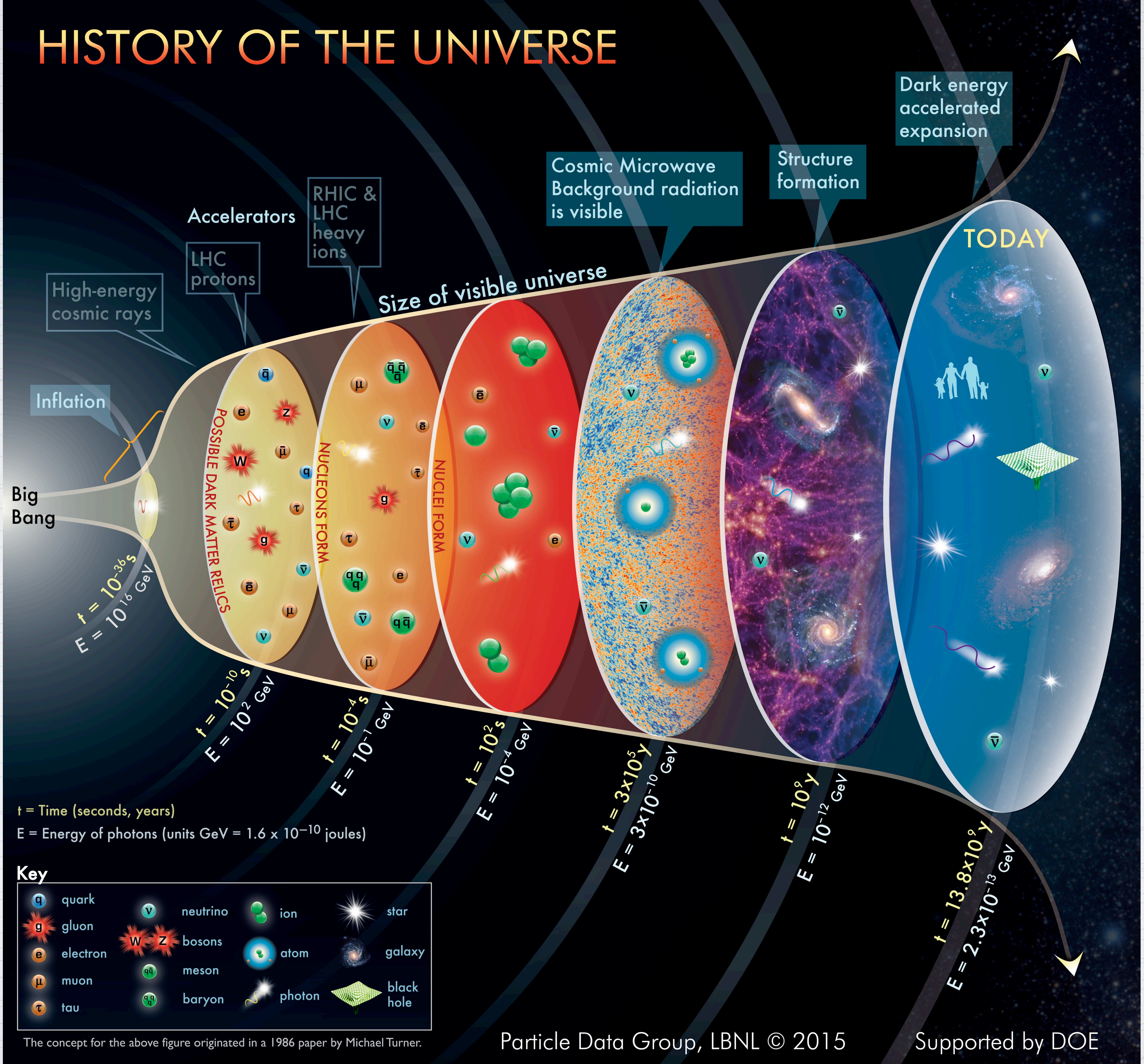
# QCD Phase Diagram

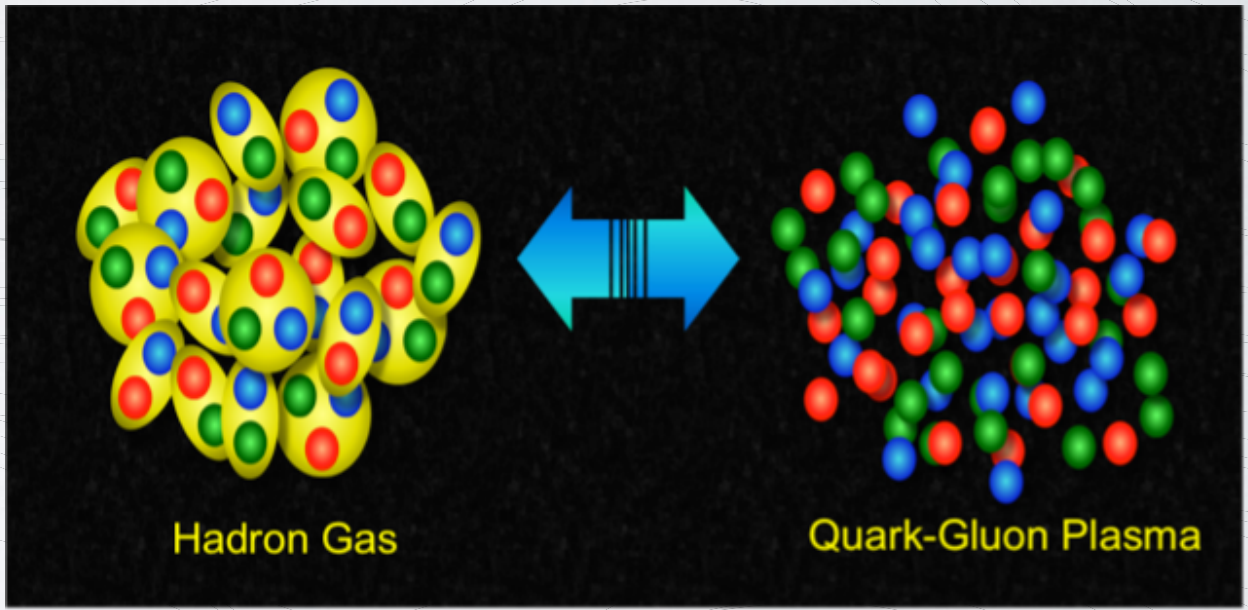


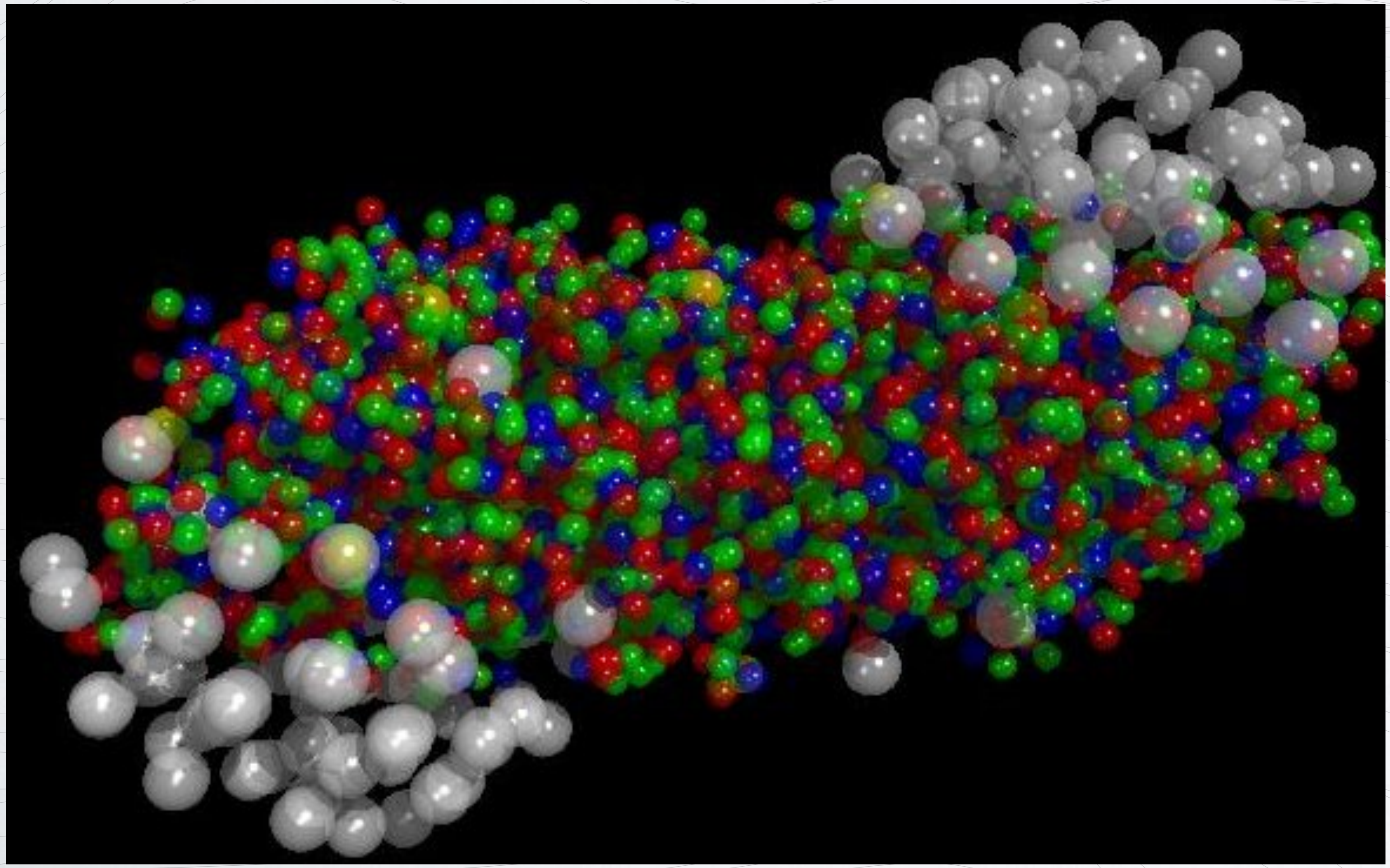


HISTORY OF THE UNIVERSE
Dark energy accelerated expansion
Structure formation
Cosmic Microwave Background radiation is visible
RHIC & LHC heavy ions
Accelerators
LHC protons
High-energy cosmic rays
Inflation
Size of visible universe
TODAY
Big Bang
POSSIBLE DARK MATTER RELICS
NUCLEONS FORM
NUCLEI FORM
$t = 10^{-36}$ 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 Phase Diagram

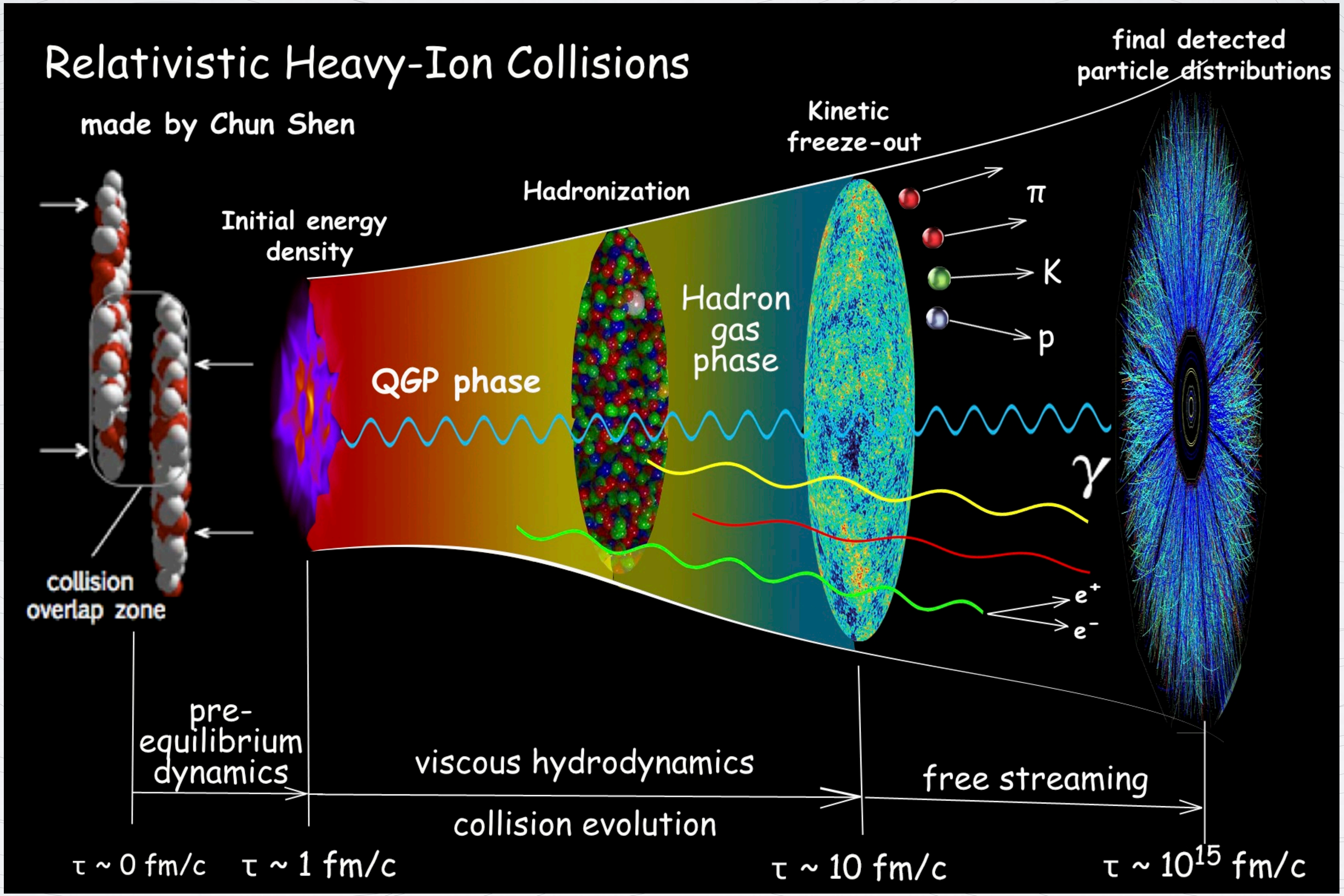
Understand the transition



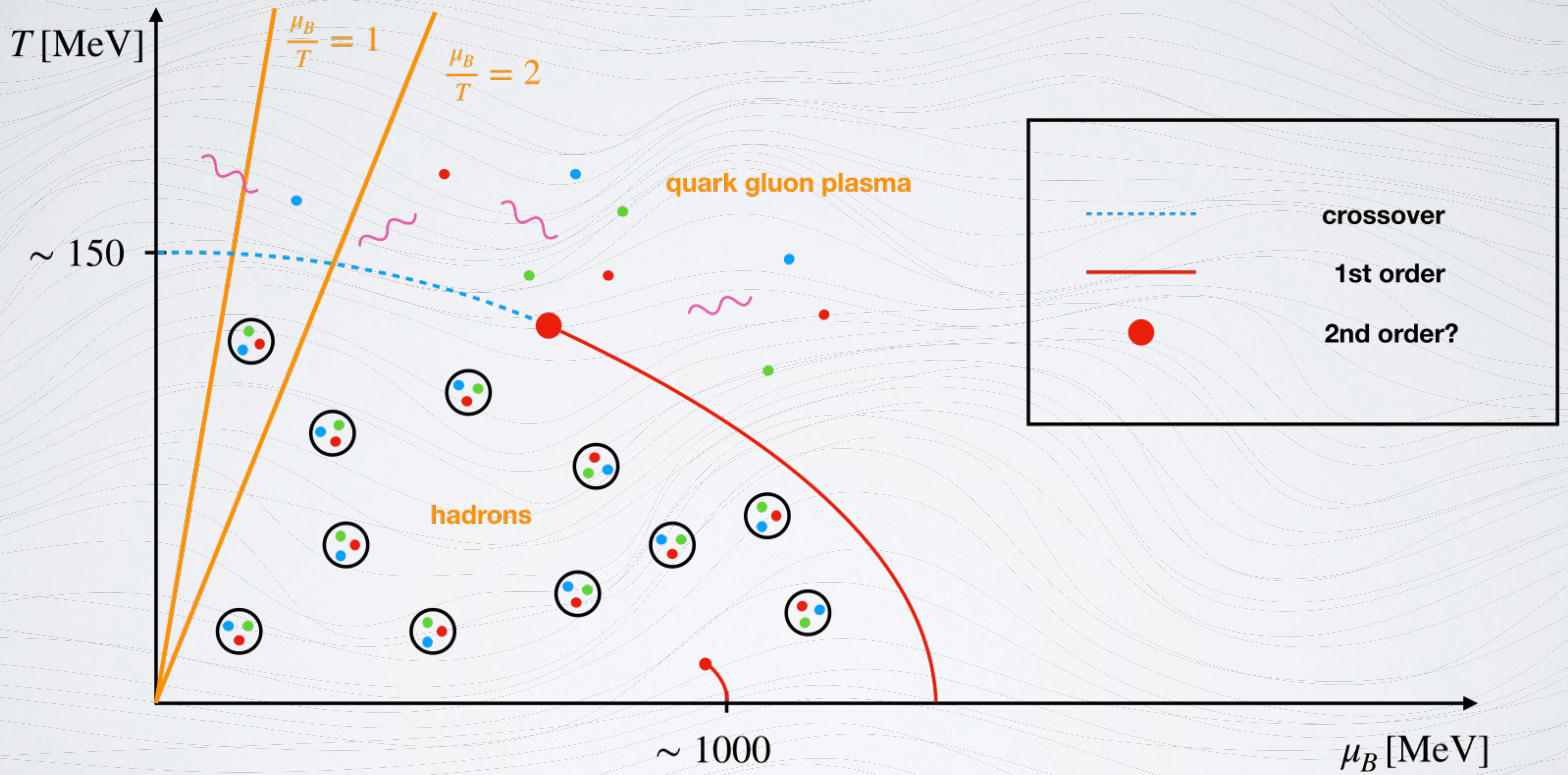



Heavy-Ion
Collision
Experiments

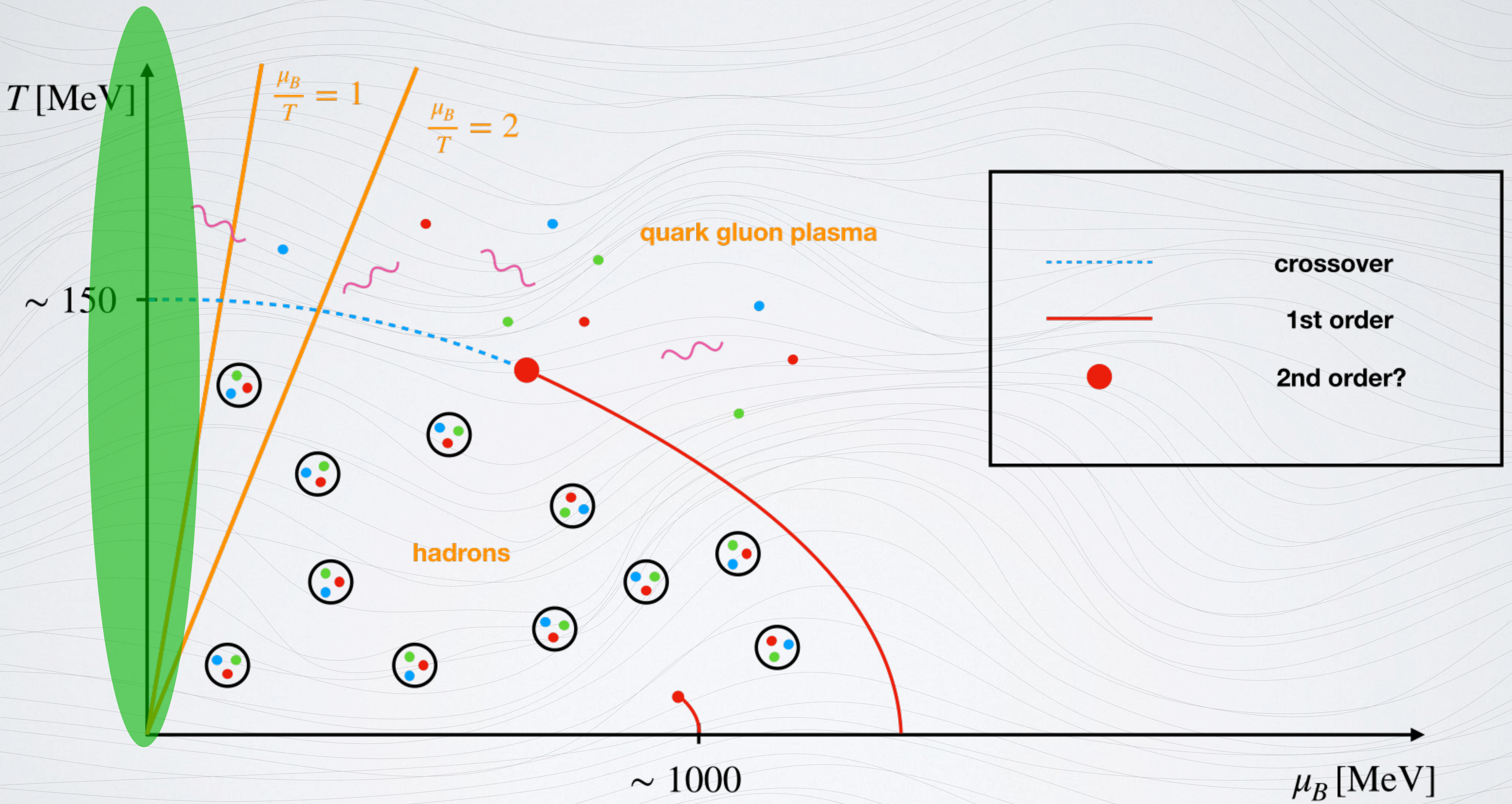
# Heavy-Ion Collision Experiments



# QCD phase diagram

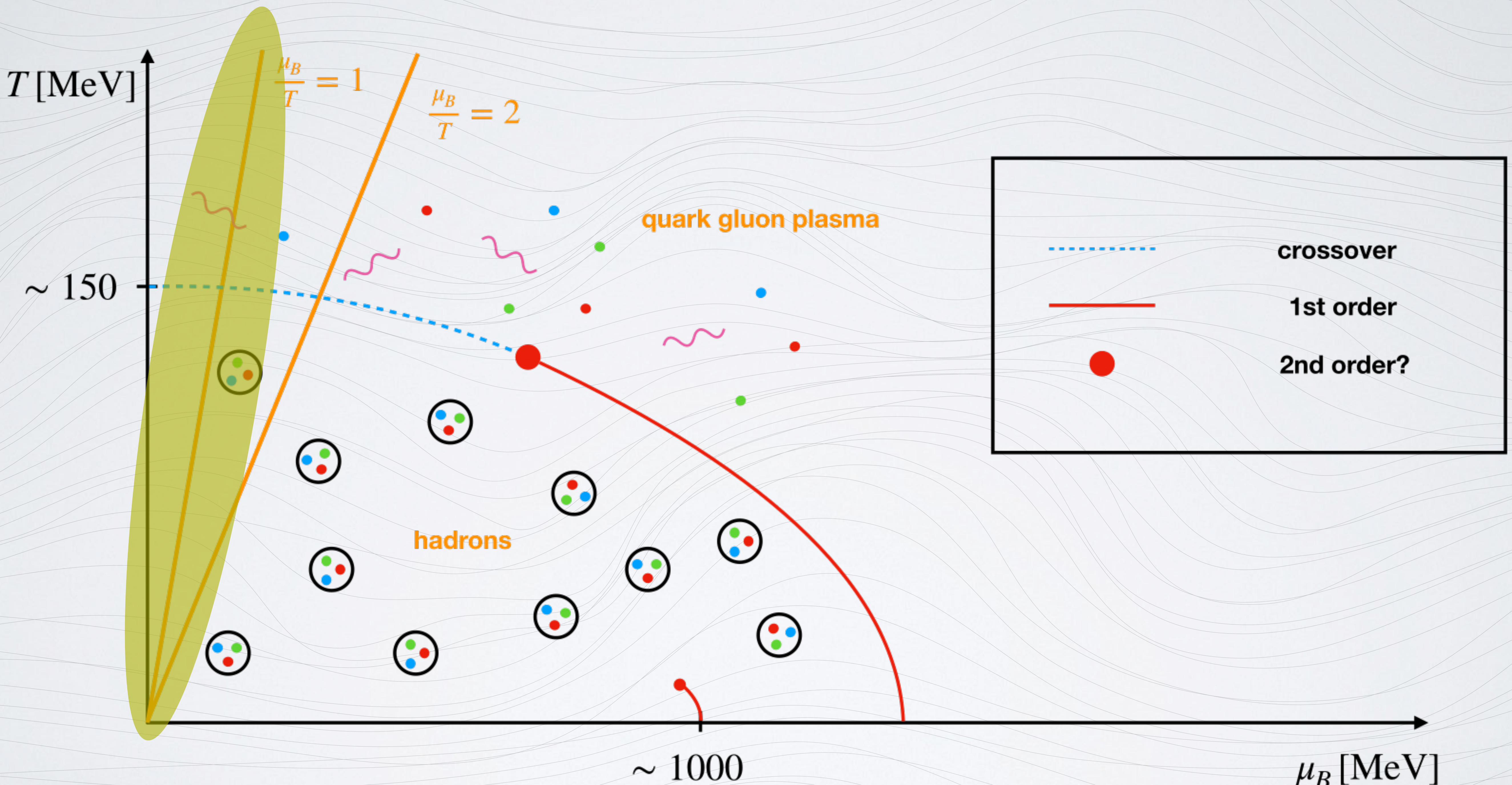


# QCD phase diagram



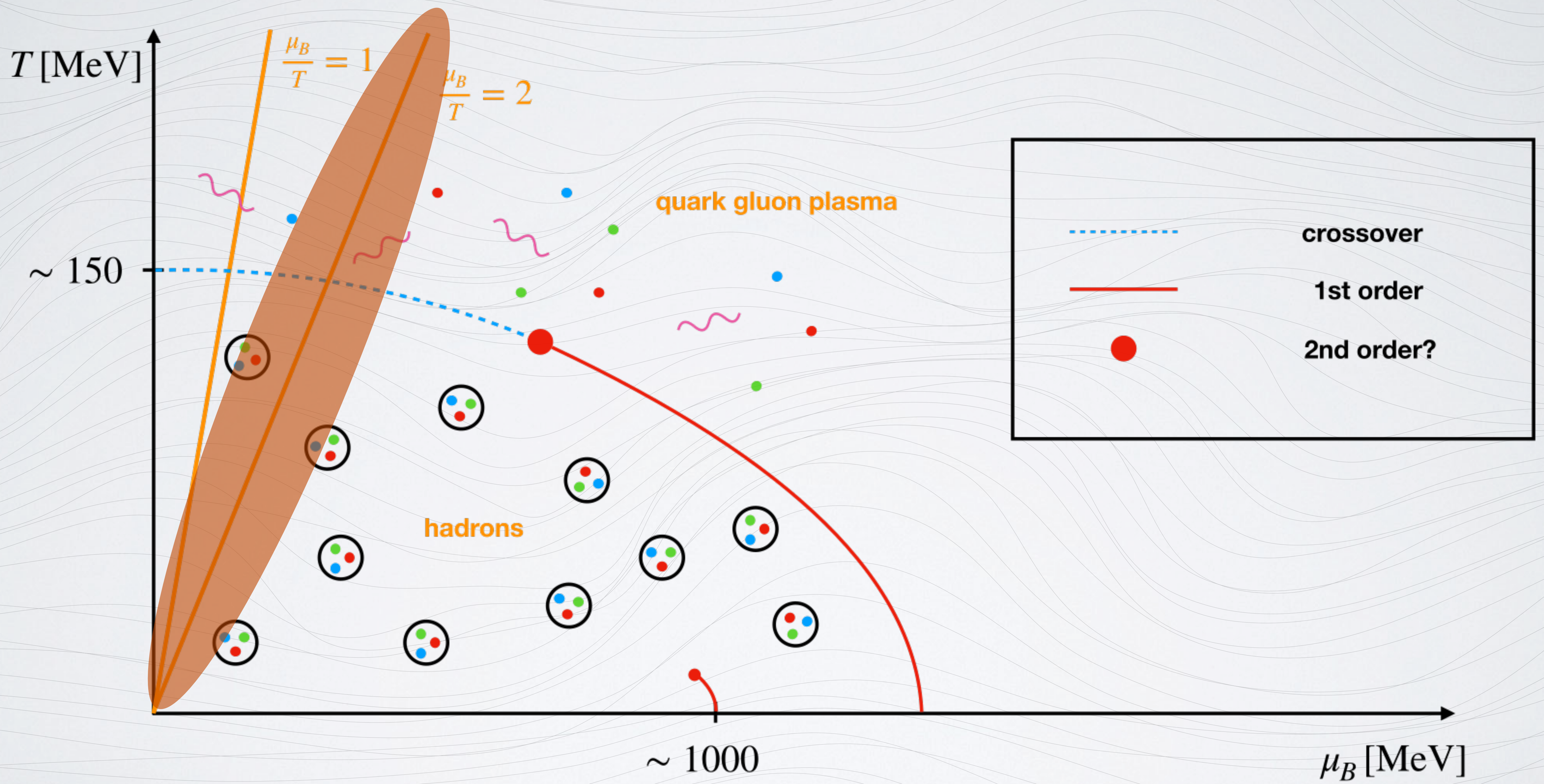

Thermodynamics ($\mu = 0$) - Easy

# QCD phase diagram



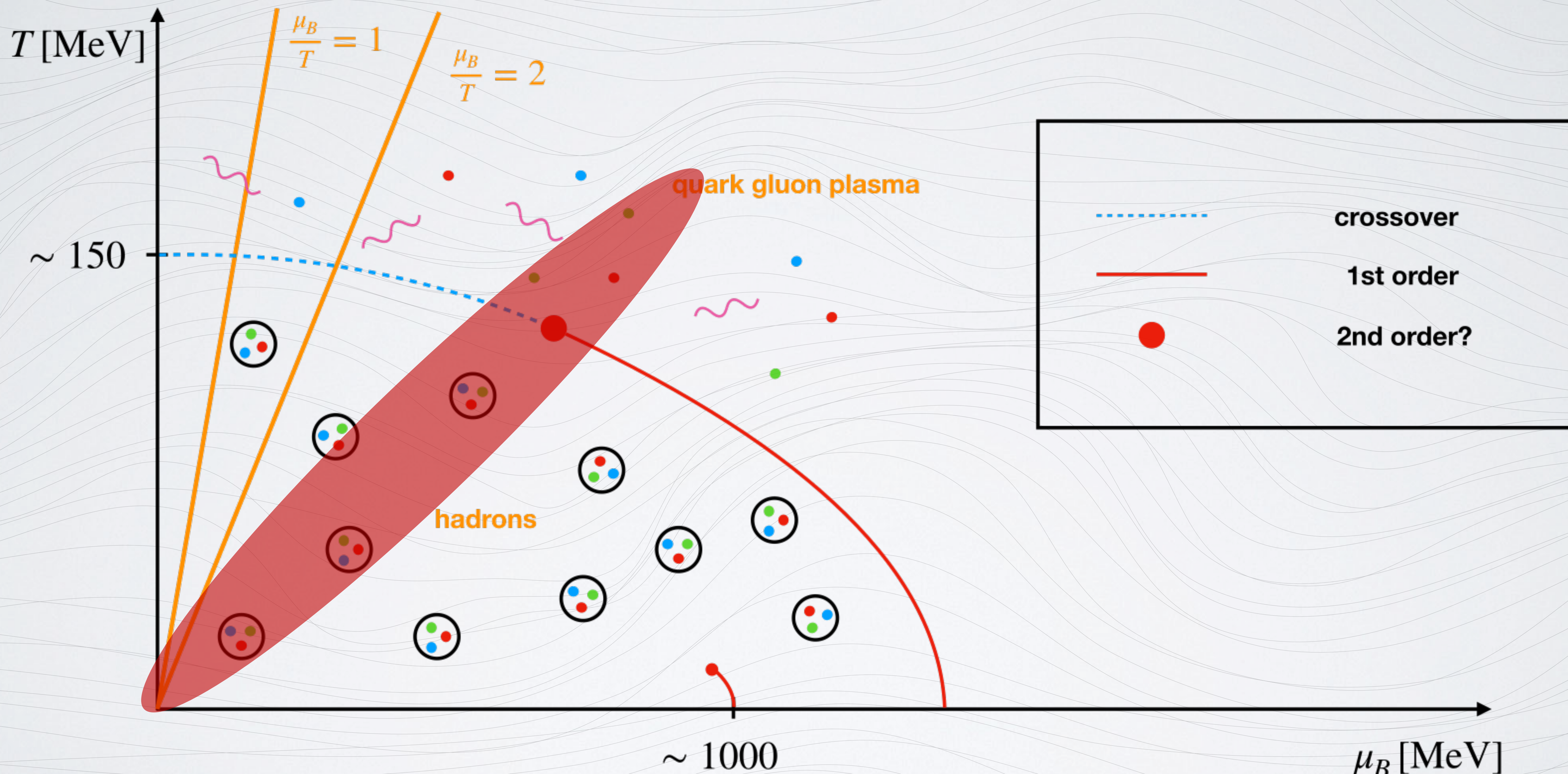

Small expansions - Medium

# QCD phase diagram



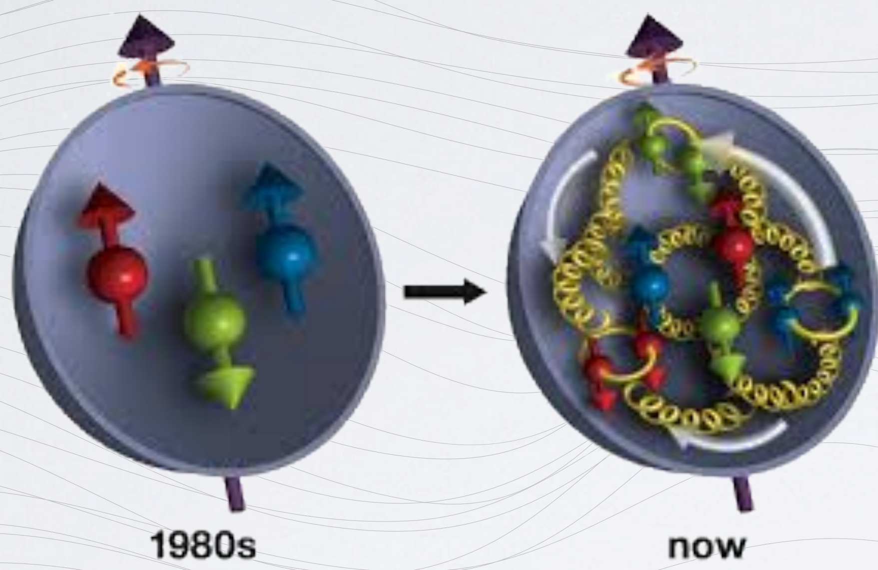

Larger expansions - Hard

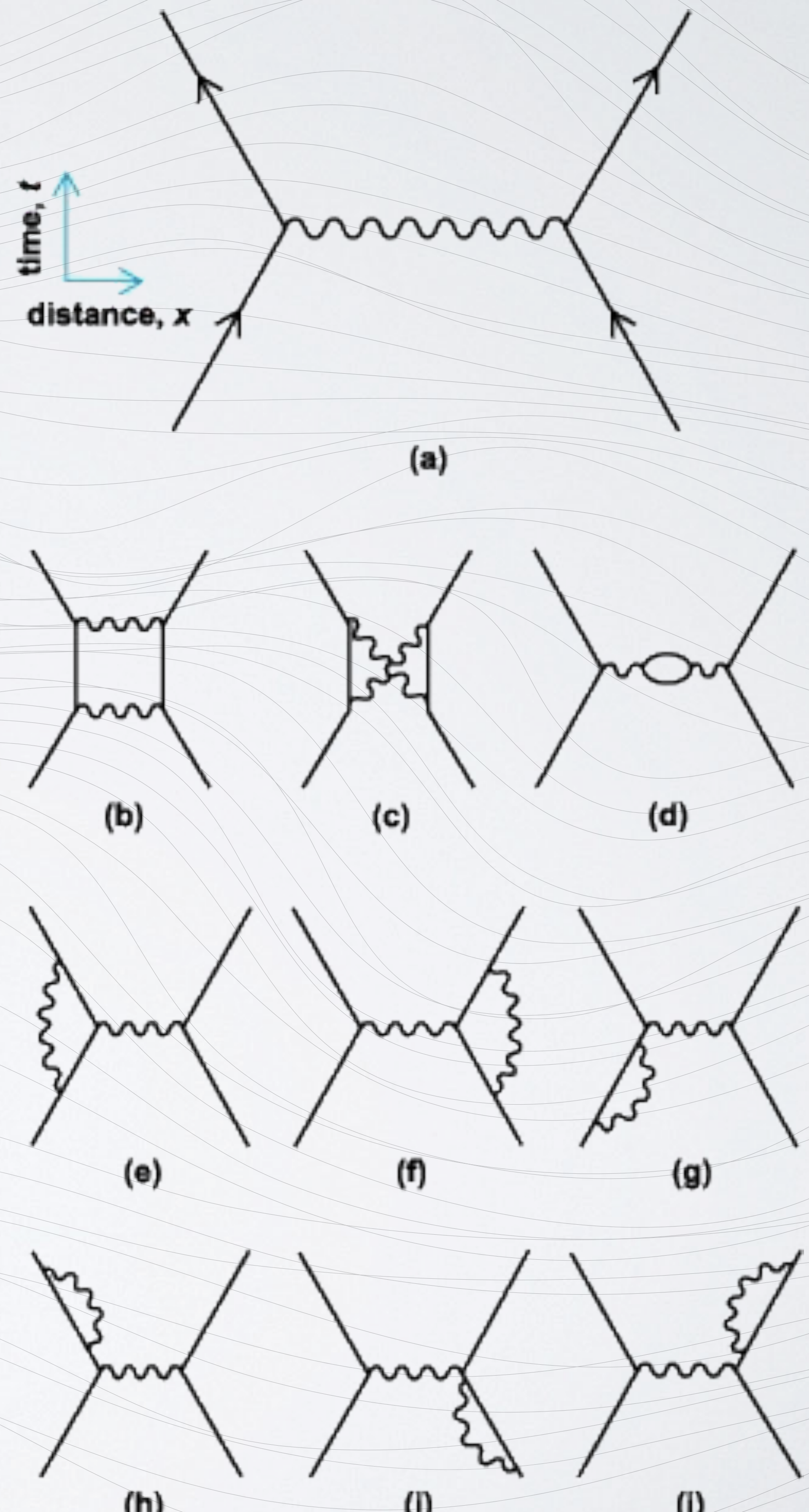
# QCD phase diagram




Finite $\mu$ - Very hard (exponential in volume)

# QCD @ small Energies?



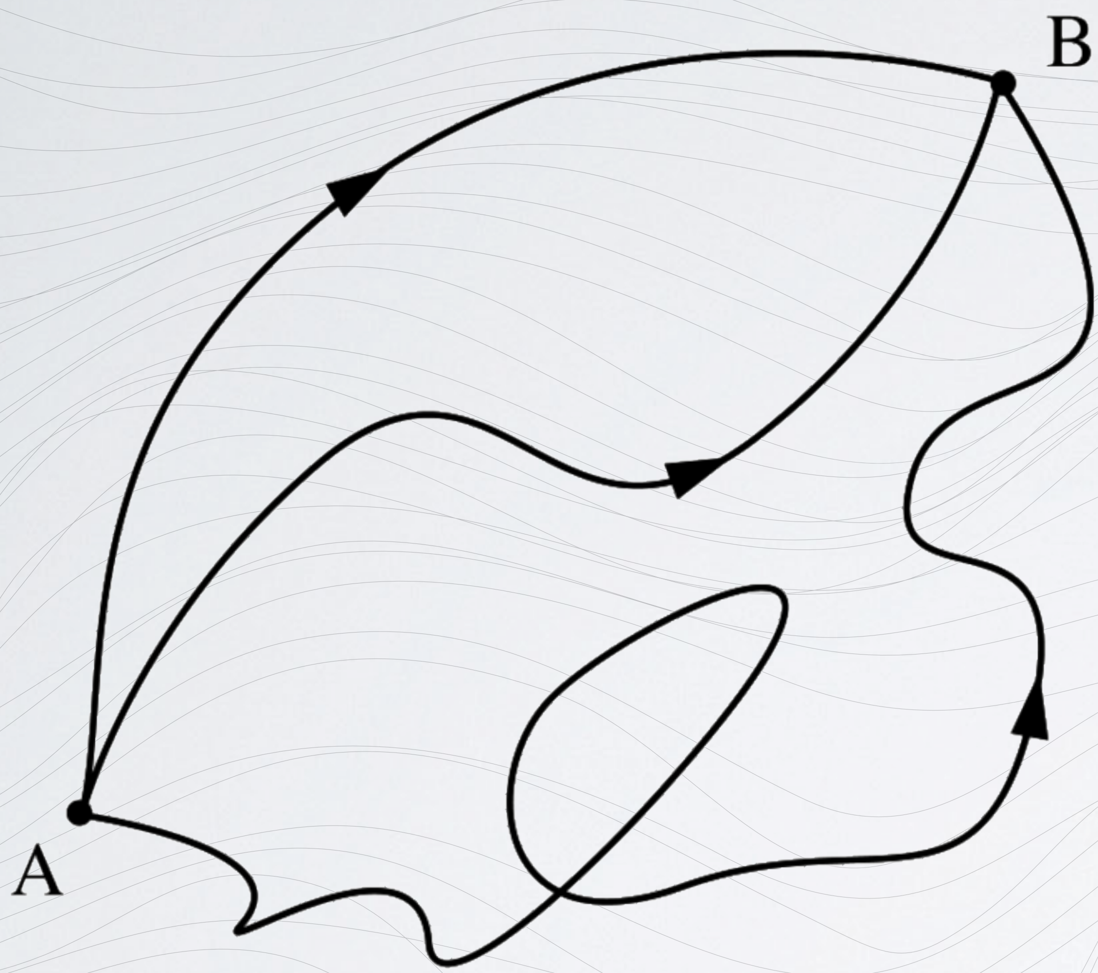

- Usually: Expand observables

$$O = \sum_{n=0}^{\infty} c_n \, \alpha^n$$

- At low energies

$$\alpha \sim 1$$

# Path Integrals




**Path integral formalism**

- Integrate over all possible paths

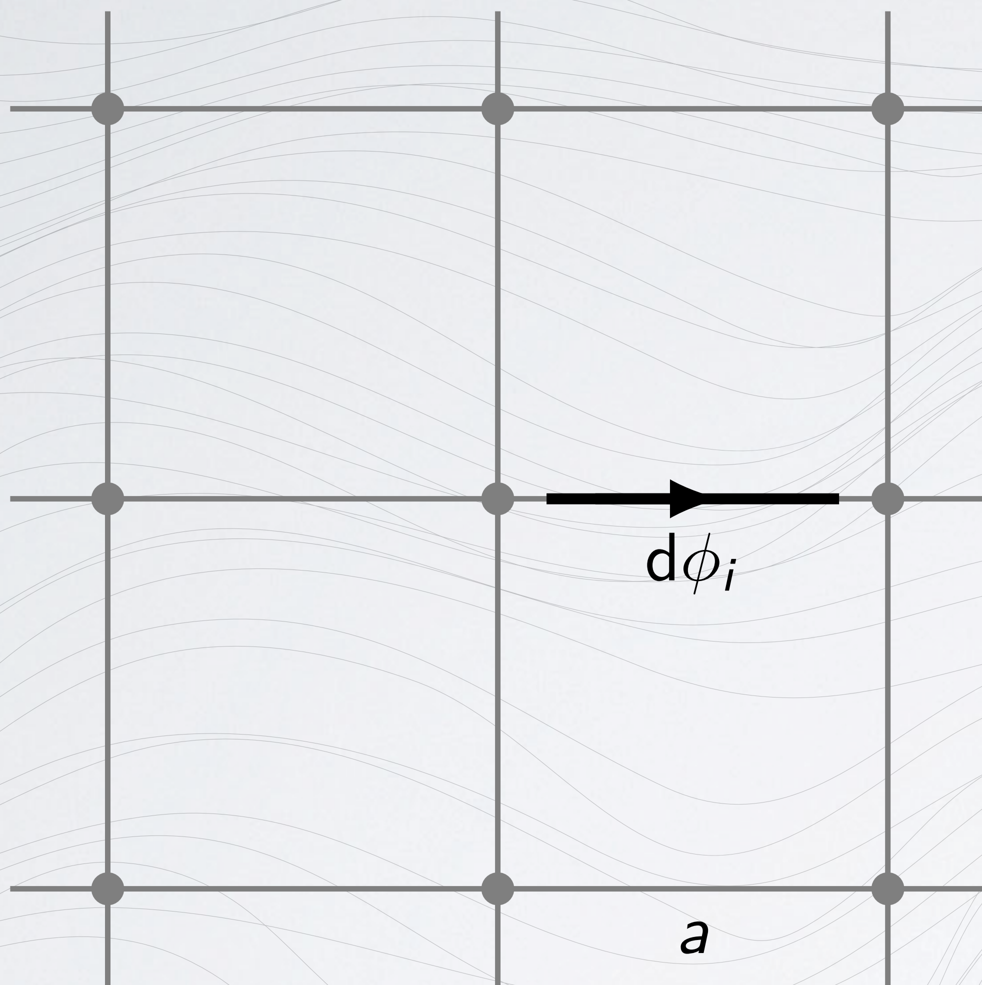
$$A \to B$$

$$Z = \int \mathcal{D}\phi \; \mathrm{e}^{-S[\phi]}$$

- Mathematically not well defined

$$\mathcal{D}\phi = \prod_{i=1}^{\infty} \mathrm{d}\phi_i$$

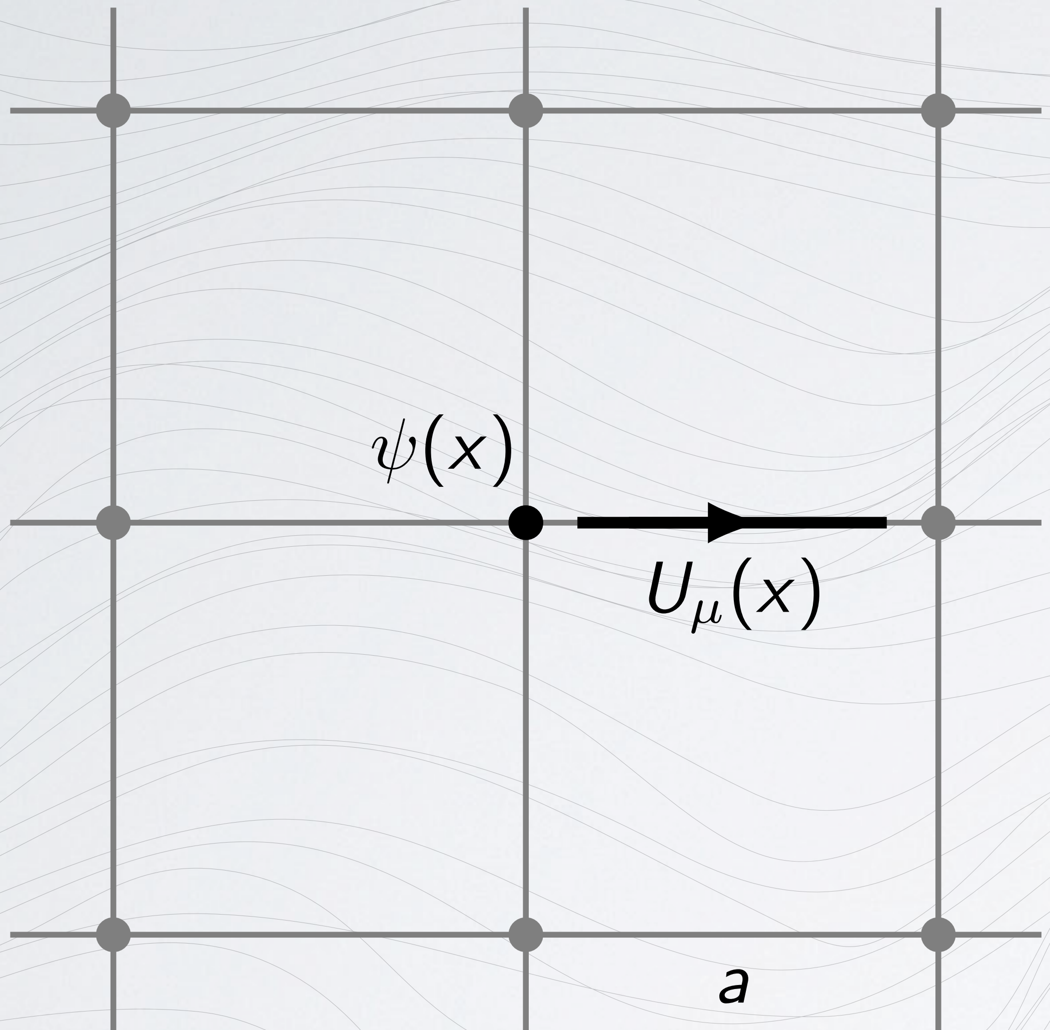
# Lattice Simulations




- 4d - Lattice in space and time
- Path integration possible

$$Z = \int d\phi_0 \ldots d\phi_N \; e^{-S[\phi]}$$

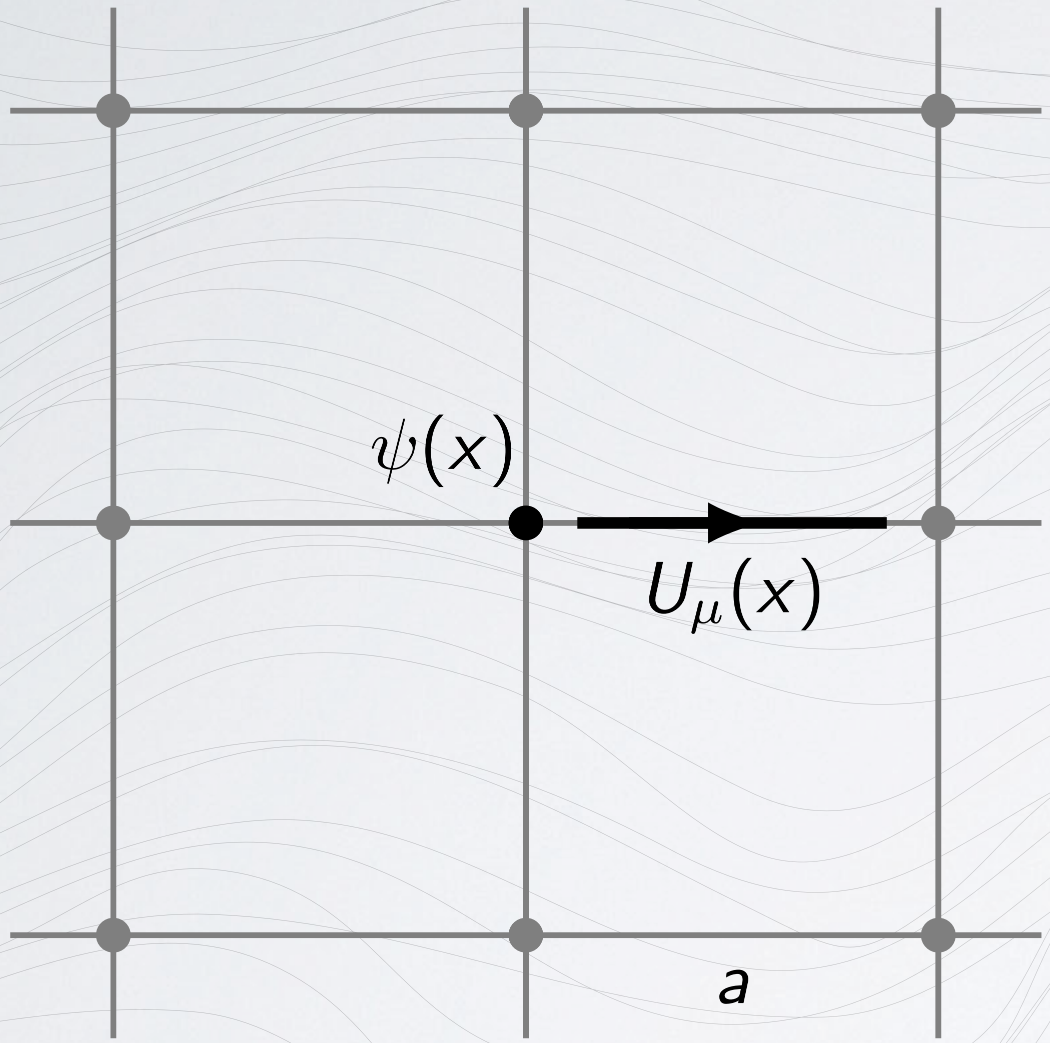
# Lattice Simulations




- **QCD**
  - Quarks: $\psi$, $\overline{\psi}$
  - Gluons: $U_\mu(x) \quad \in SU(3)$

$$Z = \int \mathcal{D}U\, \mathcal{D}\psi\, \mathcal{D}\overline{\psi}\, e^{-S[U,\psi,\overline{\psi}]}$$

# Lattice Simulations

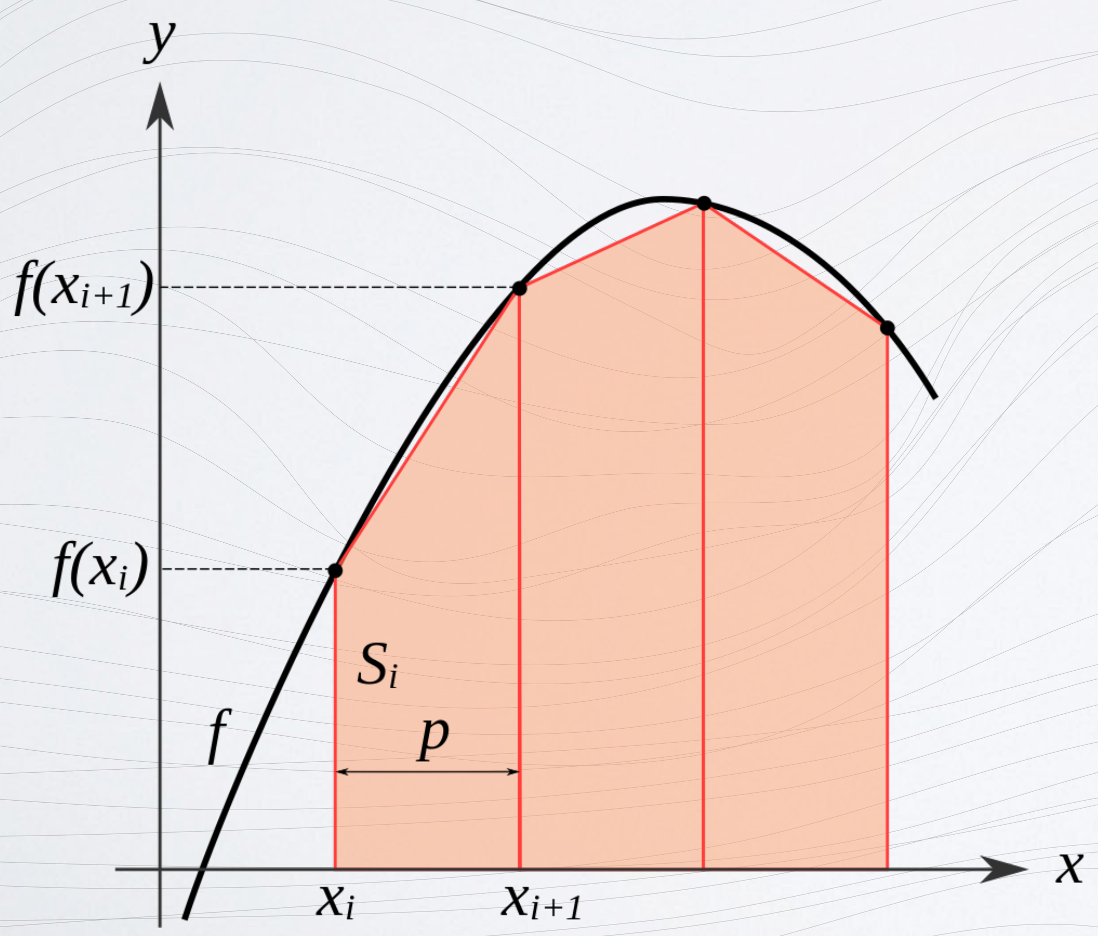



- **Quarks**: $\psi(x)$ anti-commute
  - Grassmann variables 🙁
  - Integrate out 😊
- **Gluons** $(N_c = 3)$: $U_\mu(x)$
  - SU(3) Matrices $\rightarrow$ Haar-Measure $\mathcal{D}U$

$$Z = \int \mathcal{D}U \det(M)\, \mathrm{e}^{-S_G[U]}$$

# Numerical Integration

$$Z = \int \mathcal{D}U \, \det(M) \, e^{-S_G[U]}$$




- **Dimension** (Integral)

$$D = 128 \cdot 64^3 \cdot 8 \cdot 4$$
$$= 1.073.741.824$$

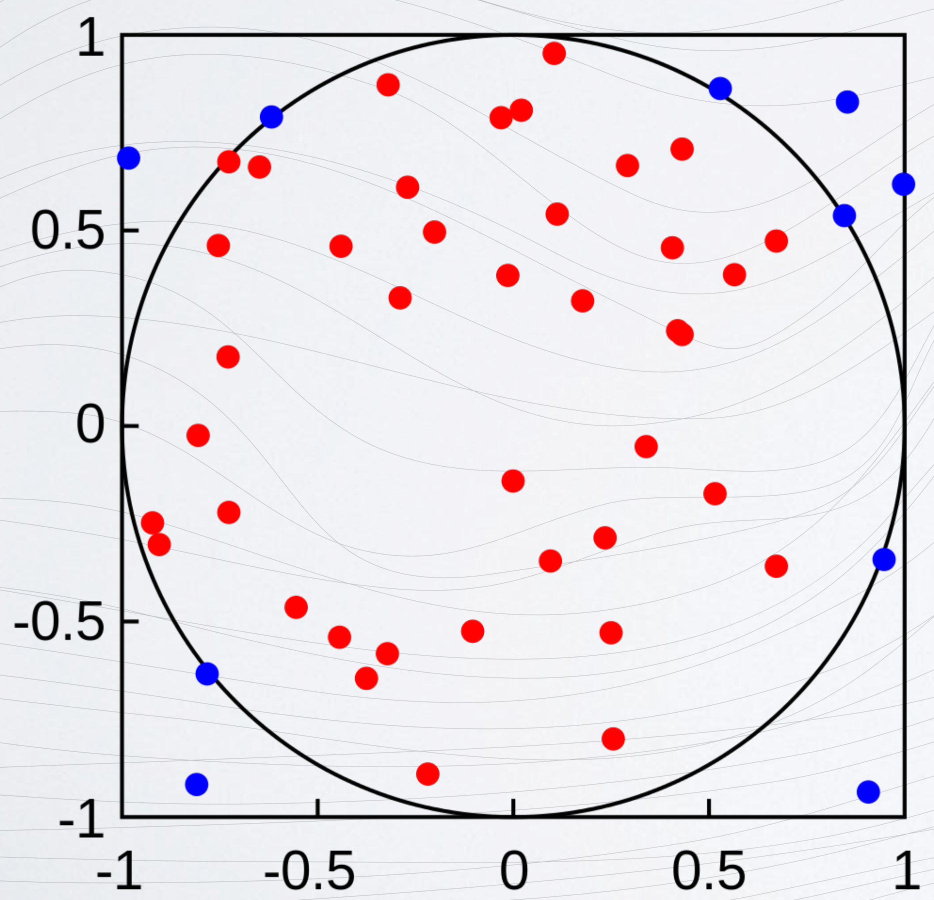
- Trapezoidal rule **impossible**

$$4^{1.073.741.824} \sim 10^{646.456.993}$$

- **Monte Carlo**

# Numerical Integration

$$Z = \int \mathcal{D}U \det(M)\, e^{-S_G[U]}$$




- **Fermion determinant**

$$\det(M)$$

$$\text{rank}(M) = 128 \cdot 64^3 \cdot 4 \cdot 3$$
$$= 402.653.184$$

- Determinant num. expensive
- Use pseudo-fermions $\phi$

$$det(M) \sim \int \mathcal{D}\phi\ e^{-\phi^\dagger M^{-1} \phi}$$

# Lattice Simulations

**Lattice simulations**

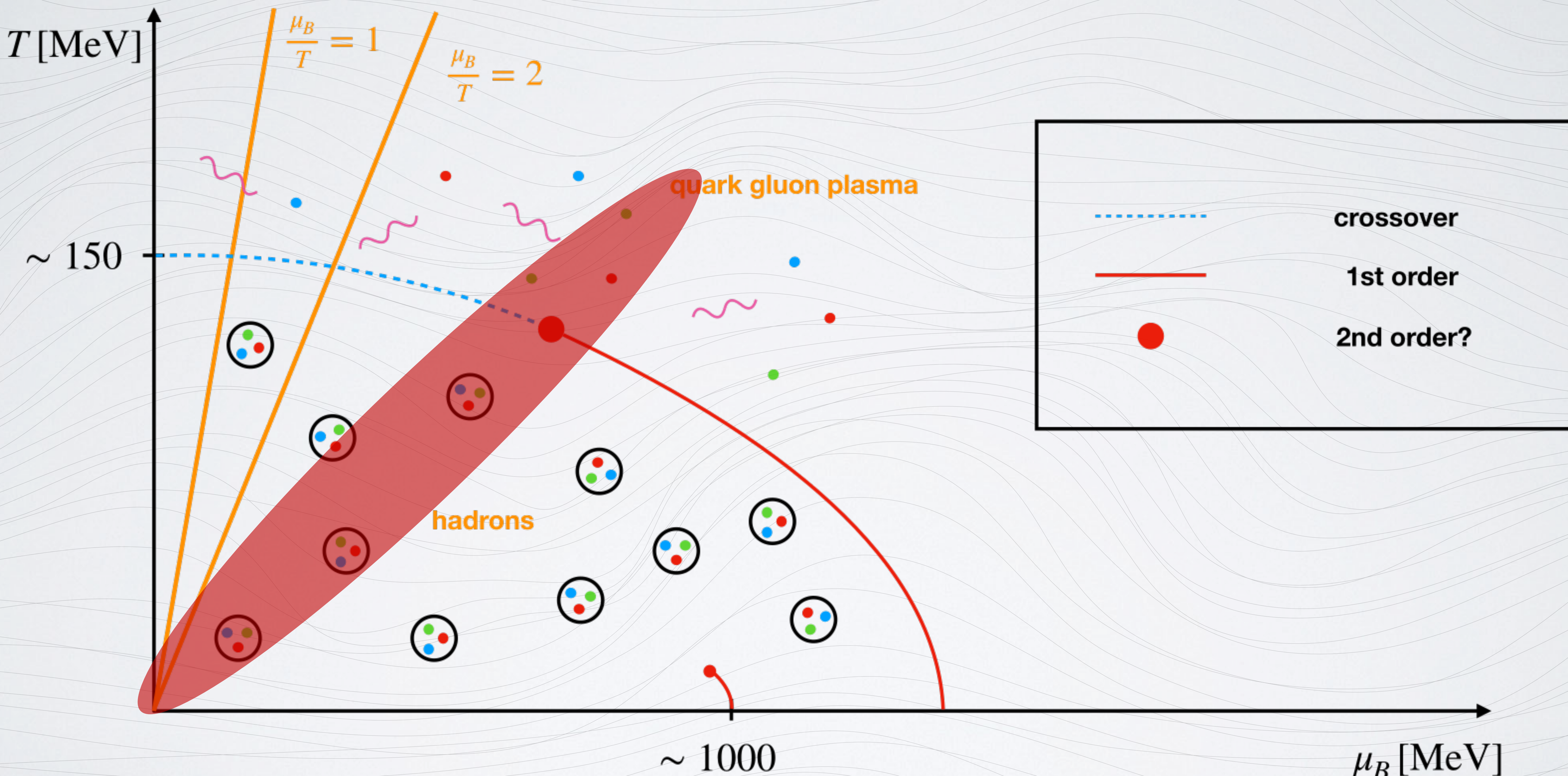
- Discretise space-time by a hyper cubic lattice
- Quantise QCD using Path Integrals
- Calculate observables using Monte Carlo techniques

$$Z = \int \mathcal{D}U \det(M)\, e^{-S_G[U]}$$

**Systematic uncertainties**

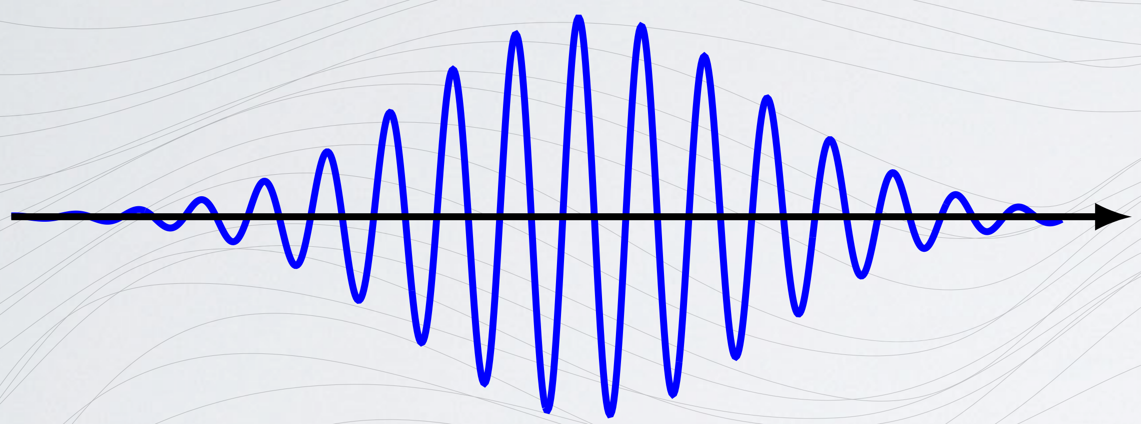
- Lattice spacing $a \to 0$
- Volume effects $V \to \infty$
- Monte Carlo method $\to$ Statistical uncertainty remains

# QCD phase diagram




Finite $\mu$ - Very hard (exponential in volume)

# Sign Problem



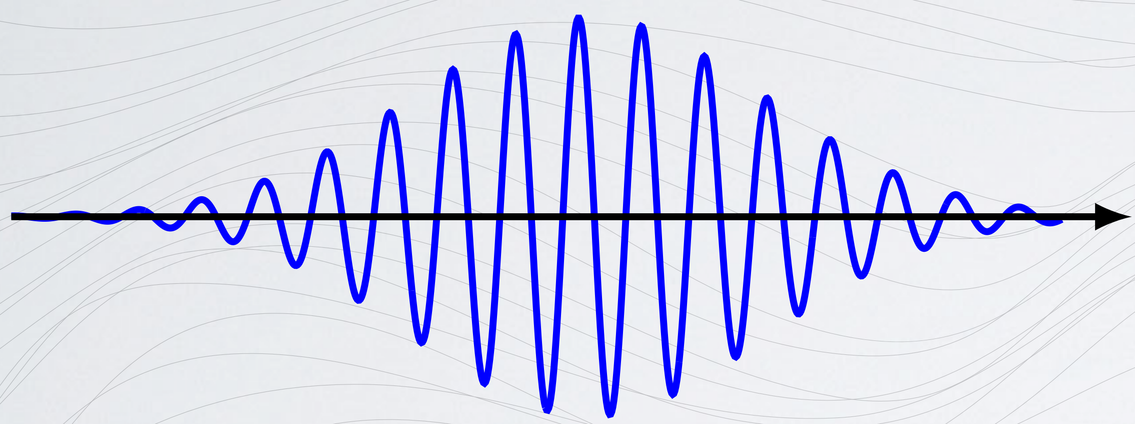
**Sign Problem**

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

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

- Importance Sampling Monte Carlo not applicable :(
- New ideas needed
- The solution not found - Many methods developed

# Example - 1dim



- Simple one-dim. integral

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

- Exact integration:

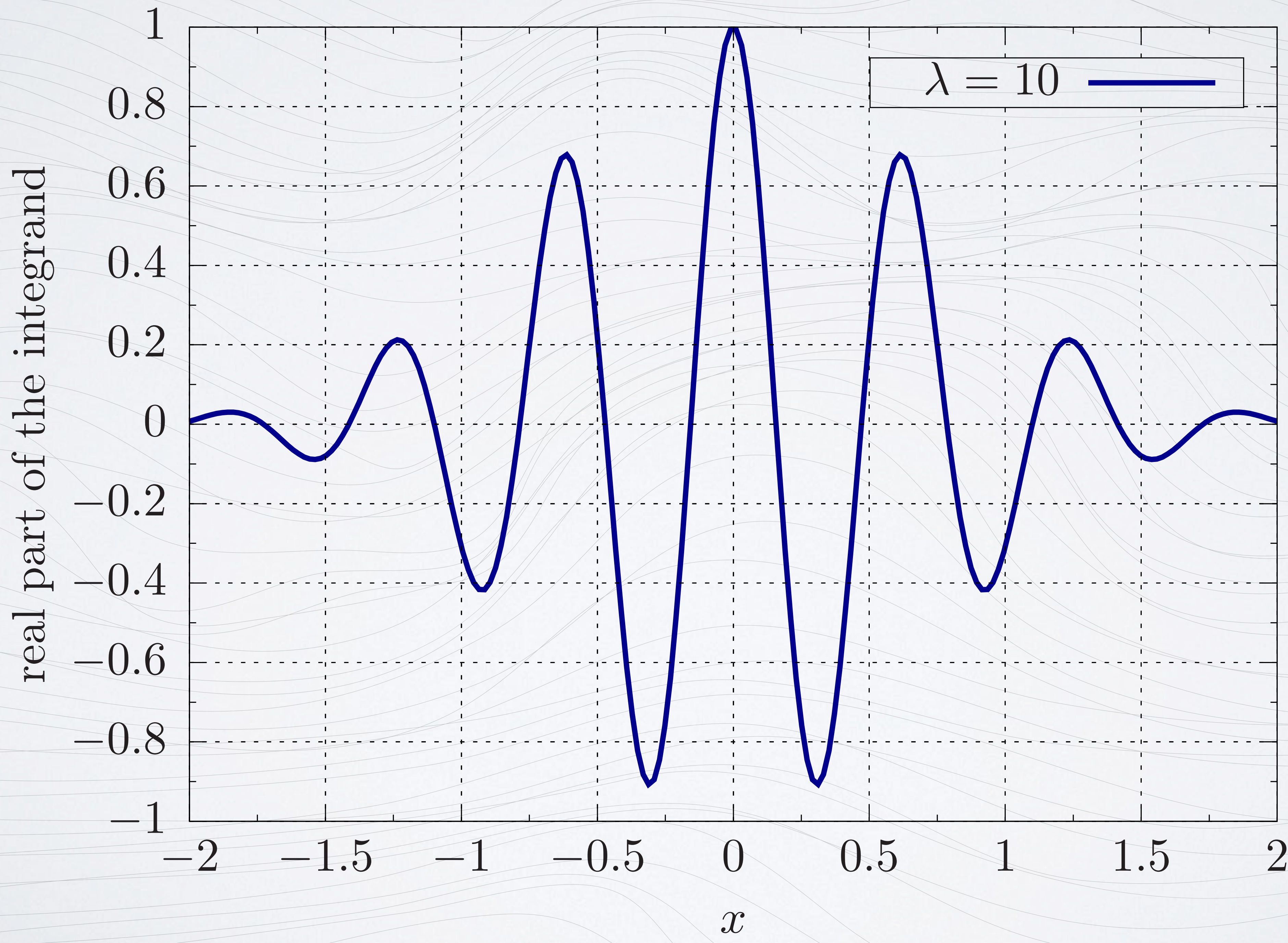
$$Z = \sqrt{\pi}\, e^{-\lambda^2/4}$$

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

# Sign Problem

**Example** ($\lambda = 10$)

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



# Sign Problem

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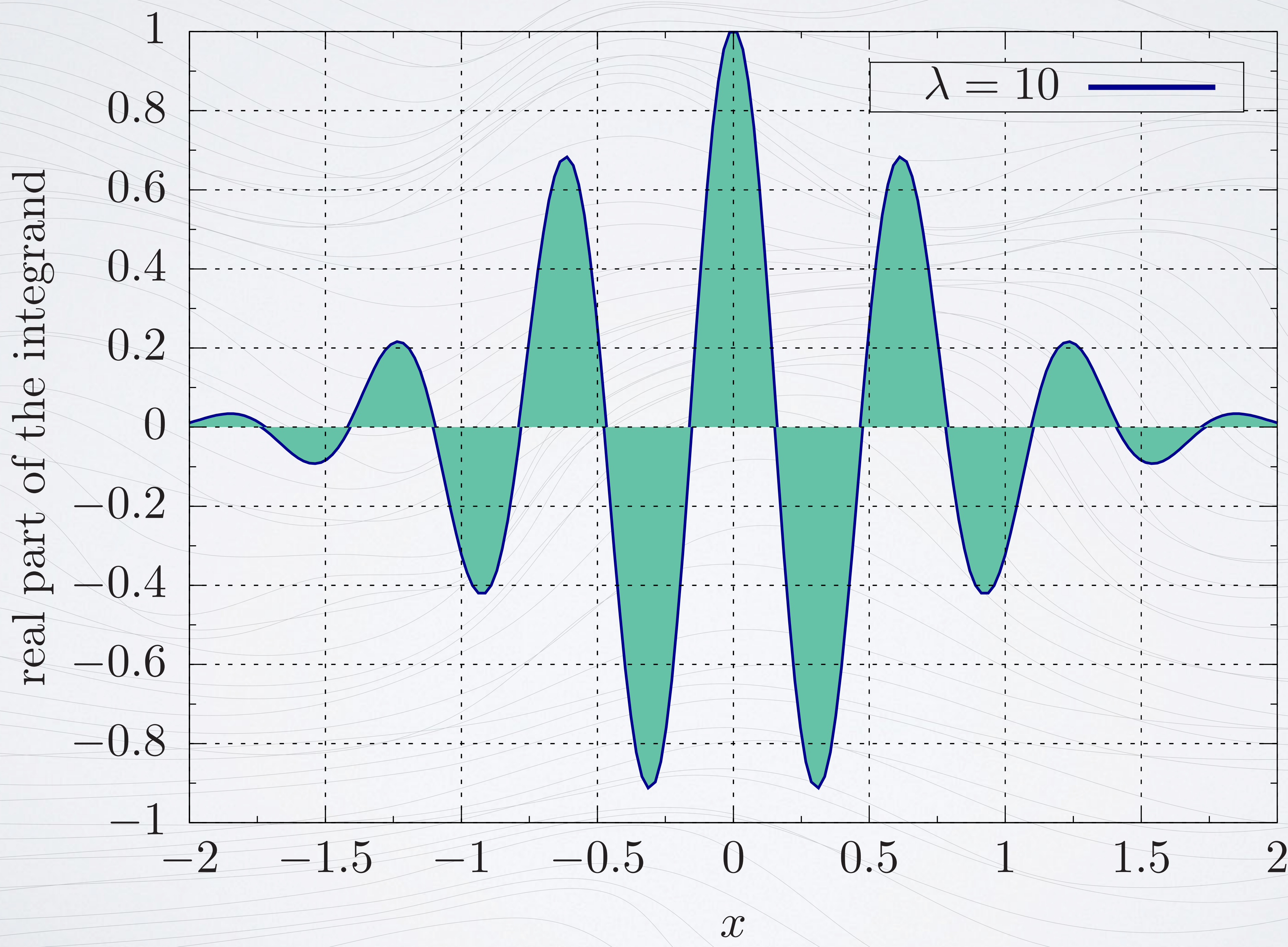

# Sign Problem

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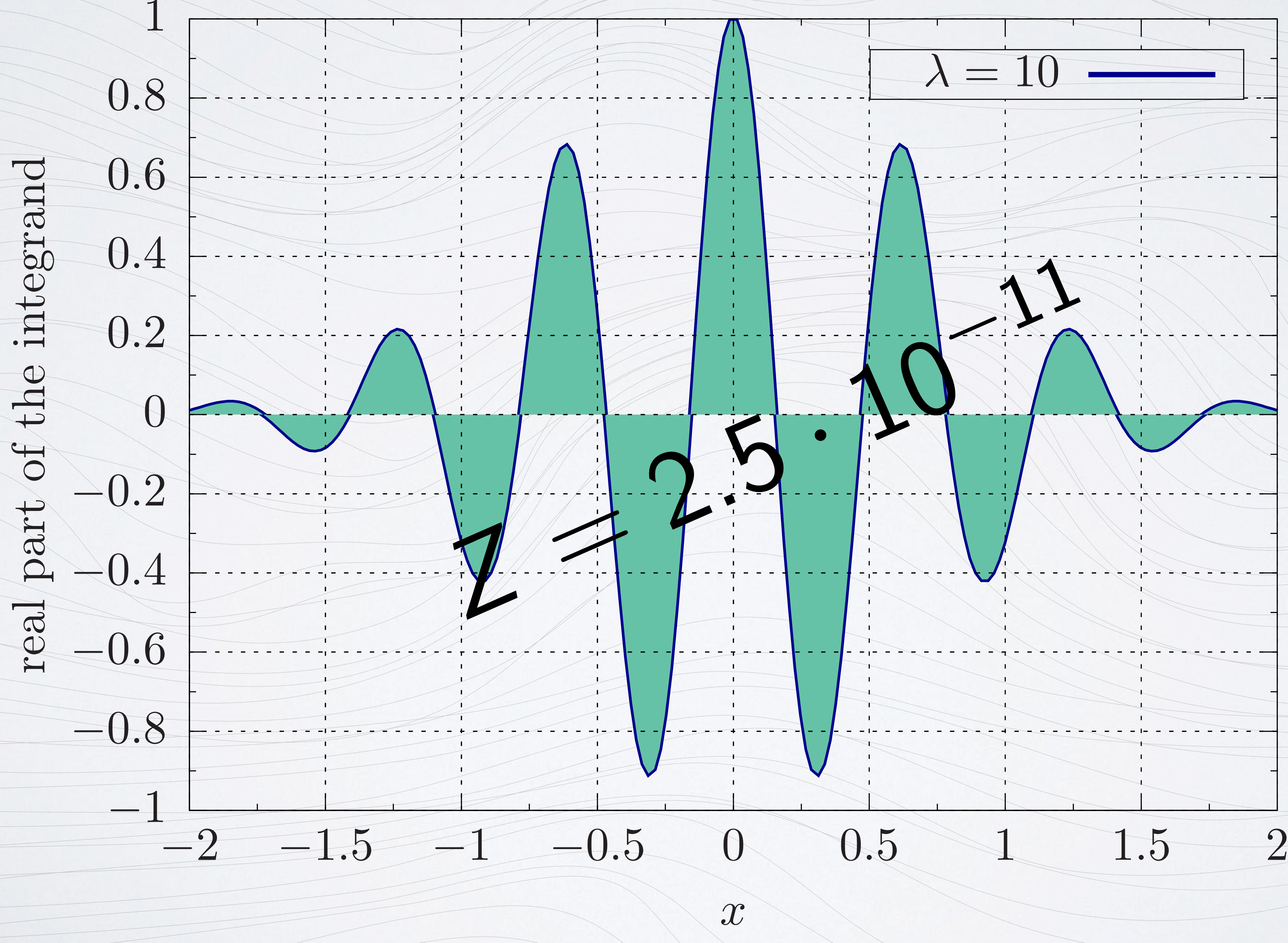
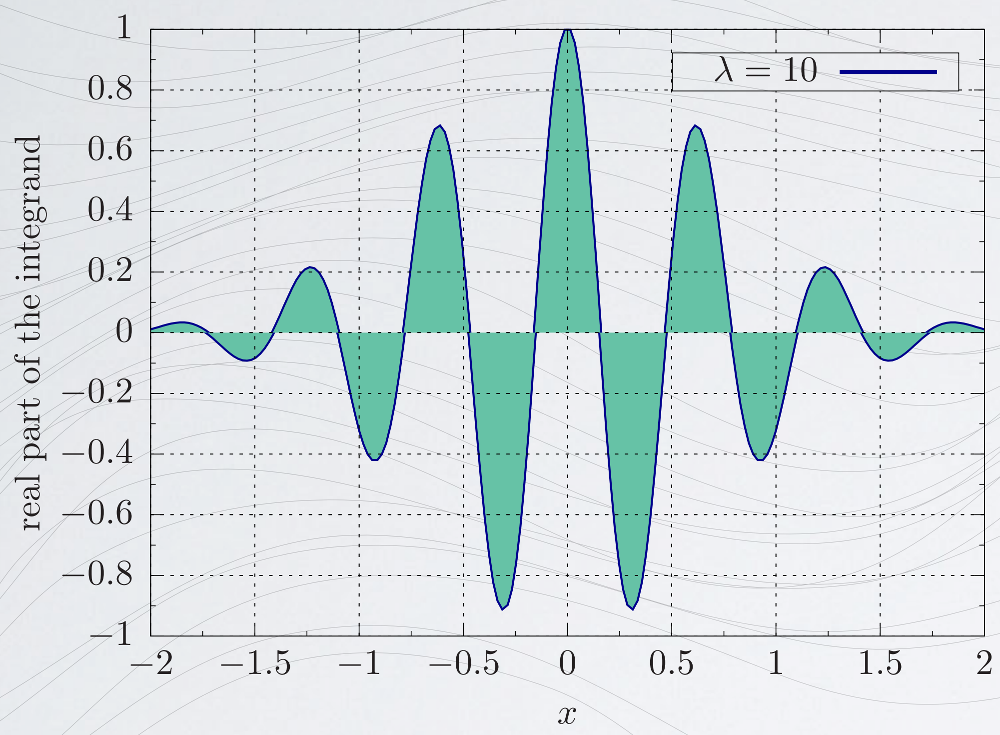


# Sign Problem



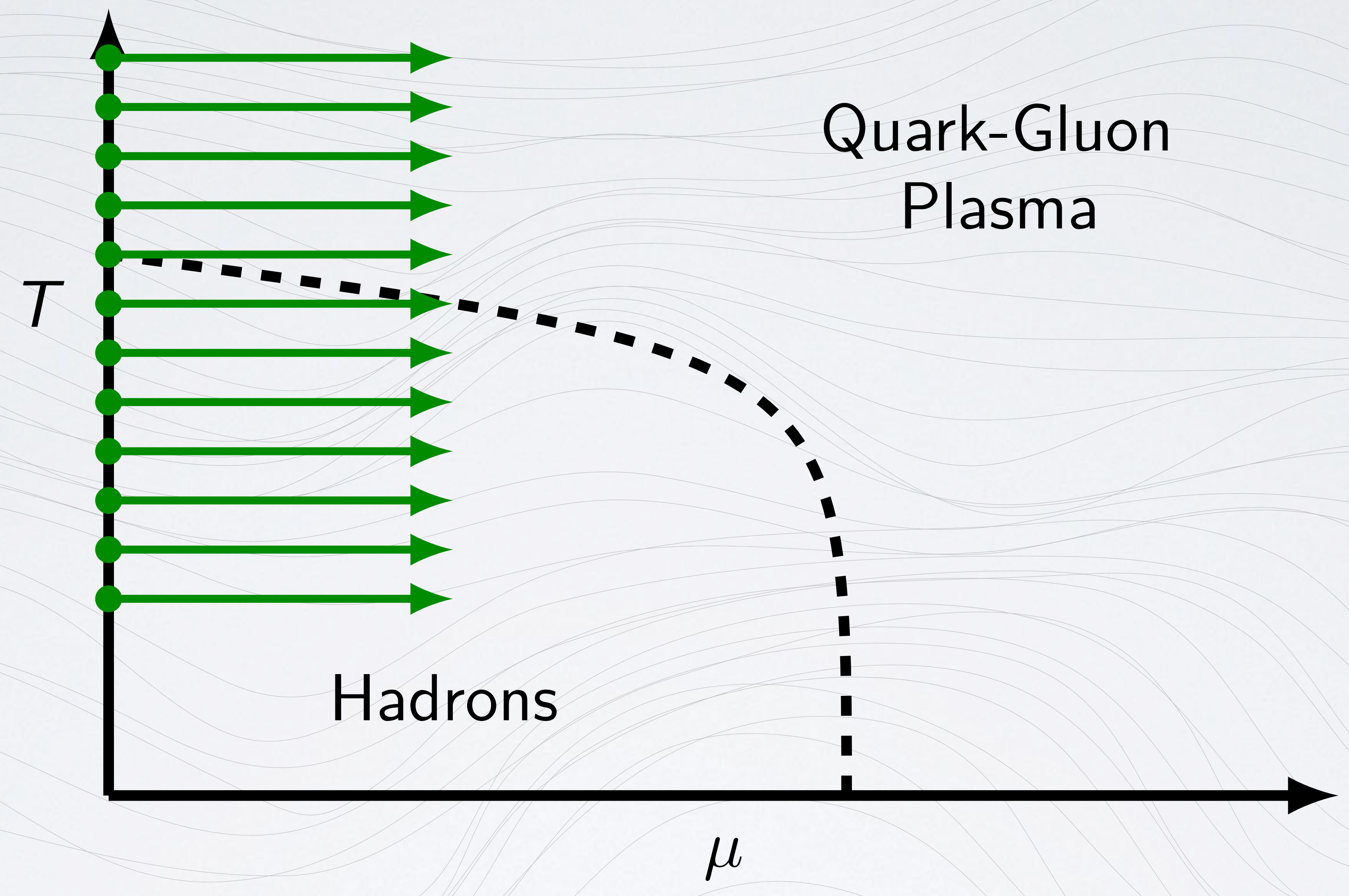

**Sign Problem**

- 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 $\mu$, Deforming the contour, …
  - Focus here: Complex Langevin

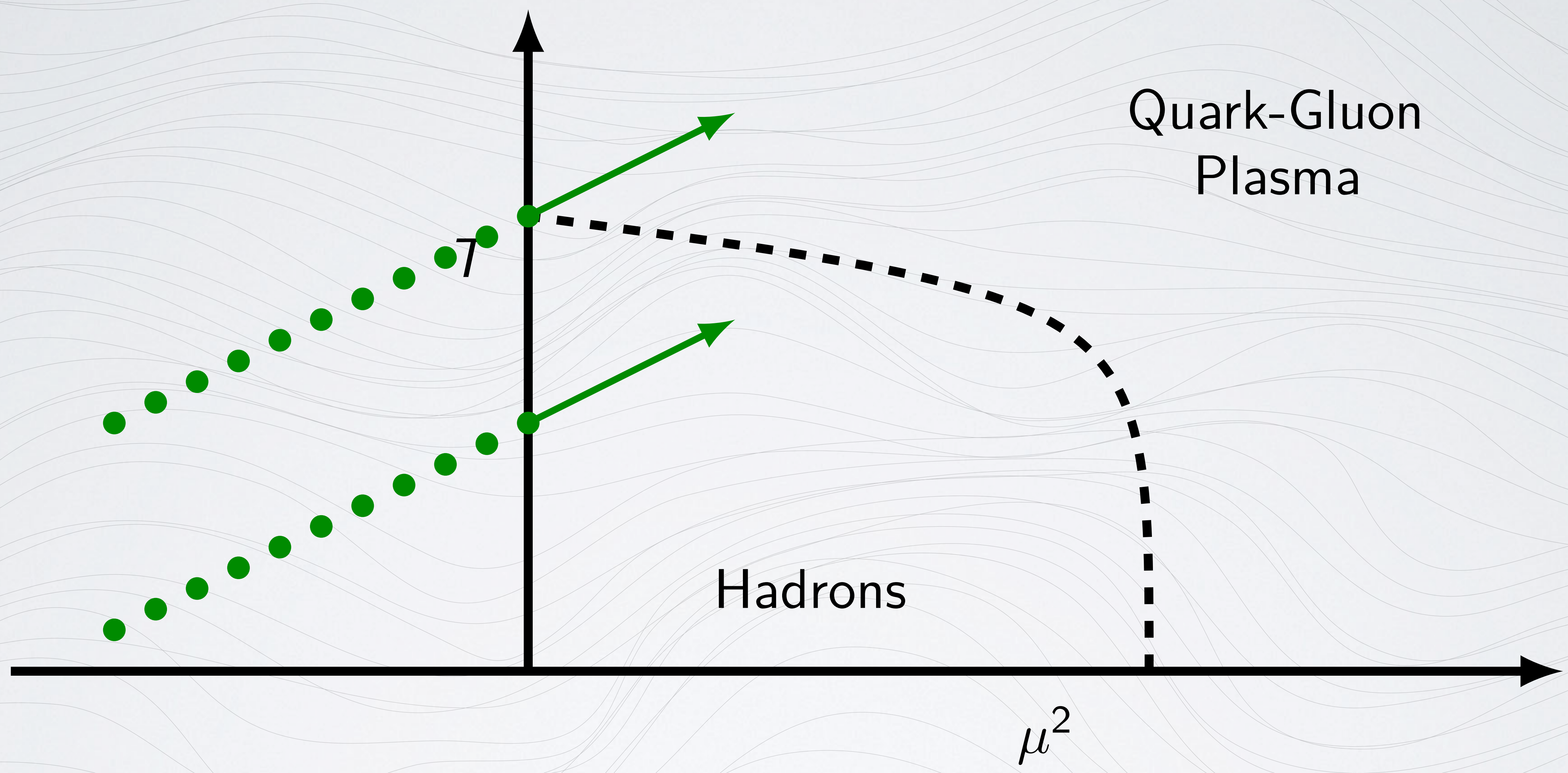
# Taylor Expansion




- Simulate at zero chemical potential and expand

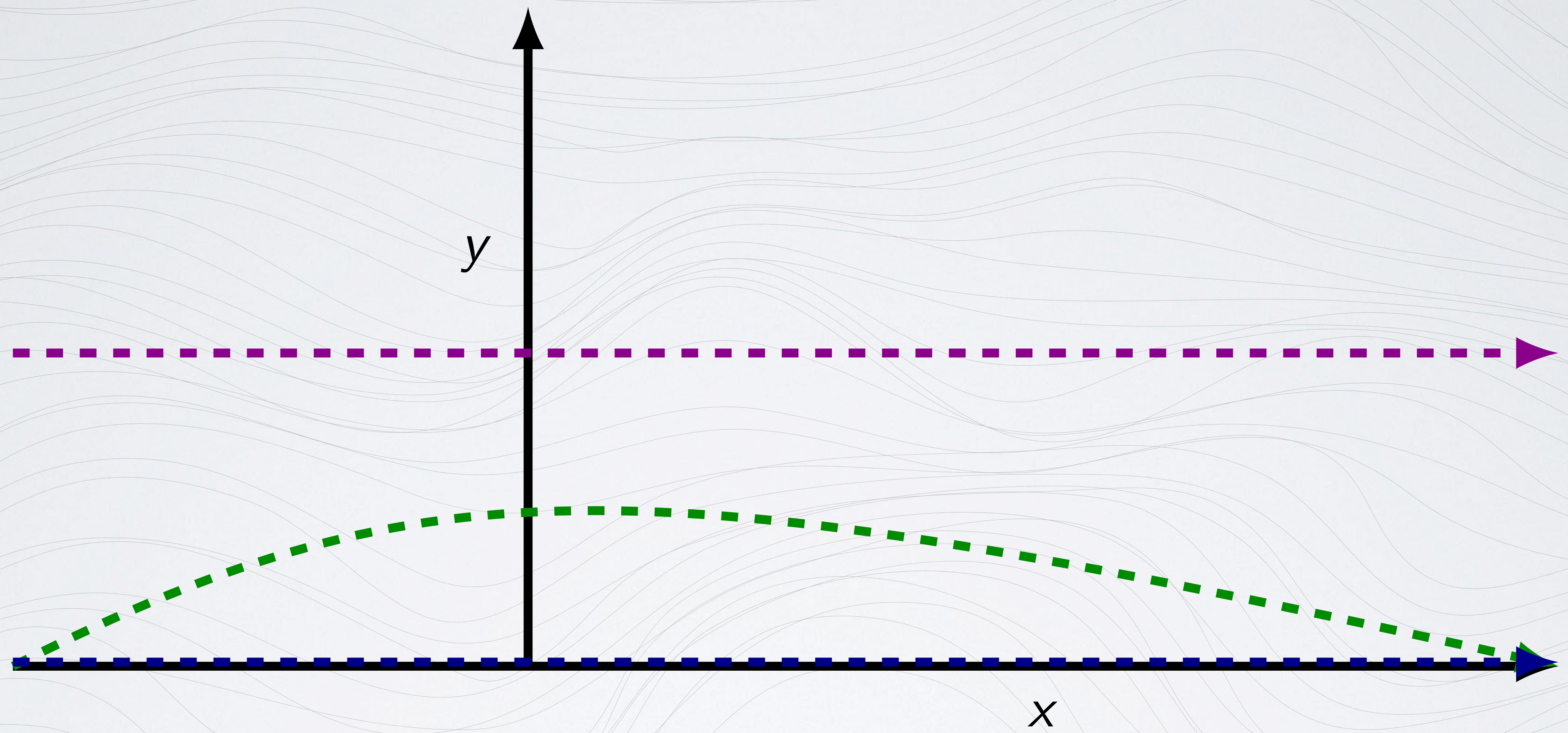
$$\frac{p}{T^4} = \sum_k c_k(T) \left(\frac{\mu}{T}\right)^k, \quad k = 0, 2, \ldots$$

# Imaginary μ



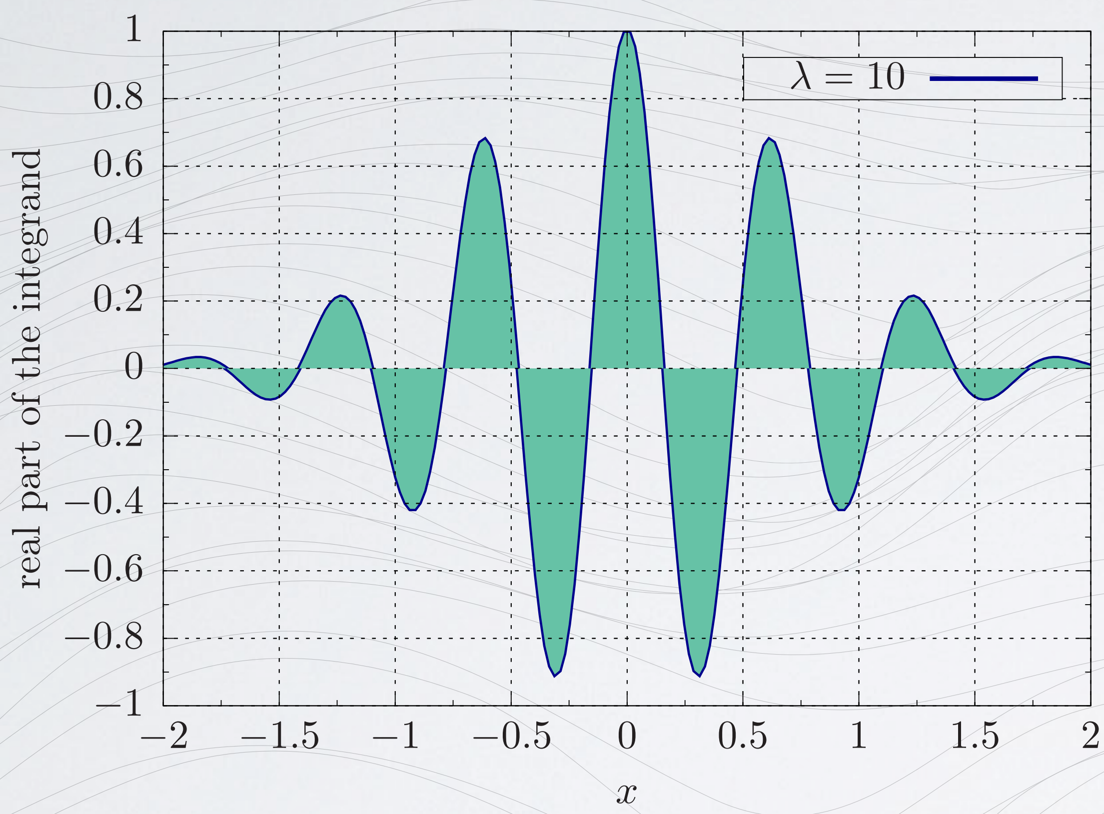

- Simulate at imaginary chemical potential and extrapolate to the QCD phase diagram

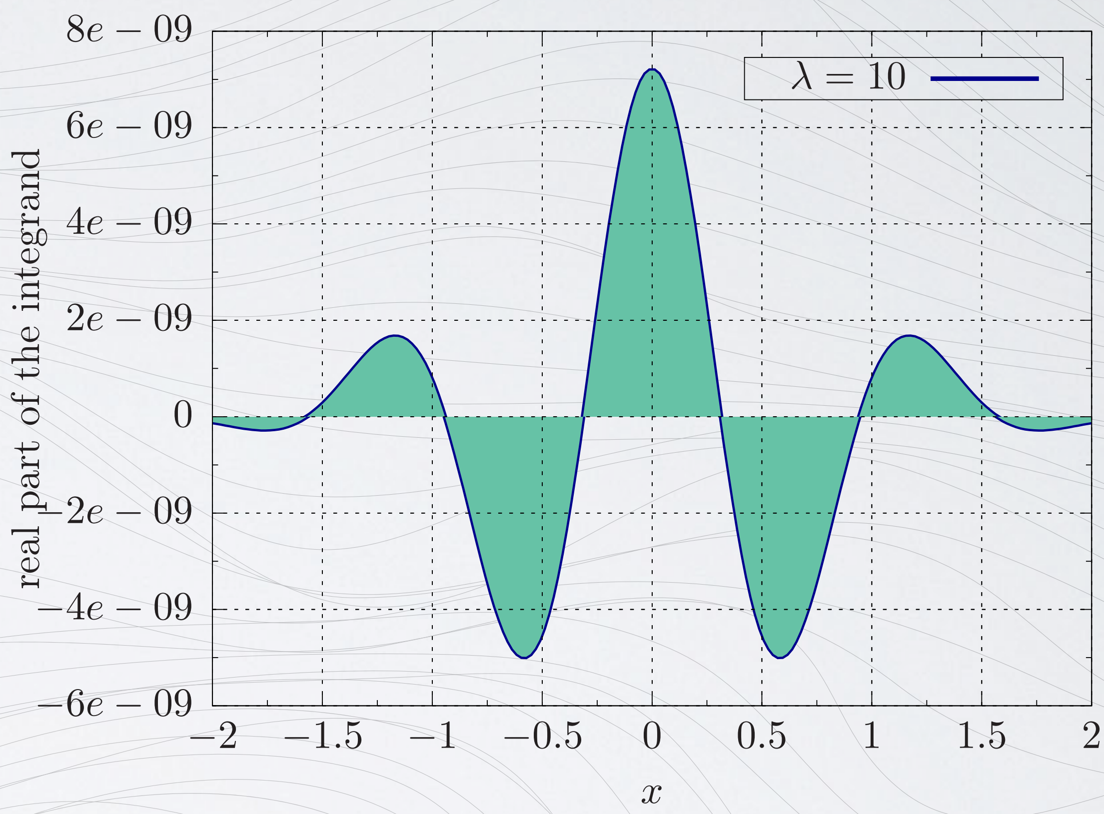
# Complex Deformation




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

# Complex Deformation



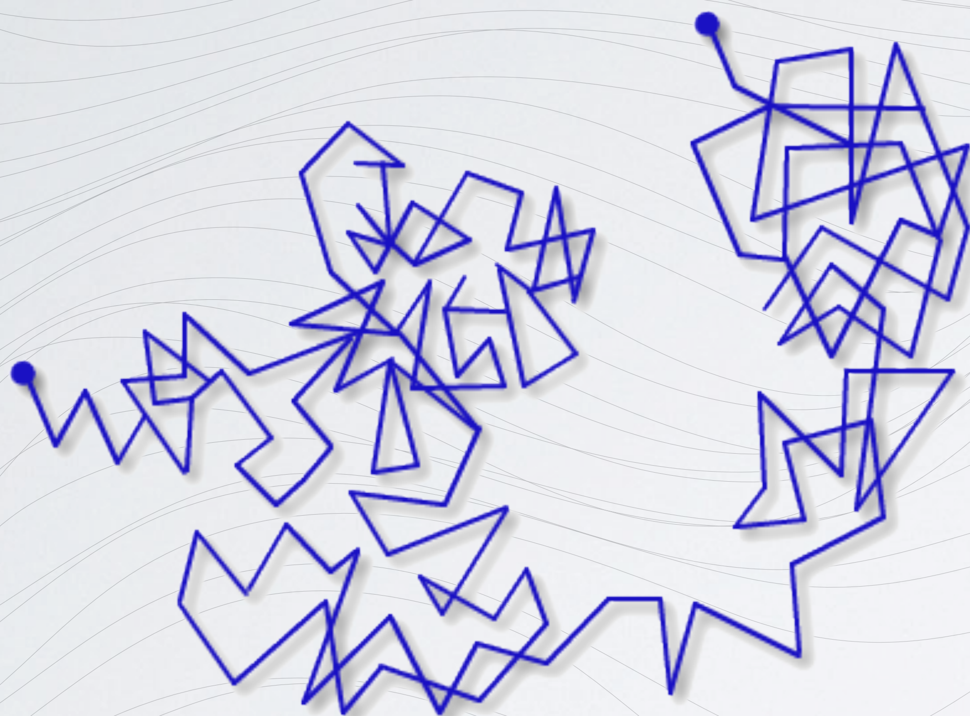




$$z = x - \frac{1}{4}\, i\, \lambda$$

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

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

# 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! :)

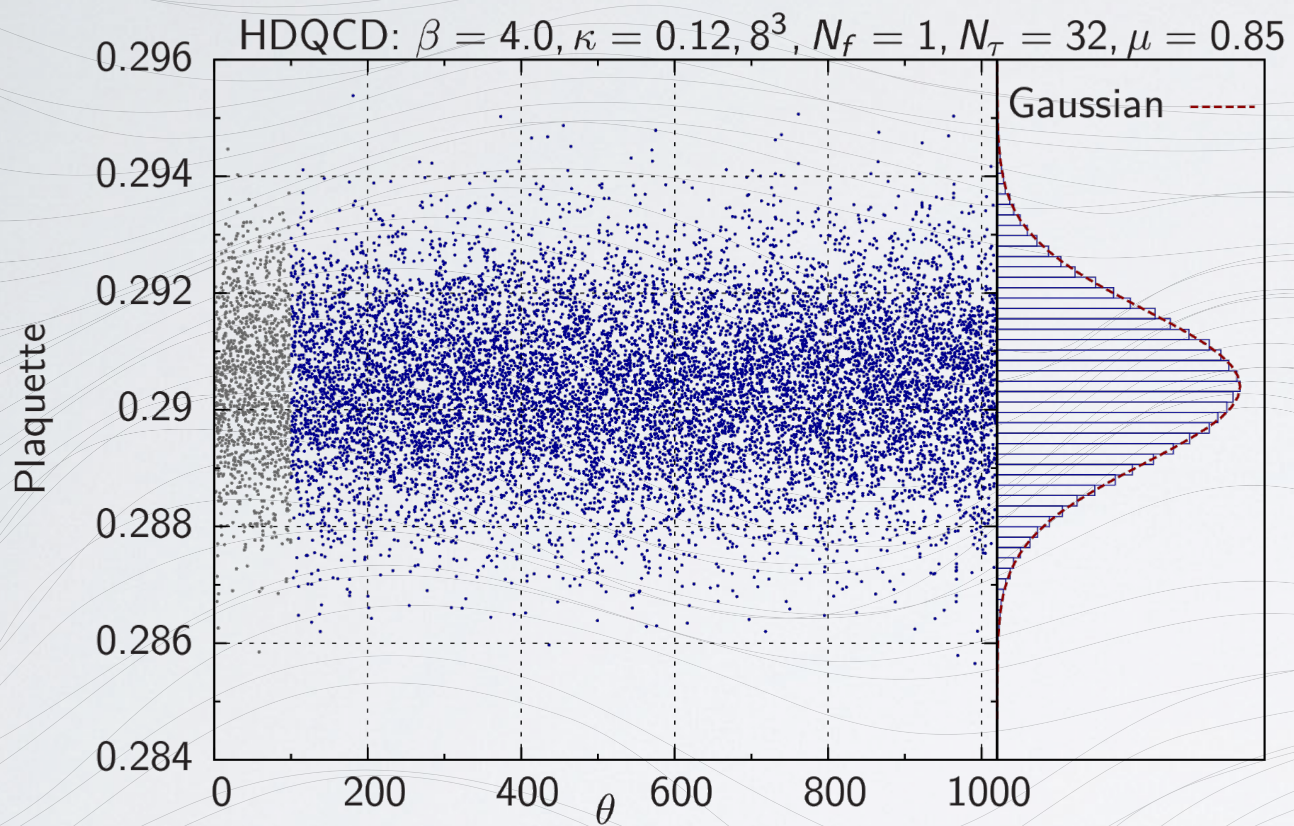
# Complex Langevin

- Complexify degrees of freedom → Complex Analysis

$$\underbrace{\int \mathrm{d}x \, \mathrm{e}^{-S[x]}}_{\text{what we want}} \overset{?}{=} \underbrace{\int\int \mathrm{d}x\mathrm{d}y \, \mathrm{e}^{-S[z]}}_{\text{what we sample}}$$

- Analytic continuation $x \to z = x + \mathrm{i}y$
- Under certain conditions both sides are equivalent
  - Action $S[z]$ and observables $O(z)$ are holomorphic
  - Imaginary direction $y$ is compact enough (No boundary)
- For gauge theories similar arguments

# 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 $\epsilon$ needed
  - For large $\mu$ 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

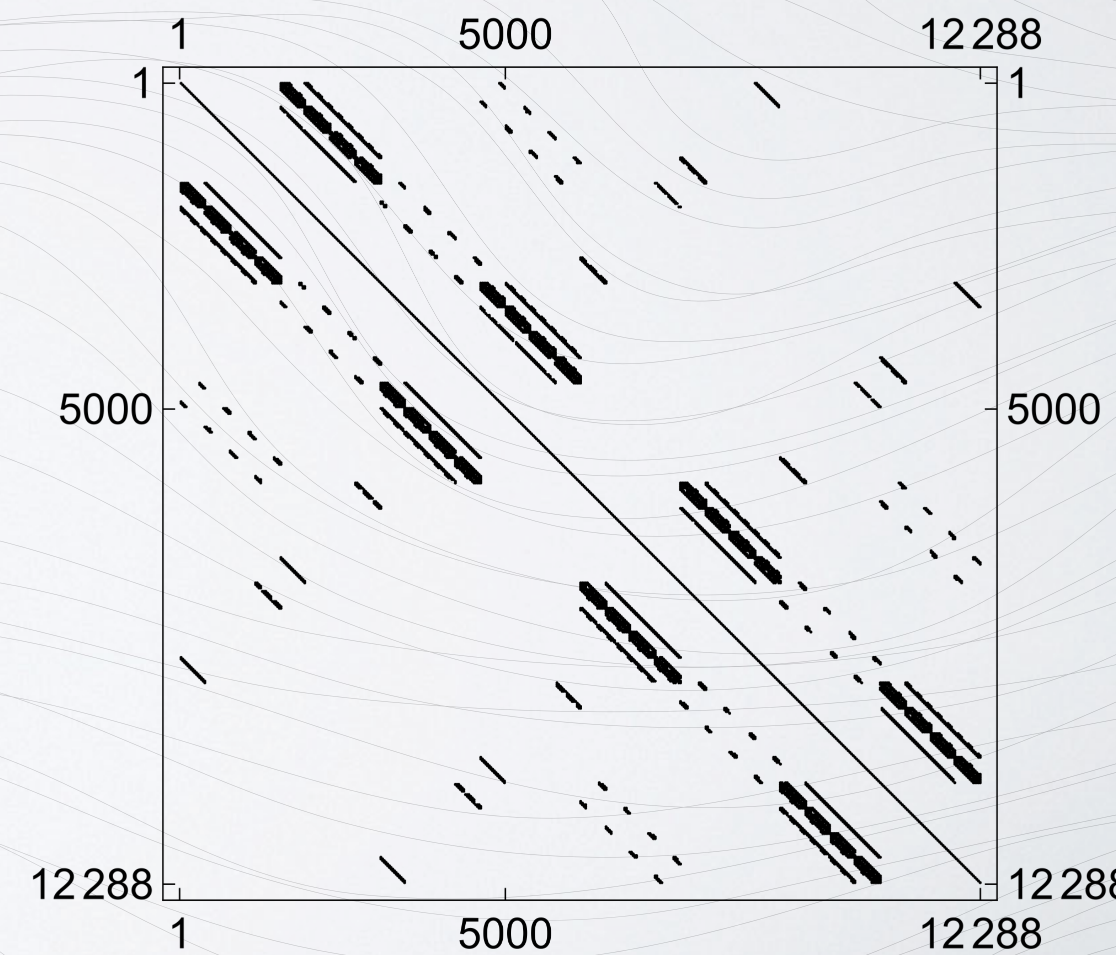
- Gauge drift (straightforward)

  $-D^a_{x,\mu} S_G$ 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 $\mu$**
  - 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…

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

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

- **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

UNIVERSITY OF SOUTHERN DENMARK

QUANTUM THEORY CENTER

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# Lattice Setup

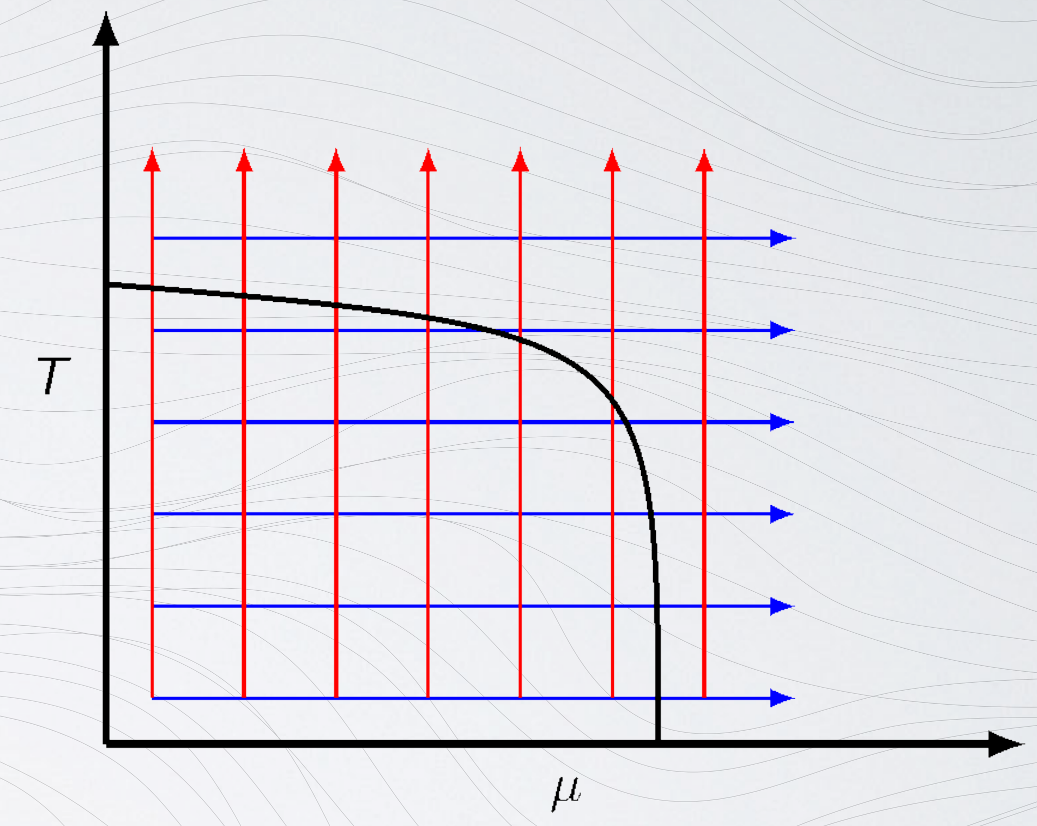
- **Lattice setup**
  - Wilson plaquette action $\beta = 5.8 \leftrightarrow a = 0.06\,fm$
  - Two-flavour dynamical fermions Wilson Fermions $(c_{sw} = 0)$
  - Pion mass $\kappa = 0.1544 \leftrightarrow m_\pi \sim 480\,MeV, m_N = 1.3\,GeV$
  - Volume $V = 24^3 \leftrightarrow m_\pi L = 3.5$

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

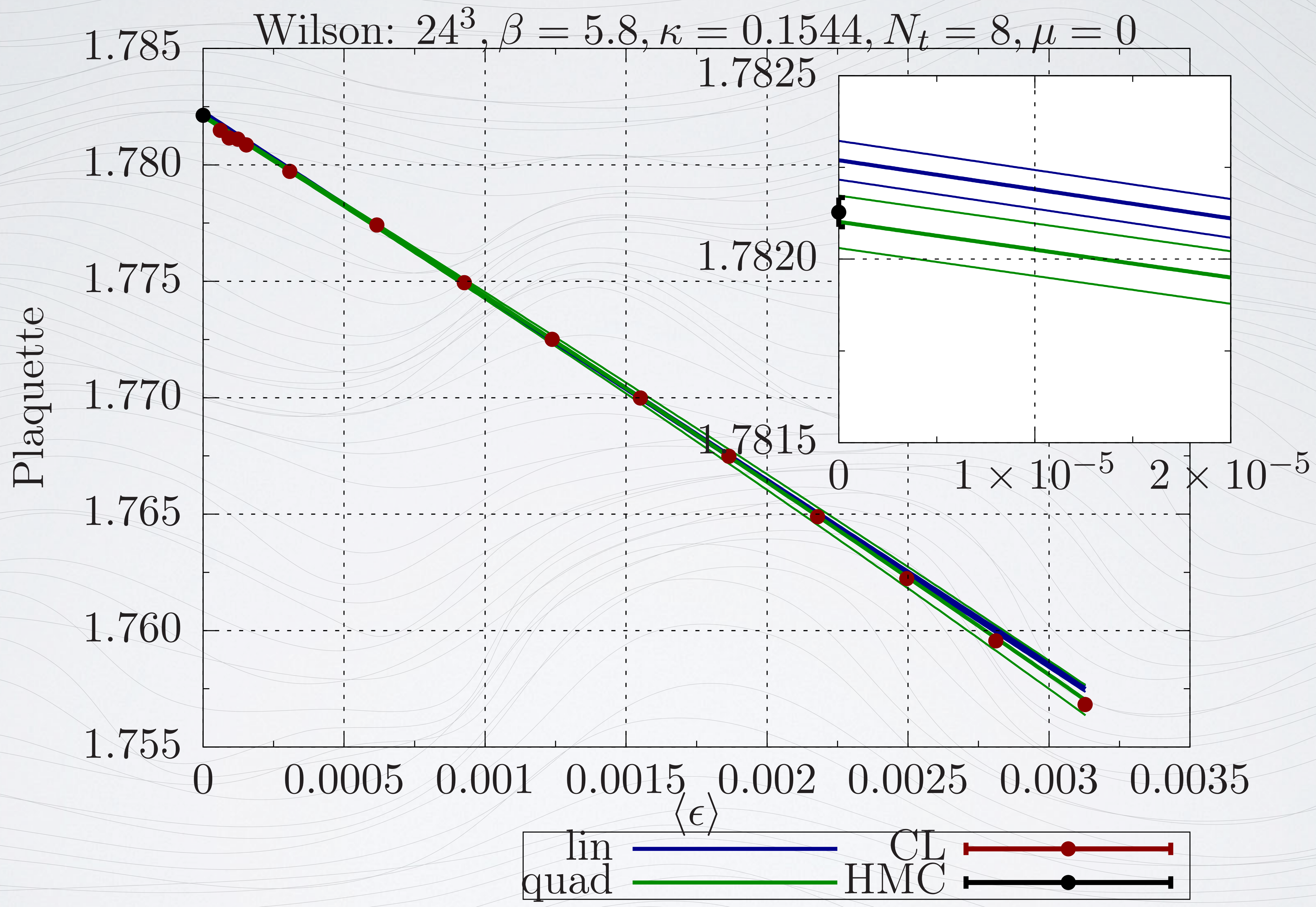
- **Consistency checks @ $\mu = 0$**
  - HMC vs. CL




- **Observables**
  - Fermion density
  - Polyakov loop

- **Equation of state**

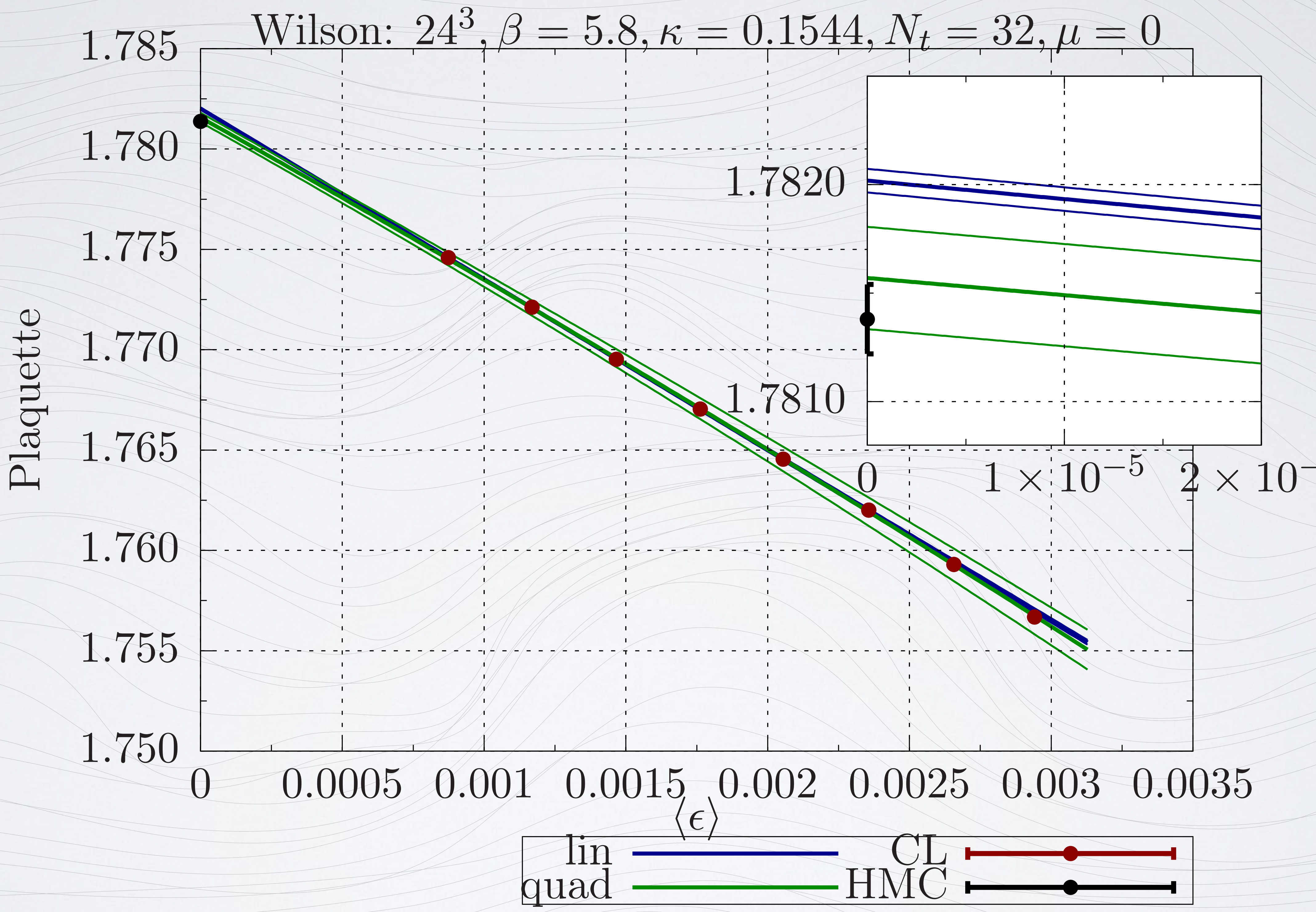
# HMC vs CL - deconfined phase




@ $\mu = 0$

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

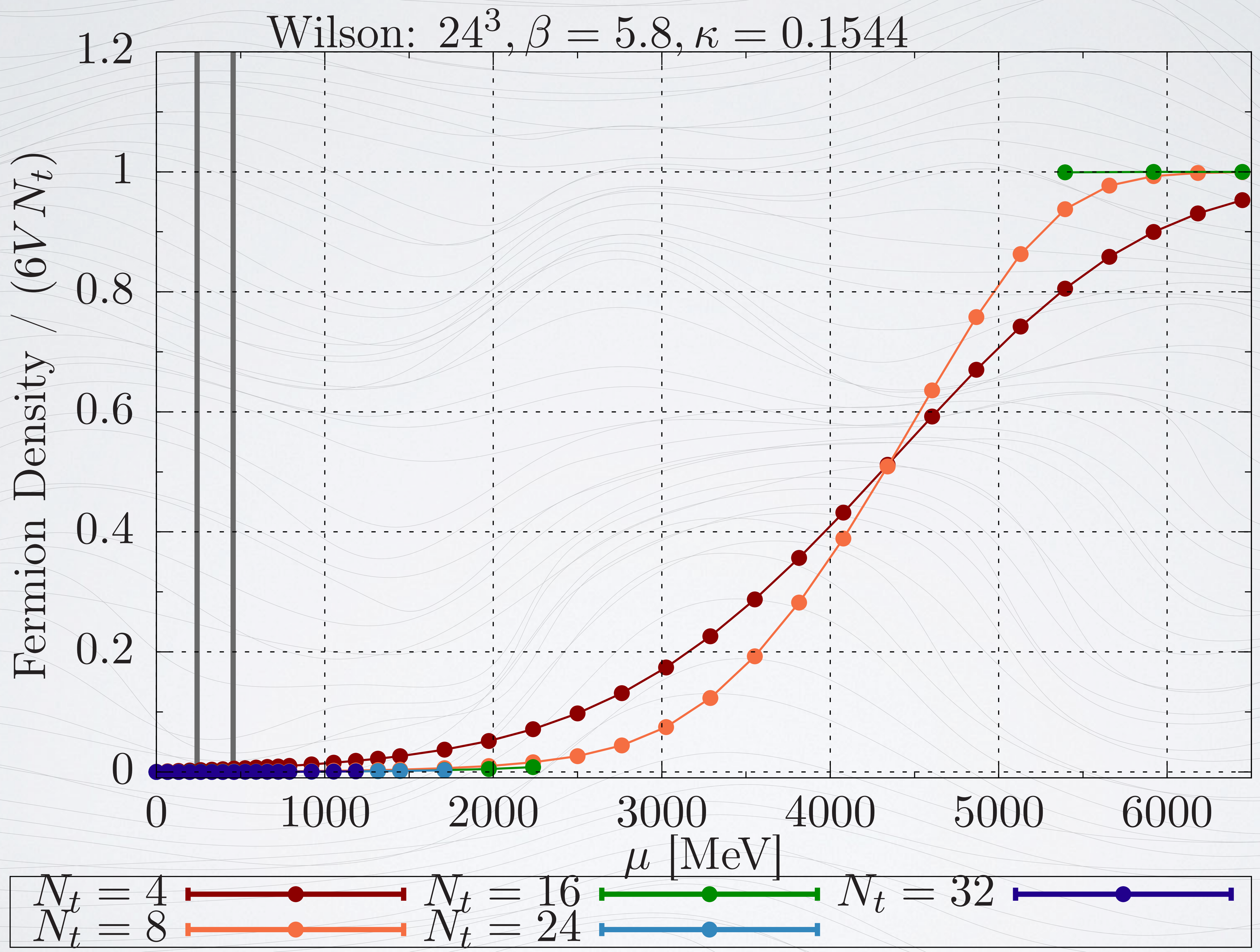
# HMC vs CL - confined phase



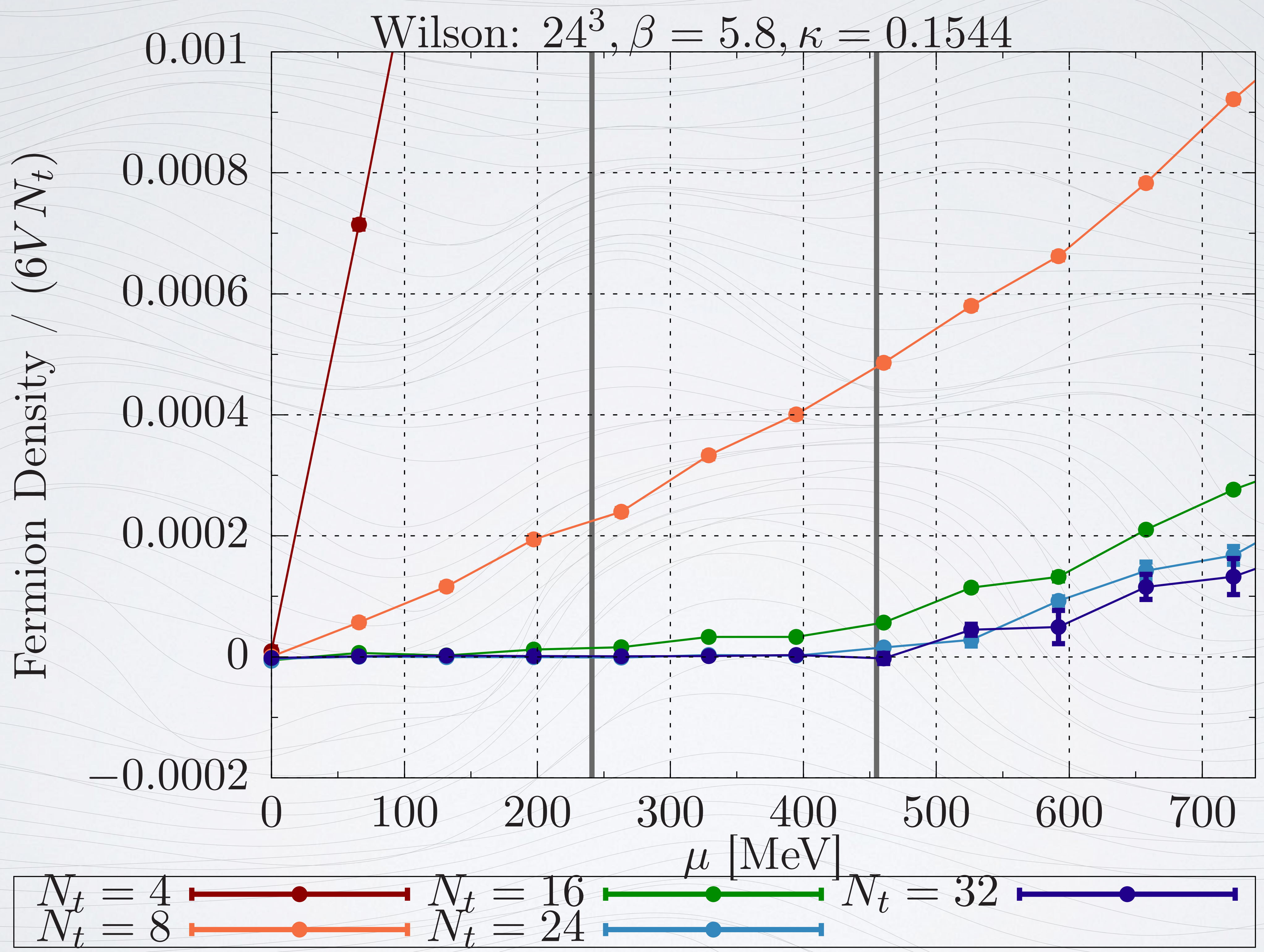

@ $\mu = 0$

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

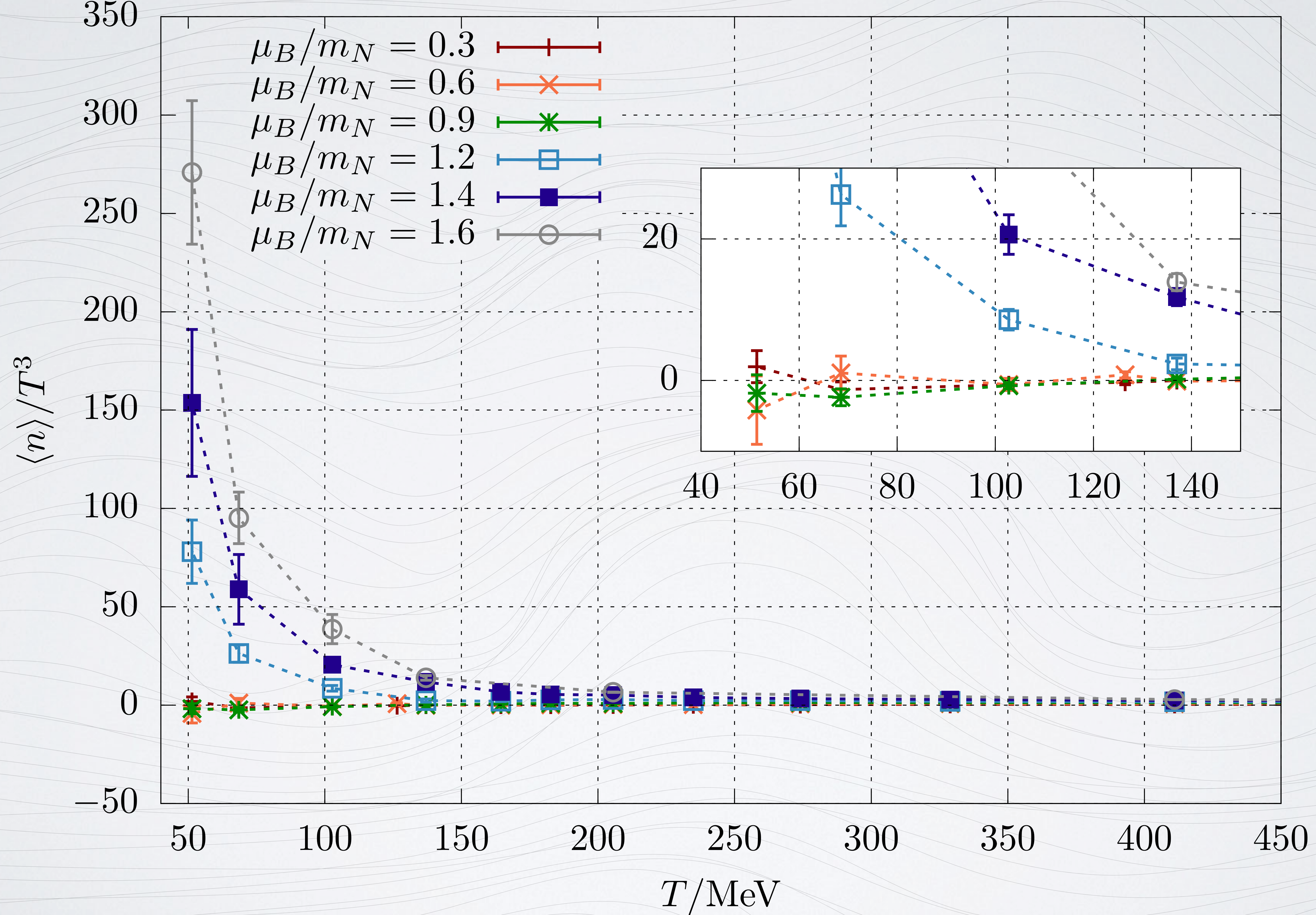
# Fermion Density



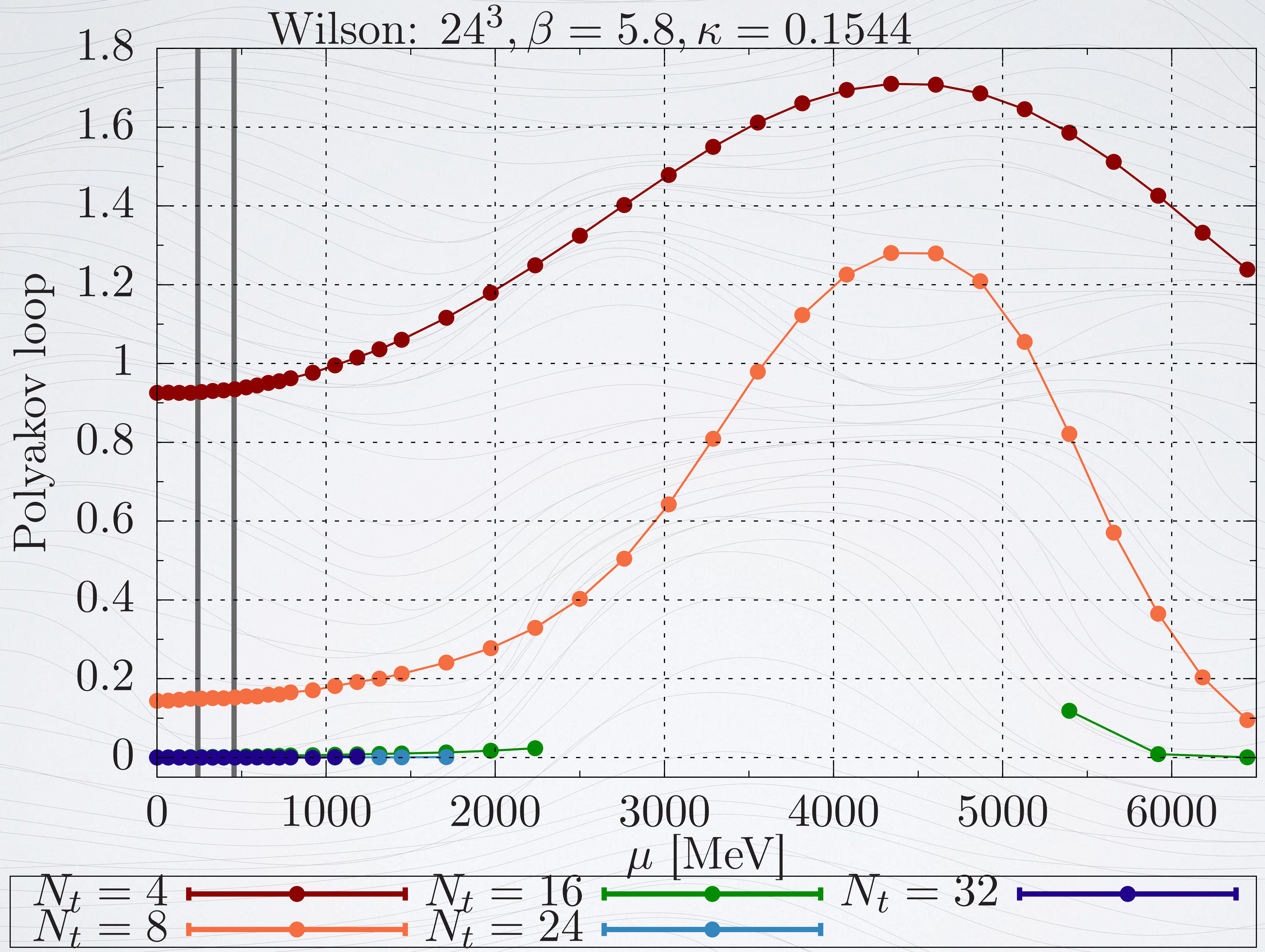
# Fermion Density



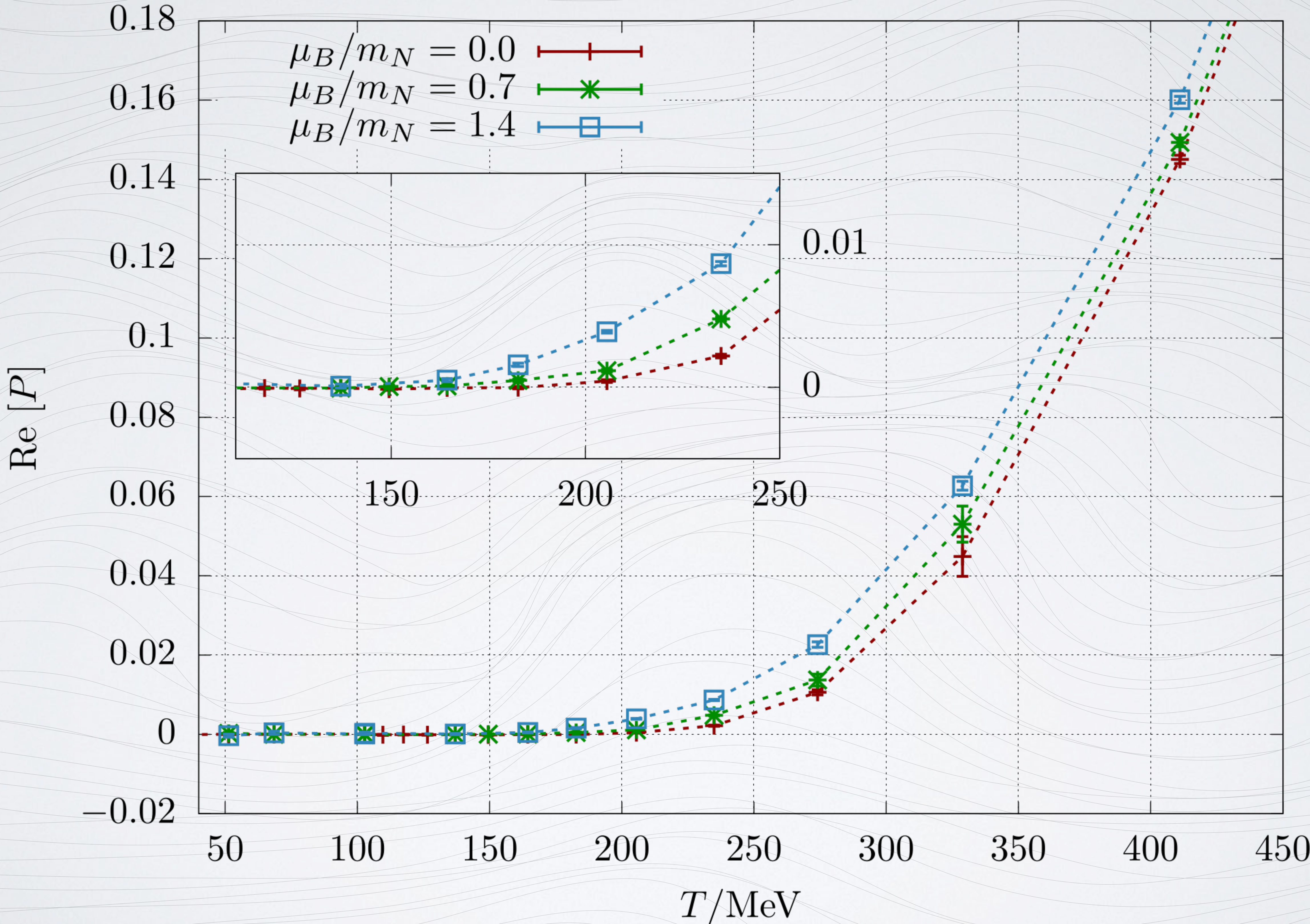
# Fermion Density



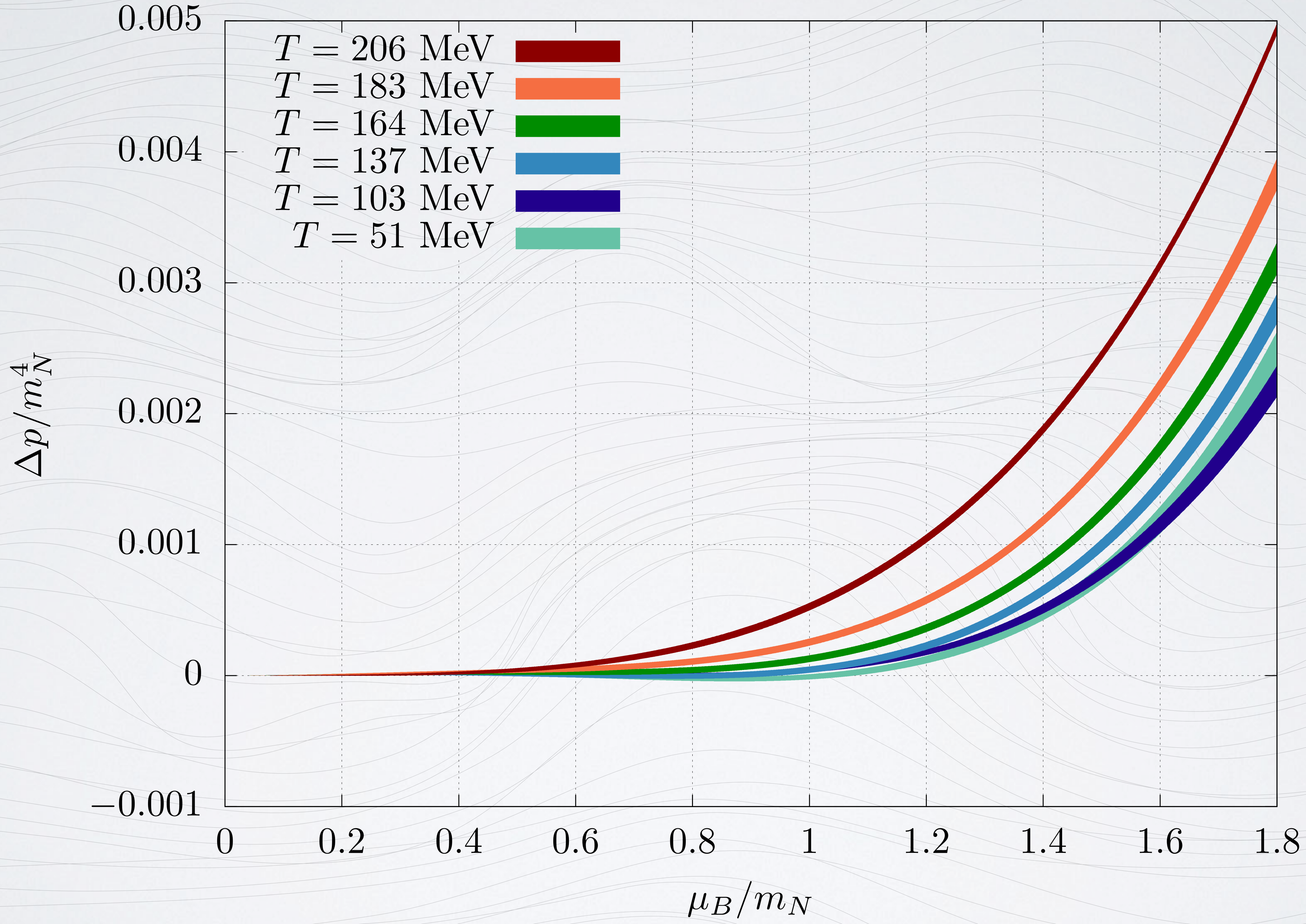
# Polyakov Loop



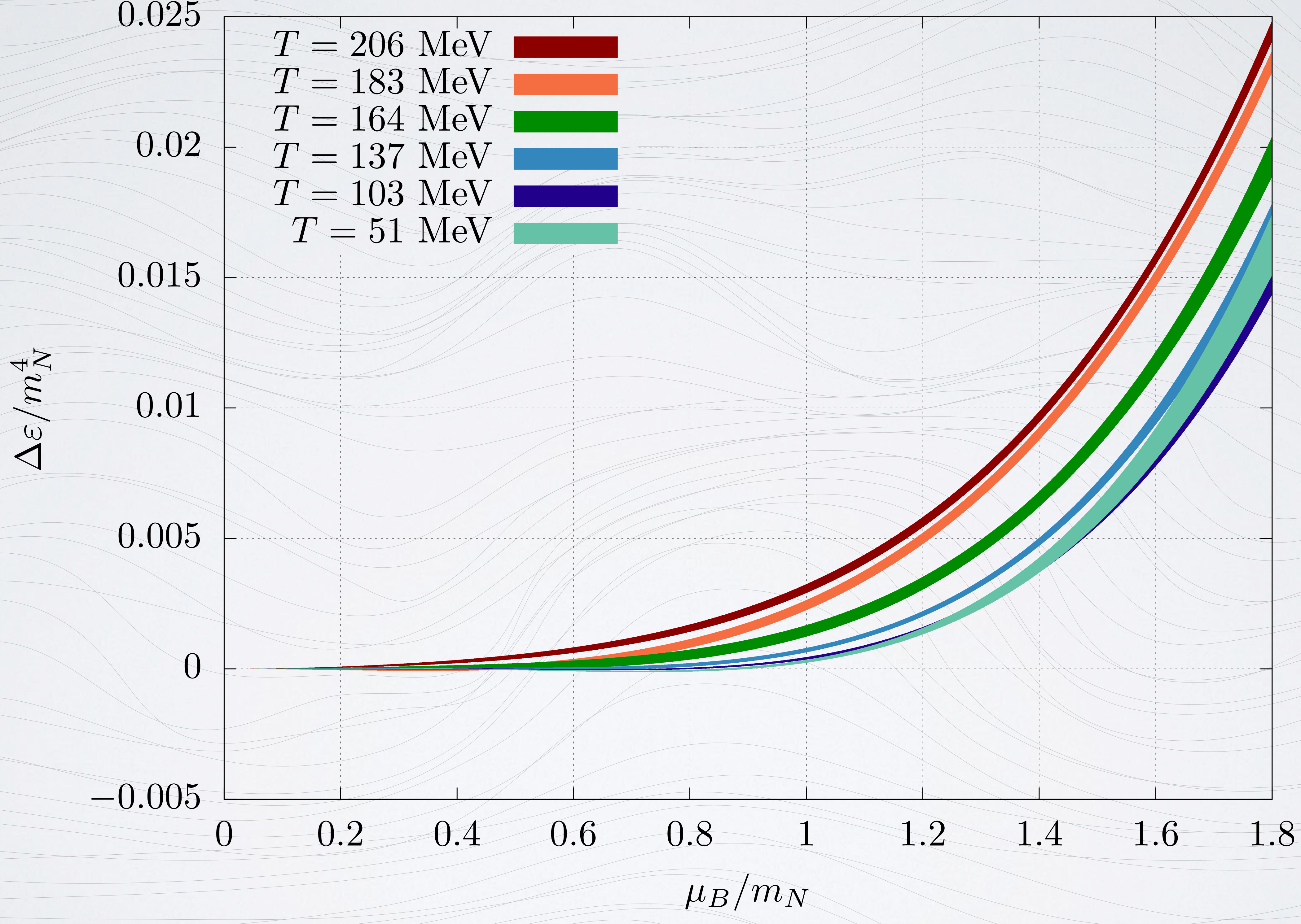
# Polyakov Loop



# Equation of State - Pressure

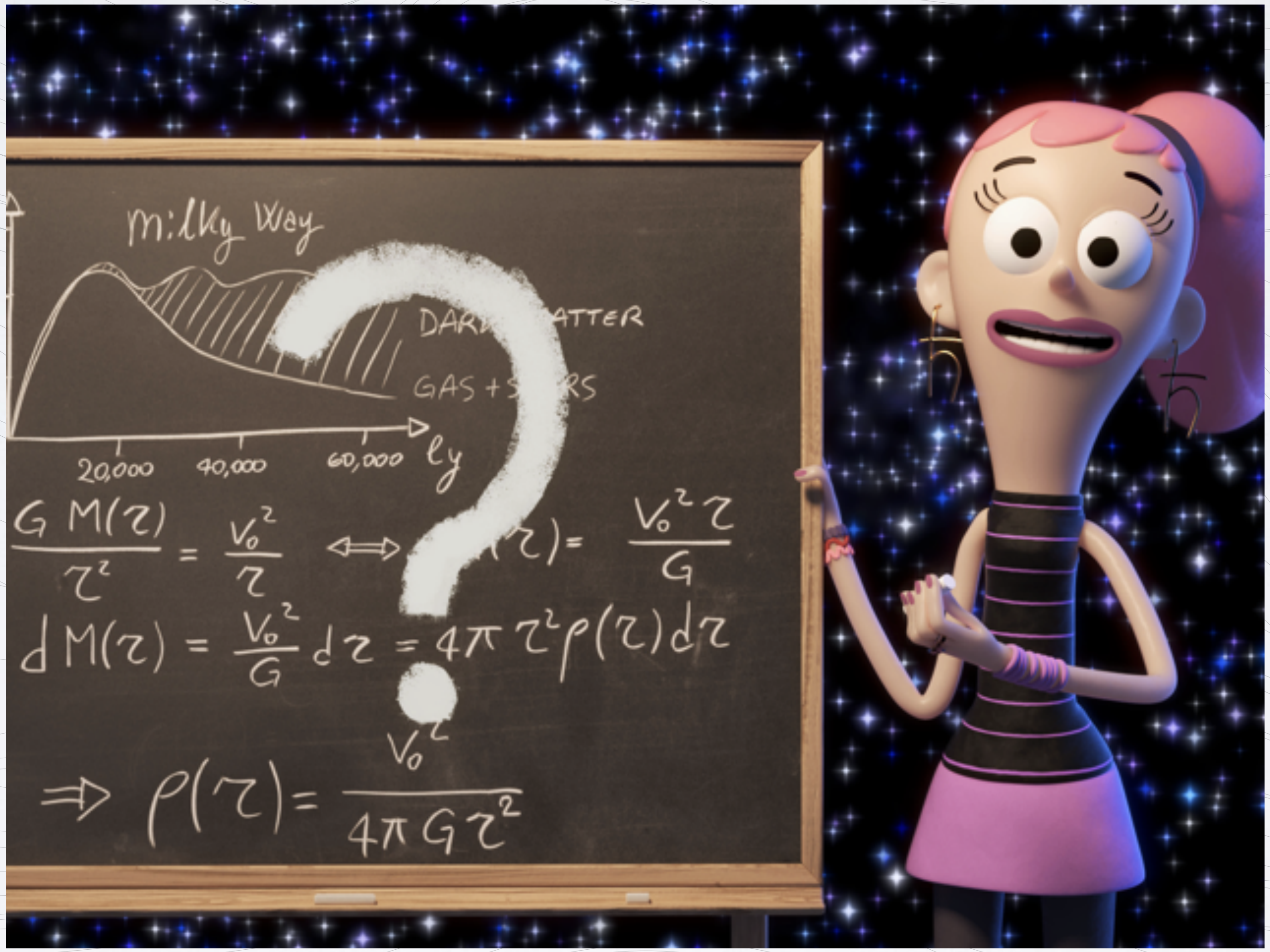


# Equation of State - Energy density



# Questions?

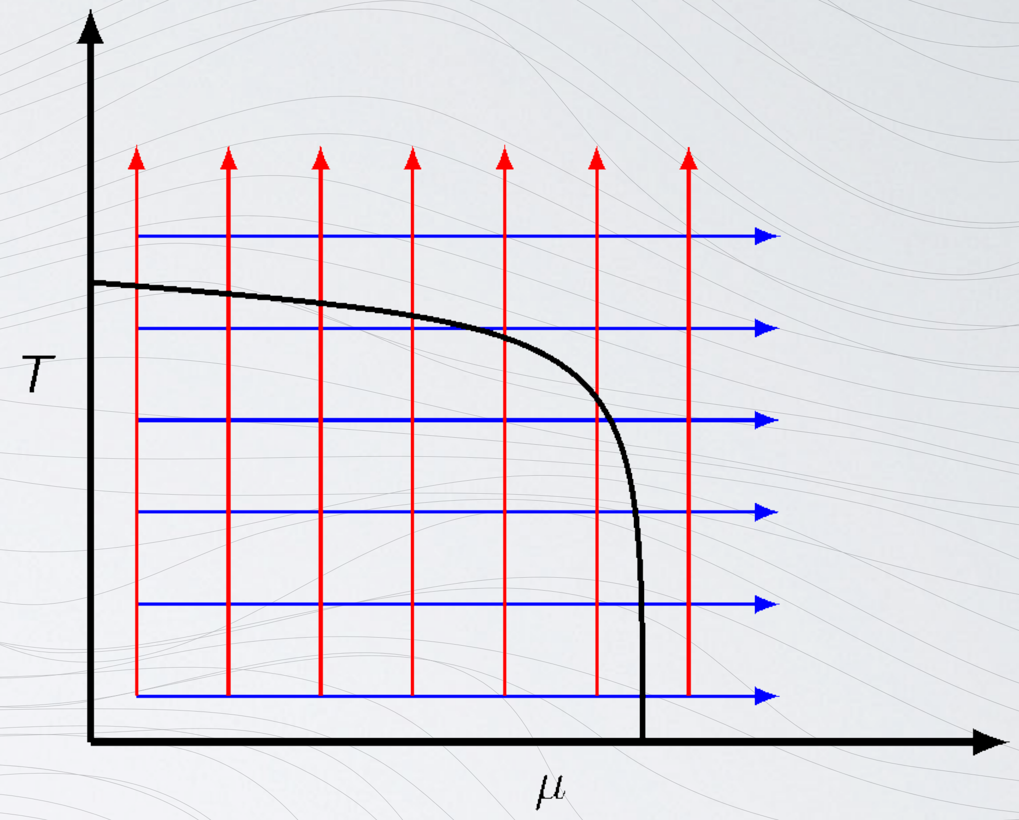
## Thank you for your attention!



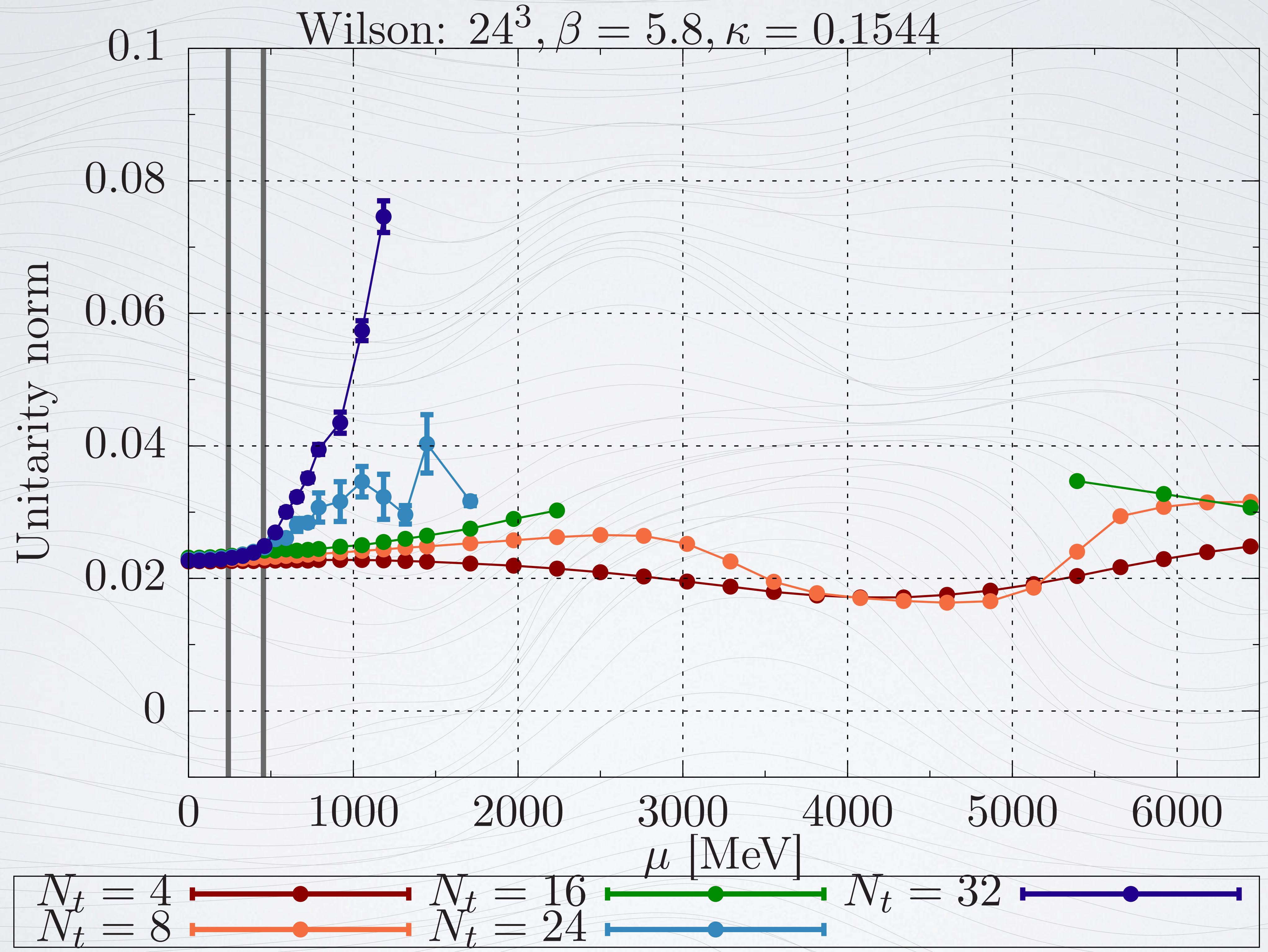

Quantum Kate (orig. Kvante Karina): CP3 Outreach http://www.kvantebanditter.dk/en

# Results

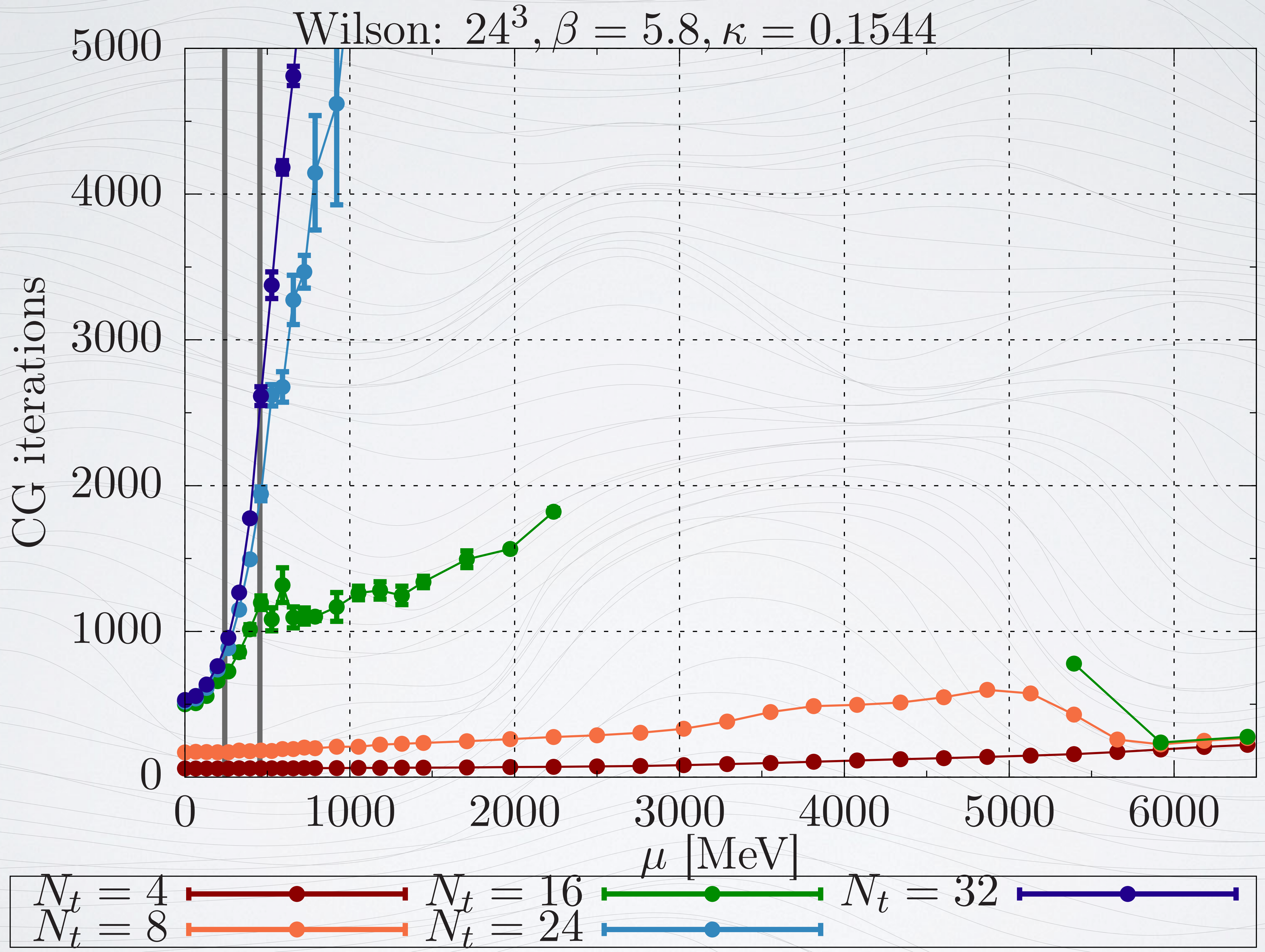
- Consistency checks @ $\mu = 0$
  - HMC vs. CL
- Observables
  - Fermion density
  - Polyakov loop
- **Numerics / Stability**
  - Unitarity norm (distance to SU(3))
  - Iterations (Conjugate Gradient)
- Equation of state



# Unitarity Norm

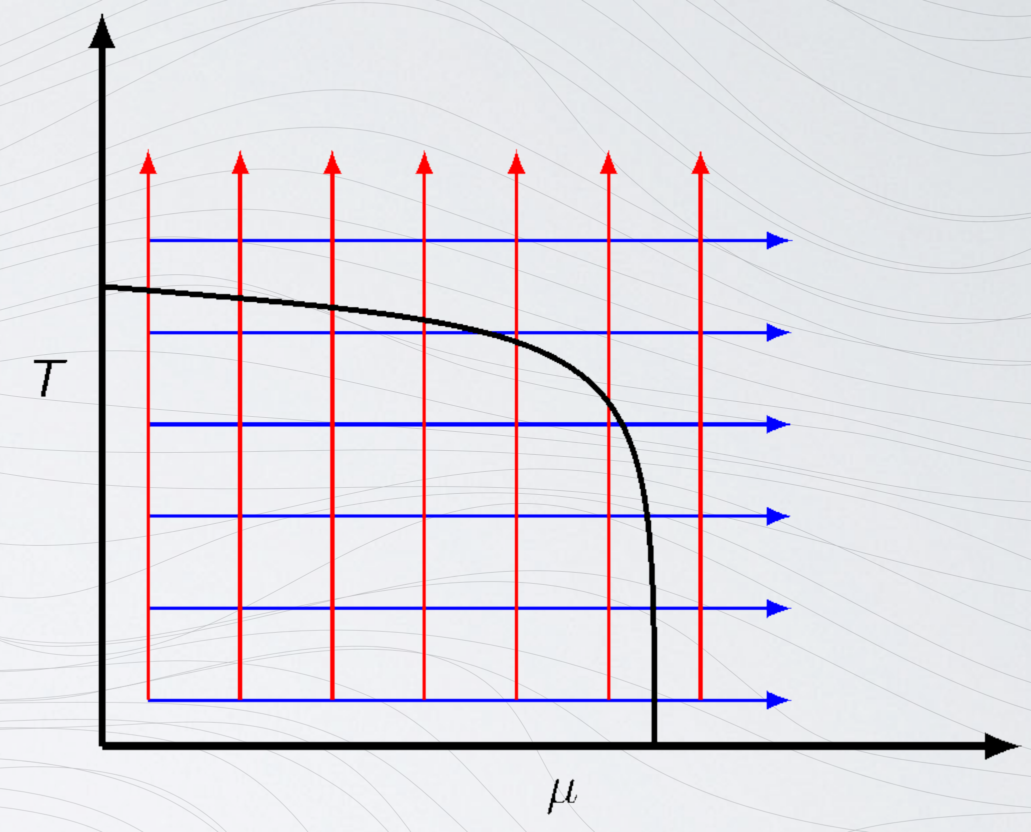


# CG Iterations



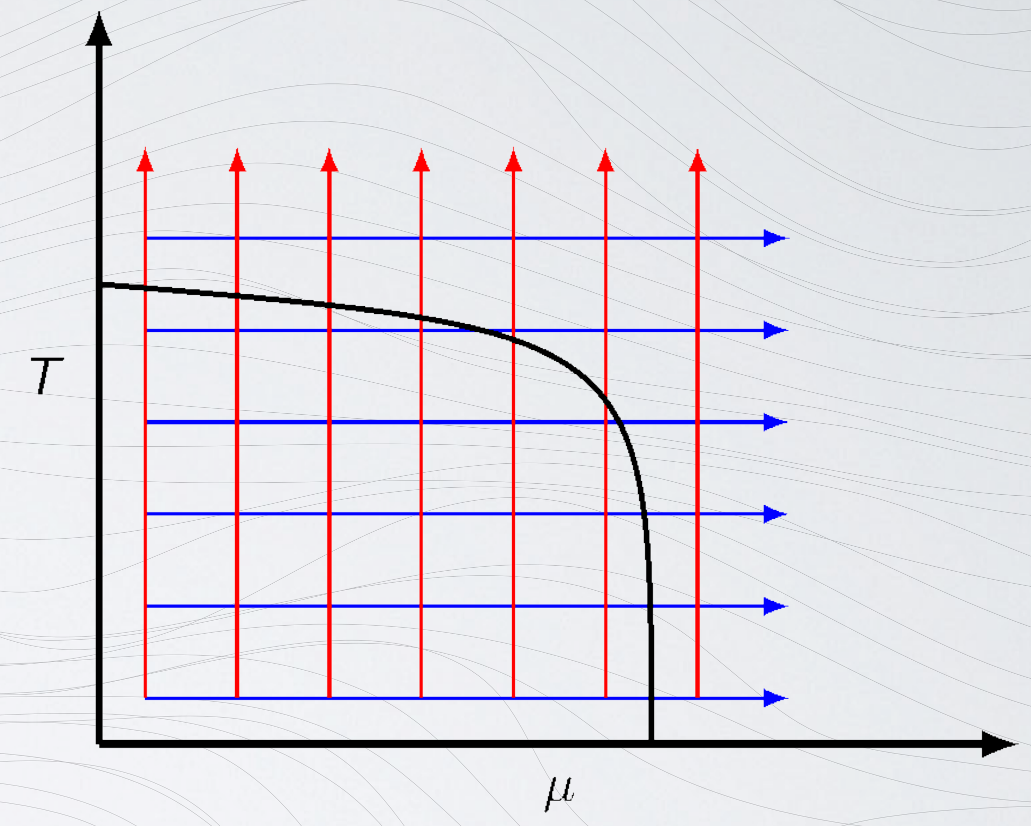
# Results

- 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**

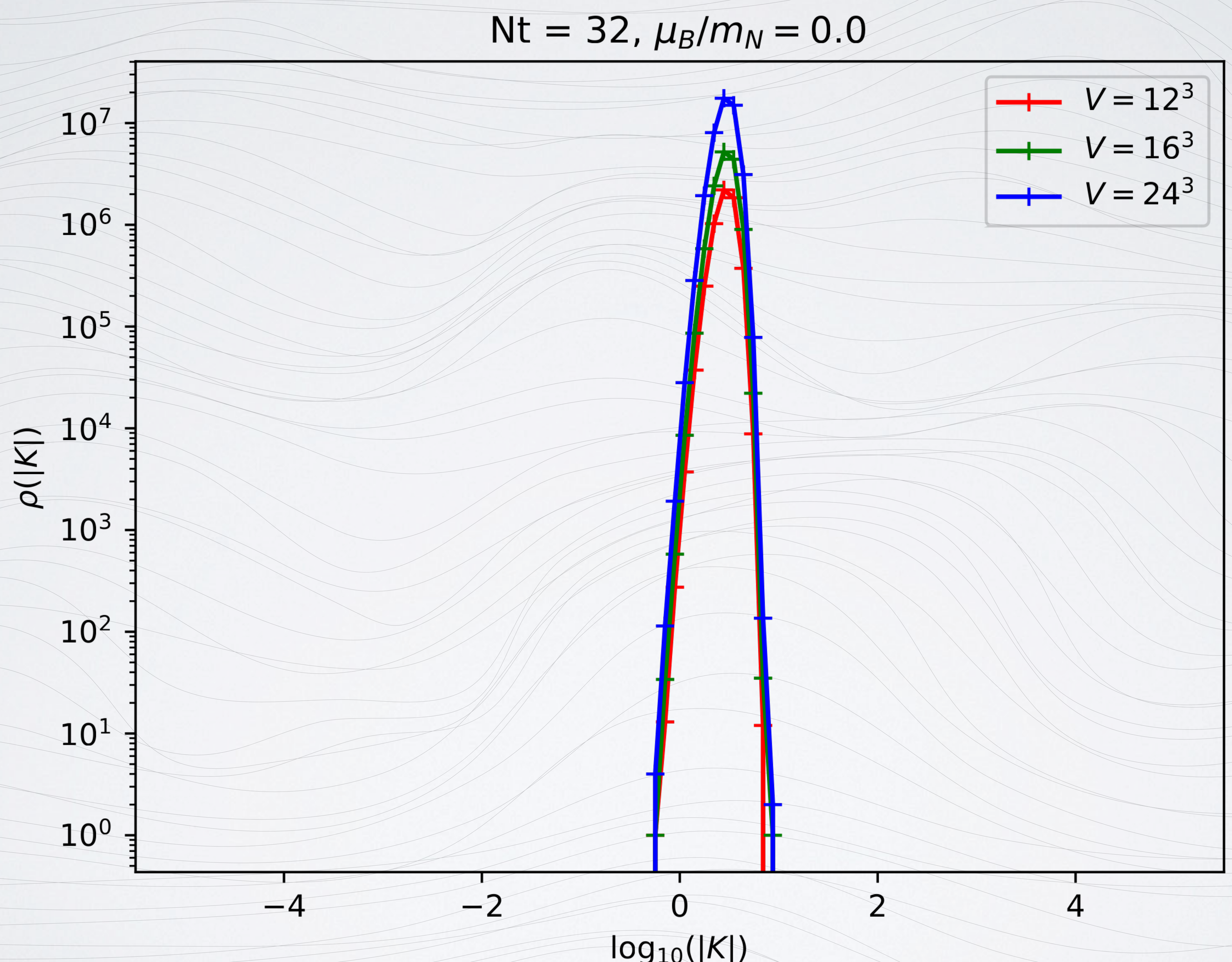


# Results

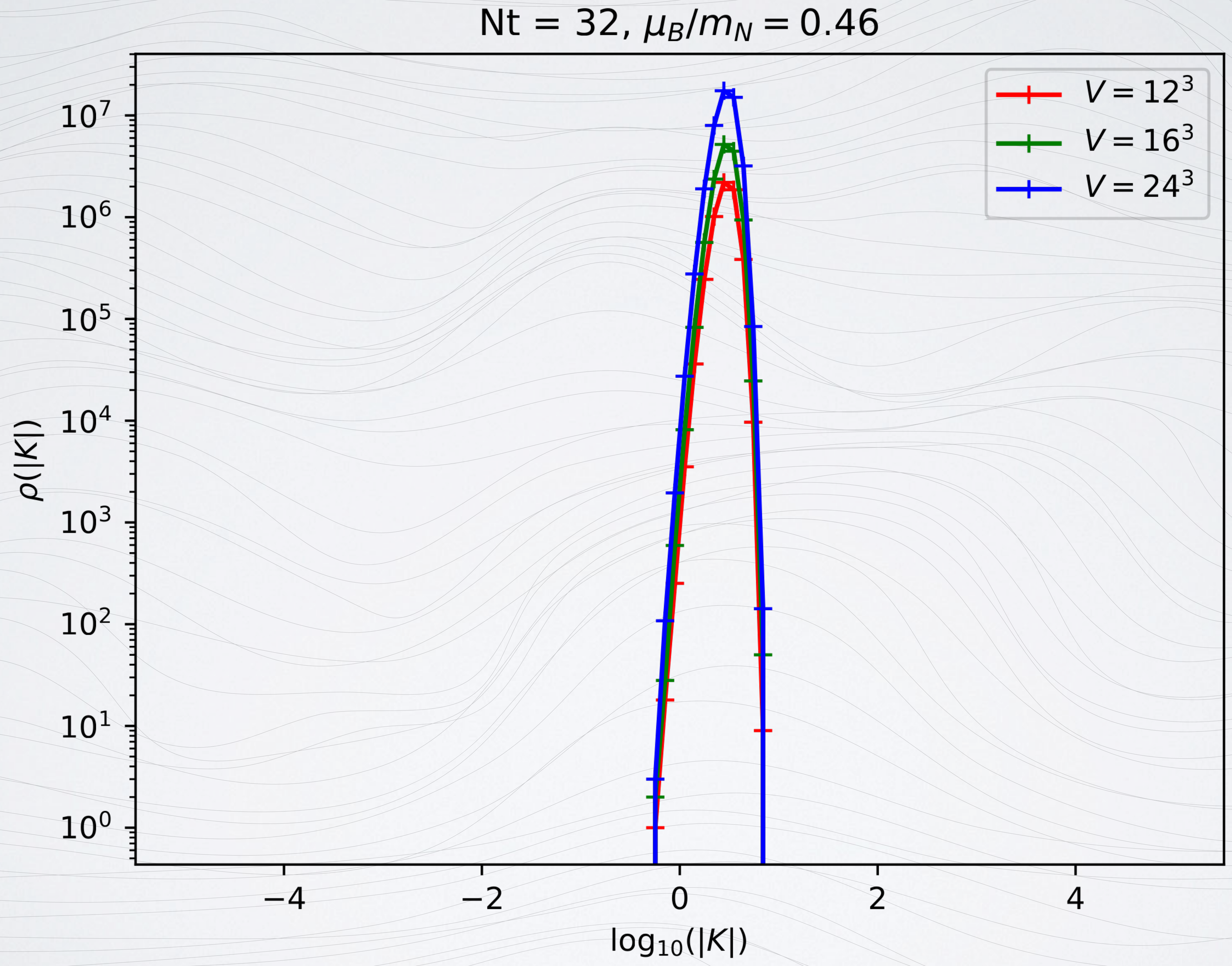
- Consistency checks @ $\mu = 0$
  - HMC vs. CL
- **Histograms**
- Observables
  - Fermion density
  - Polyakov loop
- Numerics / Stability
  - Unitarity norm (distance to SU(3))
  - Iterations (Conjugate Gradient)
- Equation of state



# Histograms

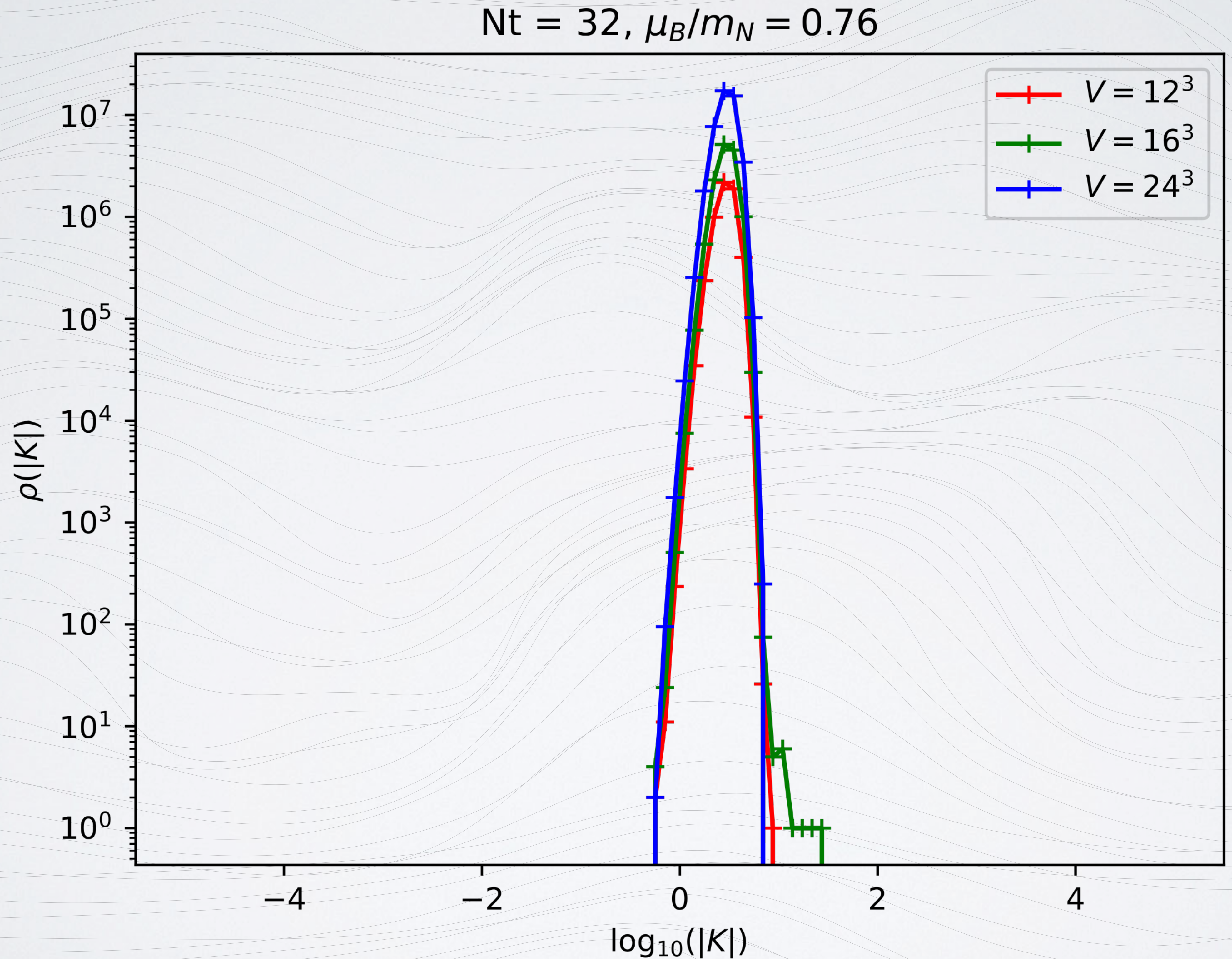


# Histograms



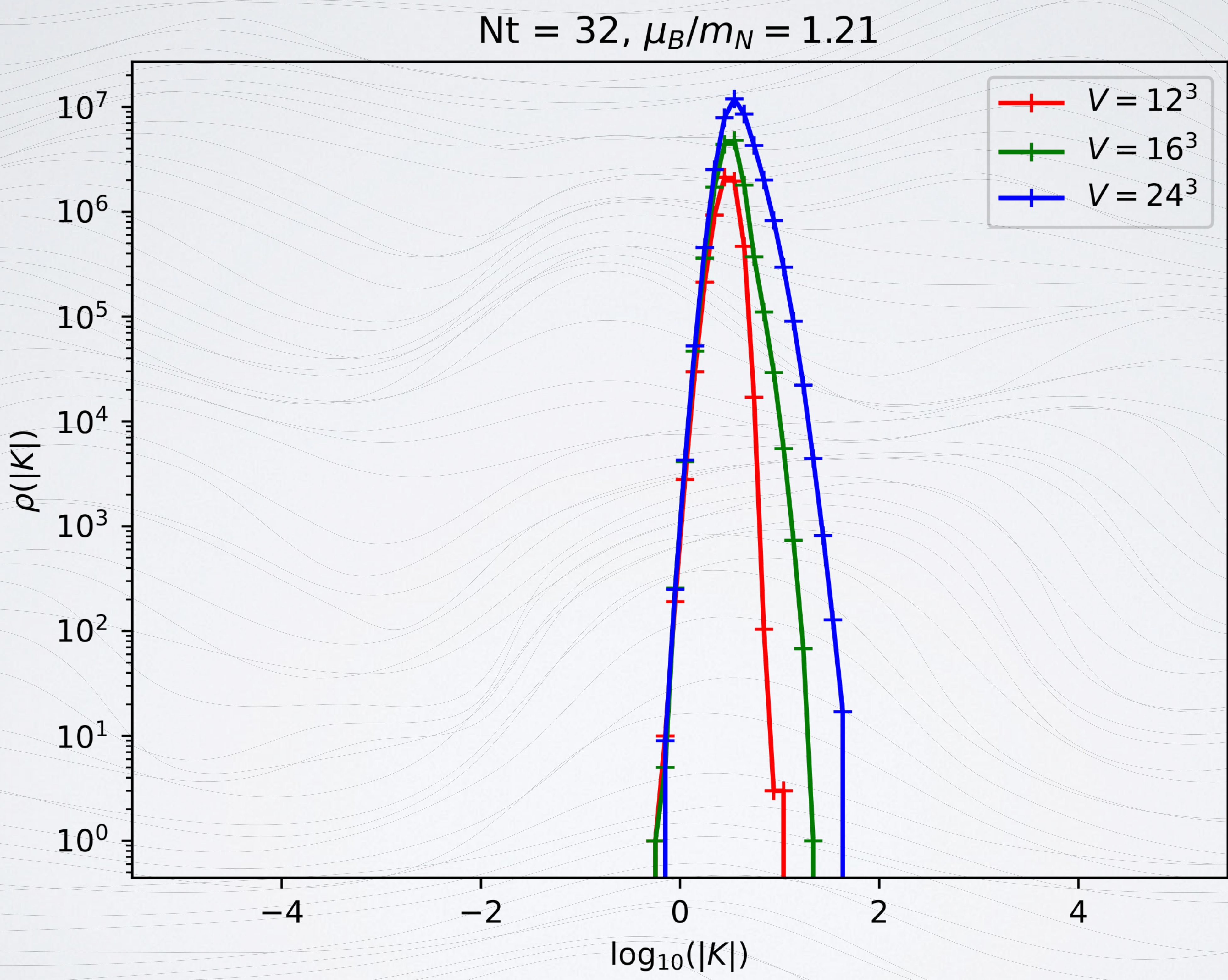
Nt = 32, $\mu_B/m_N = 0.46$
$V = 12^3$
$V = 16^3$
$V = 24^3$
$\rho(|K|)$
$10^7$
$10^6$
$10^5$
$10^4$
$10^3$
$10^2$
$10^1$
$10^0$
−4
−2
0
2
4
$\log_{10}(|K|)$

# Histograms



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

# Histograms



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

# Histograms