FASTSUM
Simulations at finite T and μ

Benjamin Jäger

on behalf of the FASTSUM collaboration

CP3 Origins
Cosmology & Particle Physics

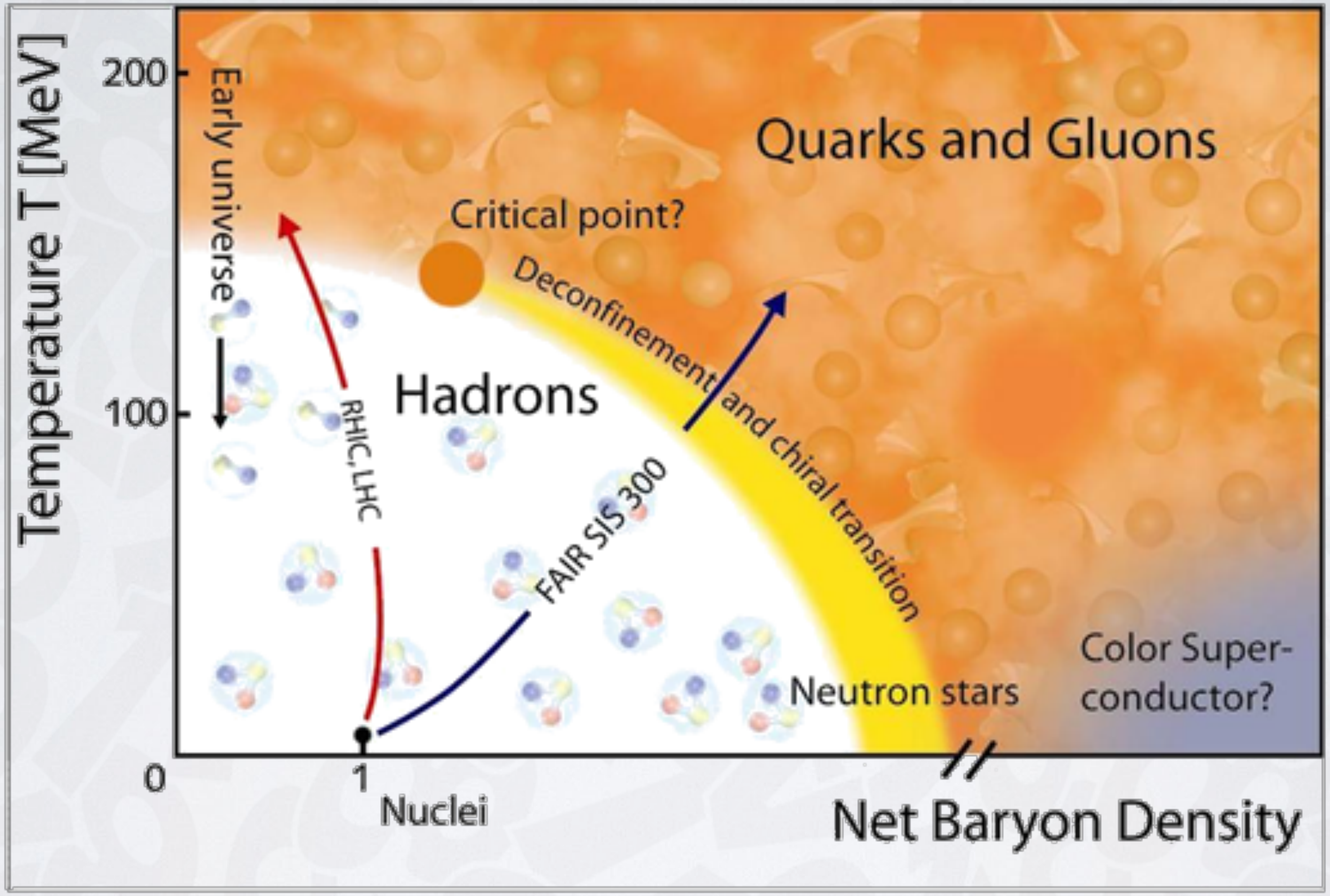
SDU
UNIVERSITY OF SOUTHERN DENMARK

D·IAS

FASTSUM

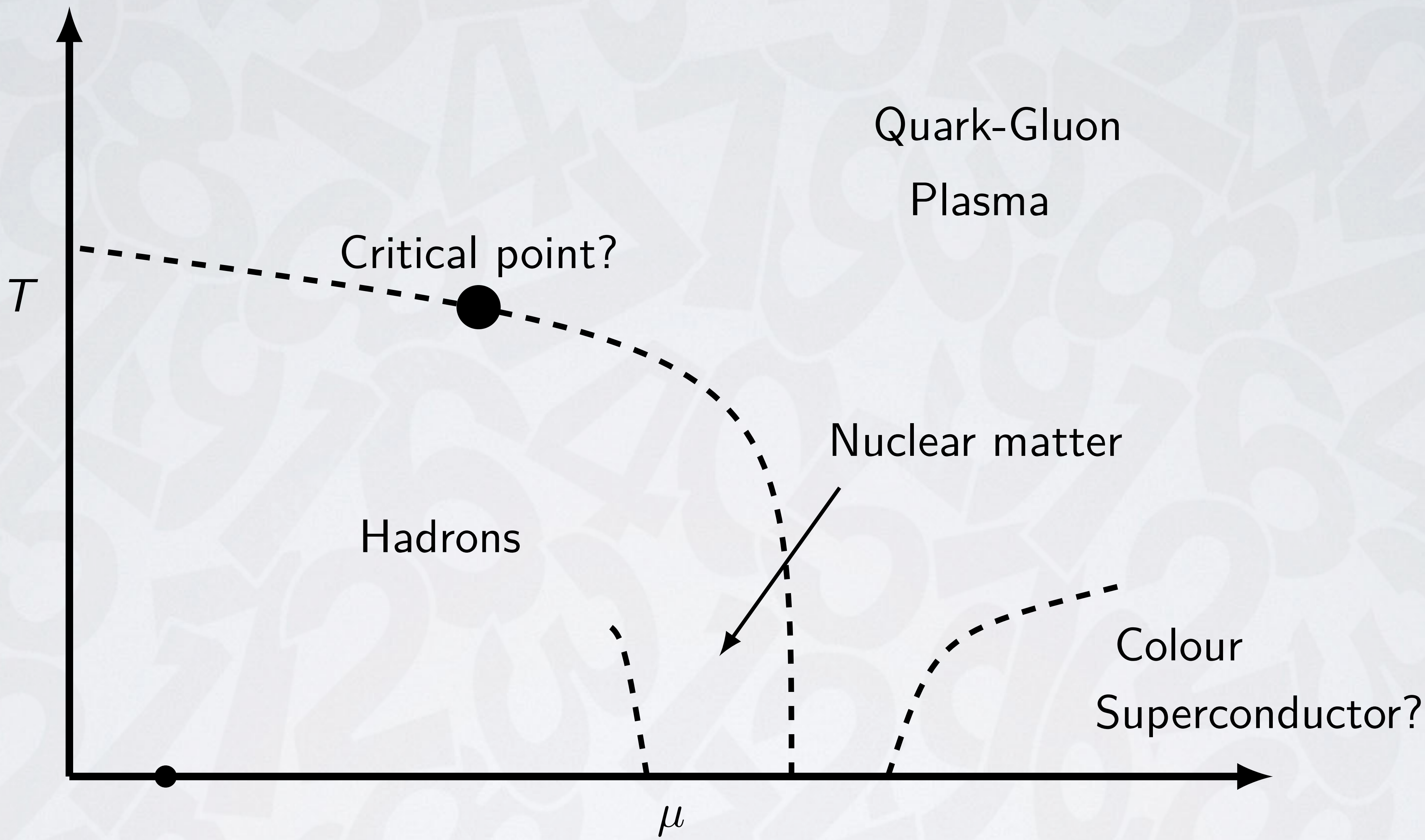
- Gert Aarts (Swansea)
- Chris Allton (Swansea)
- Simon Hands (Swansea)
- Benjamin Jäger (Odense)
- Seyong Kim (Sejong University)
- Maria-Paola Lombardo (Firenze)
- Sinead Ryan (Trinity College Dublin)
- Jonivar Skullerud (Maynooth)
- Liang-Kai Wu (Jiangsu)
- Aleksandr Nikolaev (Swansea)
- Tim Burns (Swansea)
- …

QCD Phase Diagram

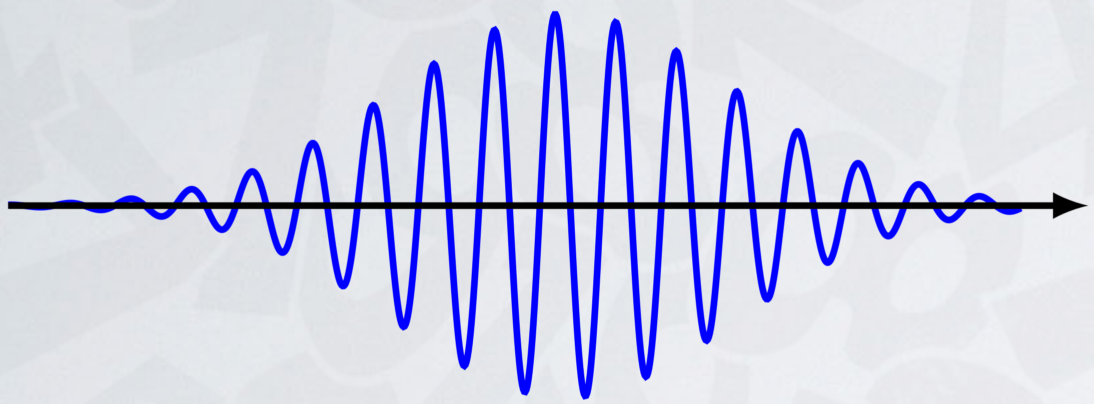


$$\textbf{Scale}: \quad T \sim 100\,\mathrm{MeV} \to 10^{12}\,\mathrm{K}, \qquad \mu \sim 10^{17}\,\frac{\mathrm{kg}}{\mathrm{m}^3}$$

What to expect?



Sign Problem



Sign Problem

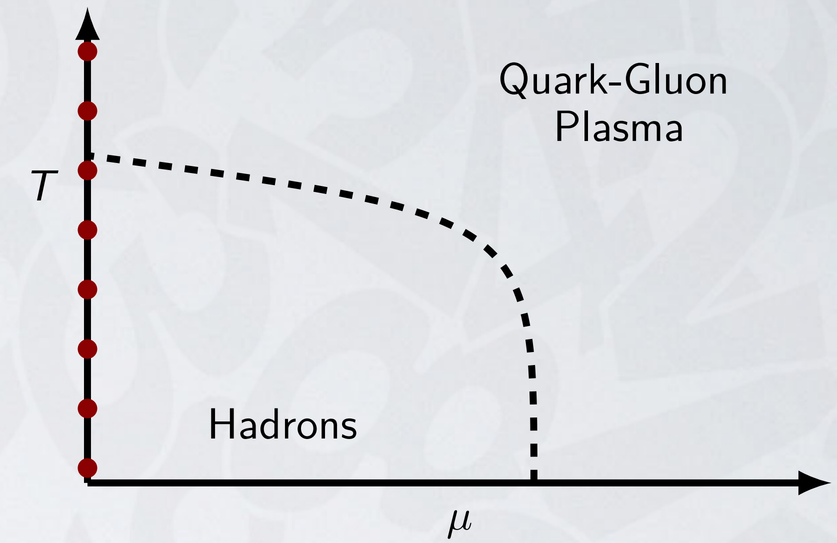
- With $\mu_B \neq 0$ the path integral becomes complex
- Since $\det(D) \in \mathbb{C}$

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

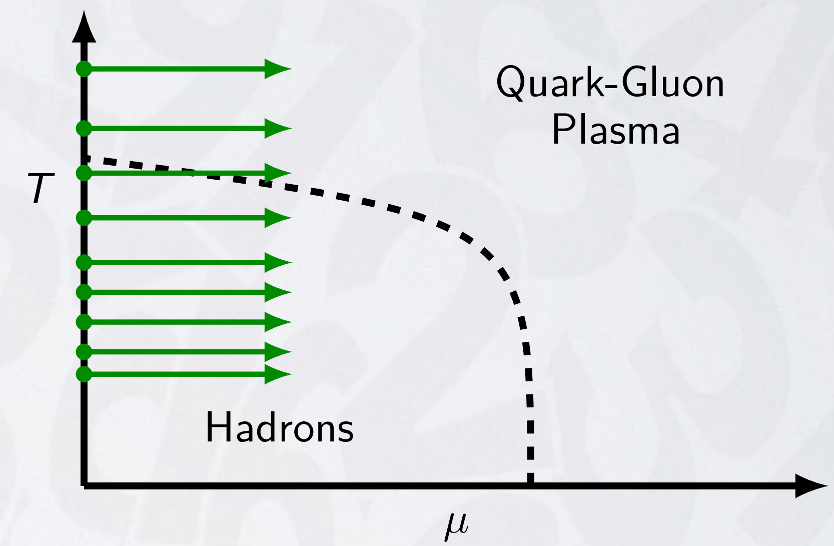
- Importance Sampling Monte Carlo not applicable
- Various other approaches used in practise
- Here: **Taylor expansion** and **Complex Langevin**

Research Projects

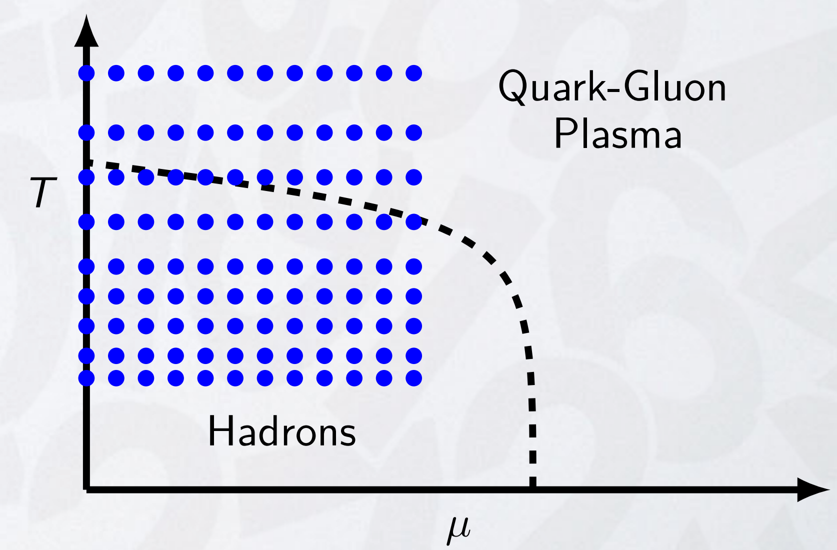
- **Thermodynamics**



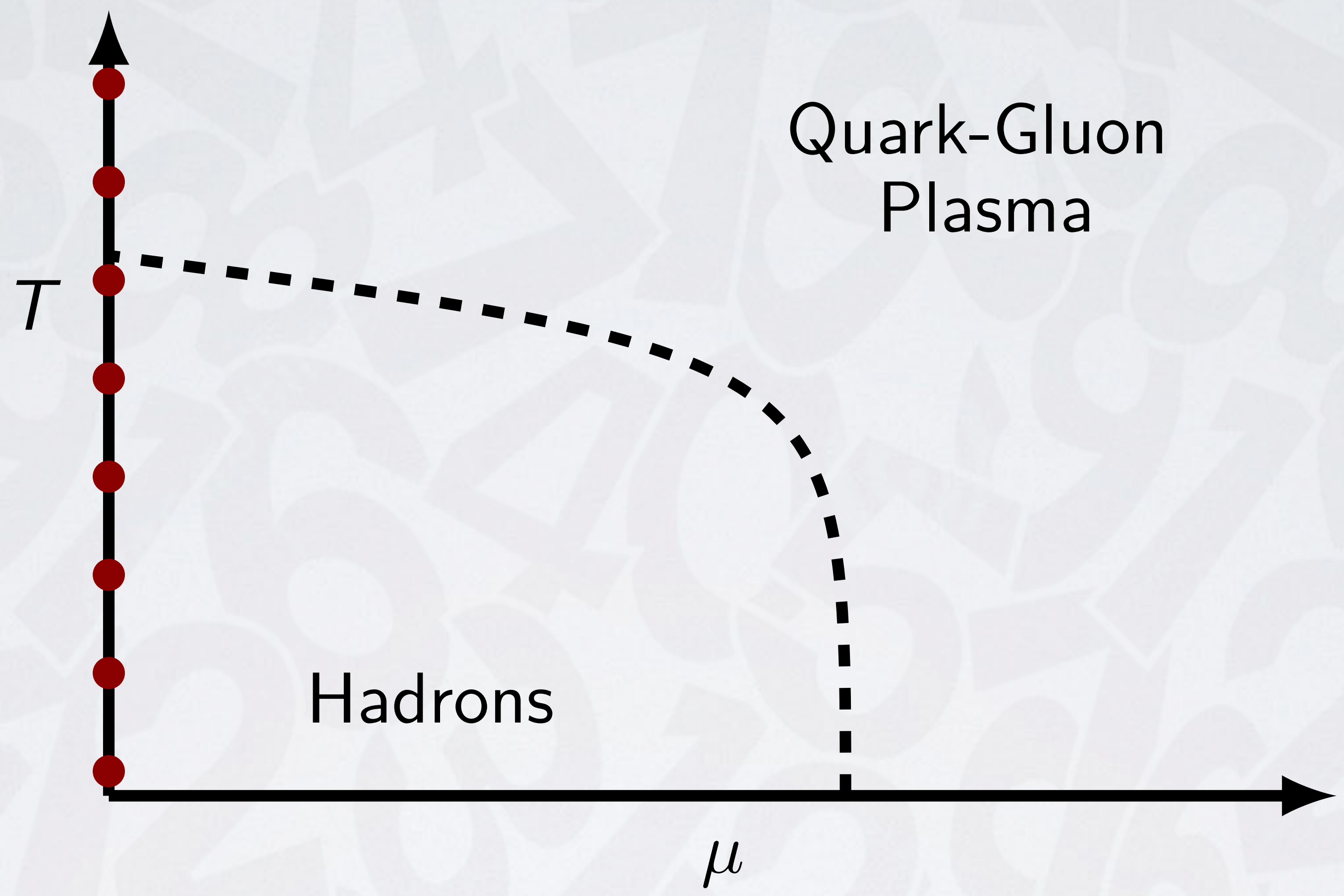
- **Taylor Expansion**



- **Complex Langevin**



Research Projects



Thermodynamics

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Collaboration

- Specialised on finite T with anisotropic lattices
- Simulations at finite μ density

Research agenda

- **Bottomonium**
- Mesons (charm, strange and light)
- **Baryons** (charm, strange and light)
- Transport
- **Finite μ corrections**
- …

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Goal

- Towards the continuum limit with physical quarks
- Anisotropic lattice $\xi = a_s/a_\tau \gg 1$

Strategies

1. continuum time limit $a_\tau \to 0$, a_s fixed, $\xi \to \infty$
2. continuum limit $a_s, a_\tau \to 0, \xi$ fixed
3. physical quarks $m_q \to m_{ud}, m_s$

Current status

- Working on 3. Gen2 $\to$ Gen2L $\to$ Gen2P
- Working on 1. Gen2 $\to$ Gen3

Lattice Setup

Current Lattice details

- $N_f = 2 + 1$ Wilson clover fermions
- Anisotropic lattice spacing $a_s/a_t \sim 3.5$ (Spectroscopy)
- Fixed scale approach, vary temperature by different N_τ
- Continuum limit and physical quark masses
- Stout smeared

	a_s [fm]	a_t [fm]	a_s/a_t	N_s	m_π [MeV]	$m_\pi L$
Gen2	0.01227(8)	0.0350(2)	3.5	24	384(4)	5.7
Gen2l	0.1136(6)	0.0330(2)	3.45	32	236(2)	4.3

Ensembles

Generation 2 ($m_\pi = 384$ MeV, $V = 24^3$)

N_τ	128*	40	36	32	28	24	20	16
T [MeV]	44	141	156	176	201	235	281	352
N_{cfg}	139	500	500	1000	1000	1000	1000	1000

Generation 2l ($m_\pi = 236$ MeV, $V = 32^3$)

N_τ	256*	128	64	56	48	40	36
T [MeV]	23	47	94	107	125	150	167
N_{cfg}	750	300	500	500	500	500	500

N_τ	32	28	24	20	16	12	8
T [MeV]	187	214	250	300	375	500	750
N_{cfg}	1000	1000	1000	1000	1000	1000	1000

*generated by HadSpec collaboration

More statistics to come: 500 $\rightarrow$ 1000 configs

Future

Future plans:

- Generation 3 (Anisotropy $\xi = a_s / a_\tau = 7$)
- Tuning in progress (multi dimensional tuning)

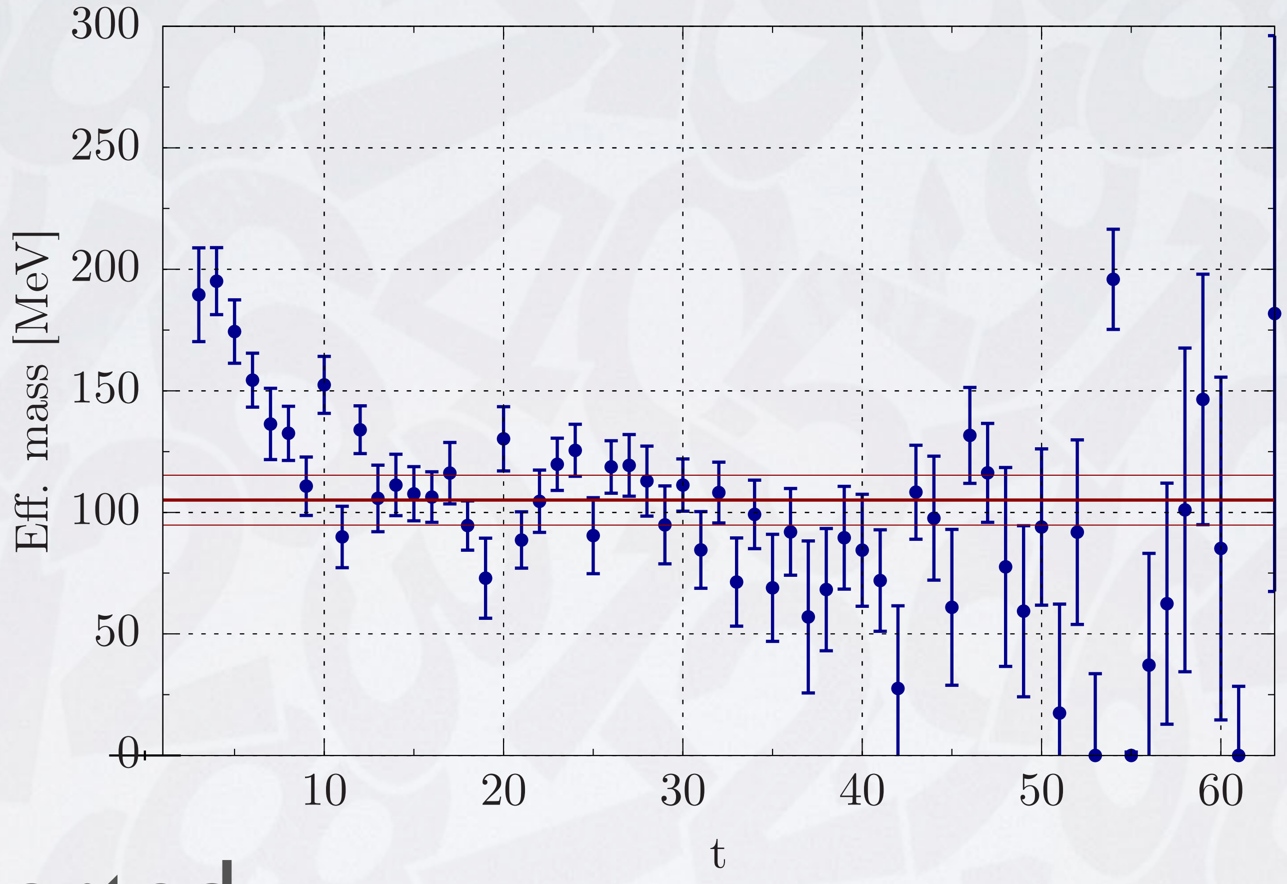
- Temporal resolution double as fine
- Important for spectral reconstruction

- Simulations will commence soon :)

Future

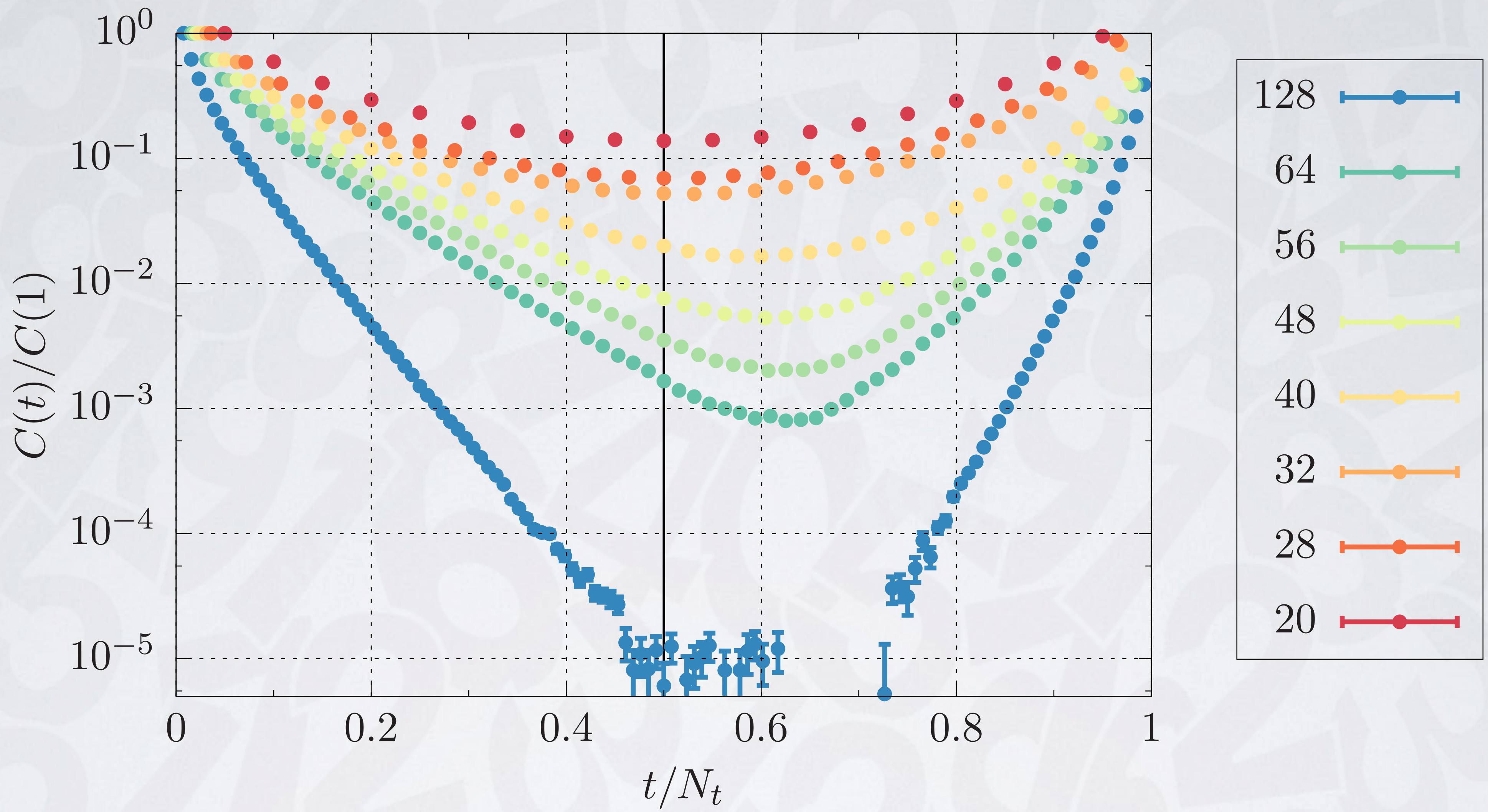
Future plans:

- Generation 2P (physical quark mass)



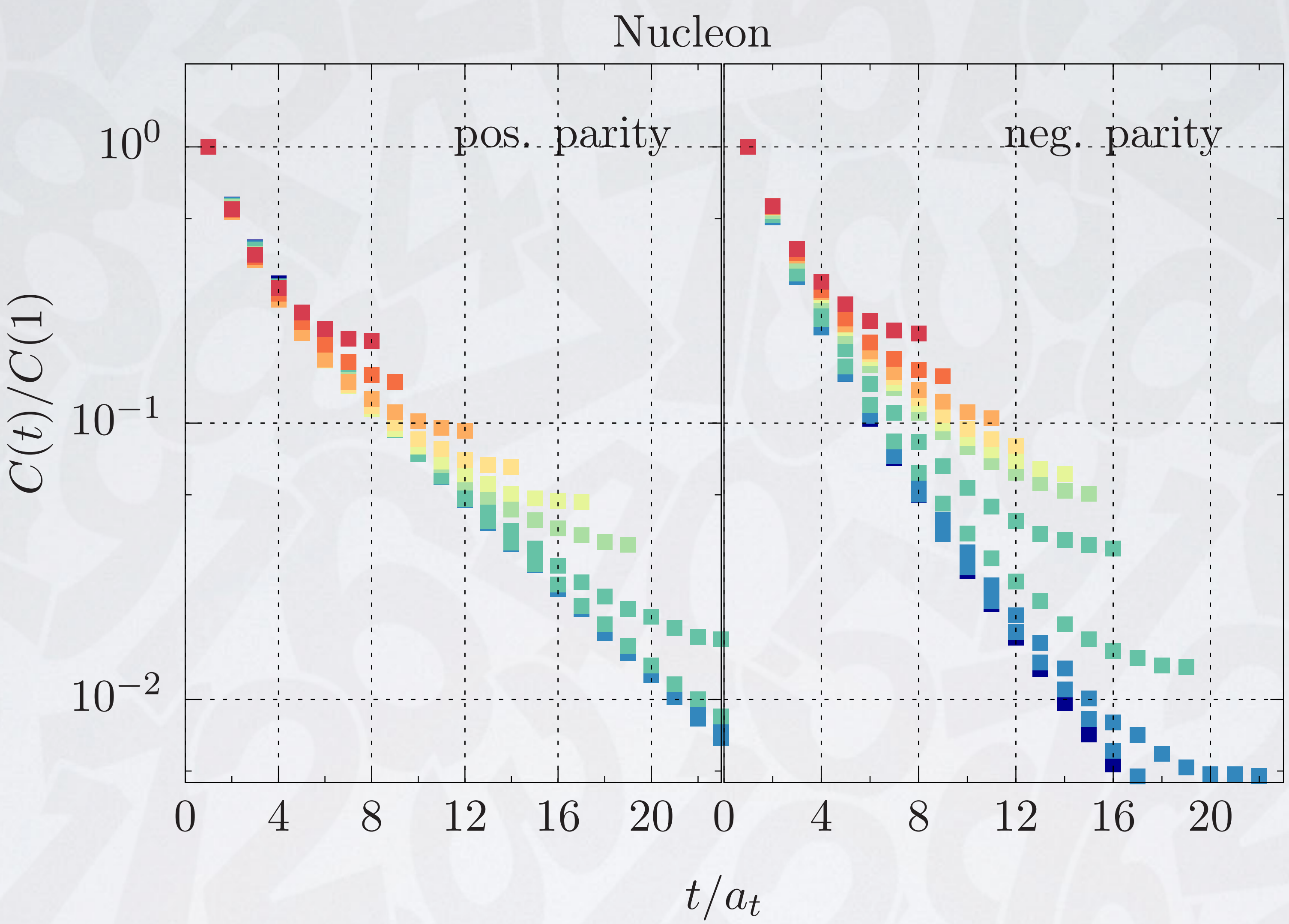
- Tuning started
- Anisotropic lattices @ physical quark masses

Baryons @ finite T



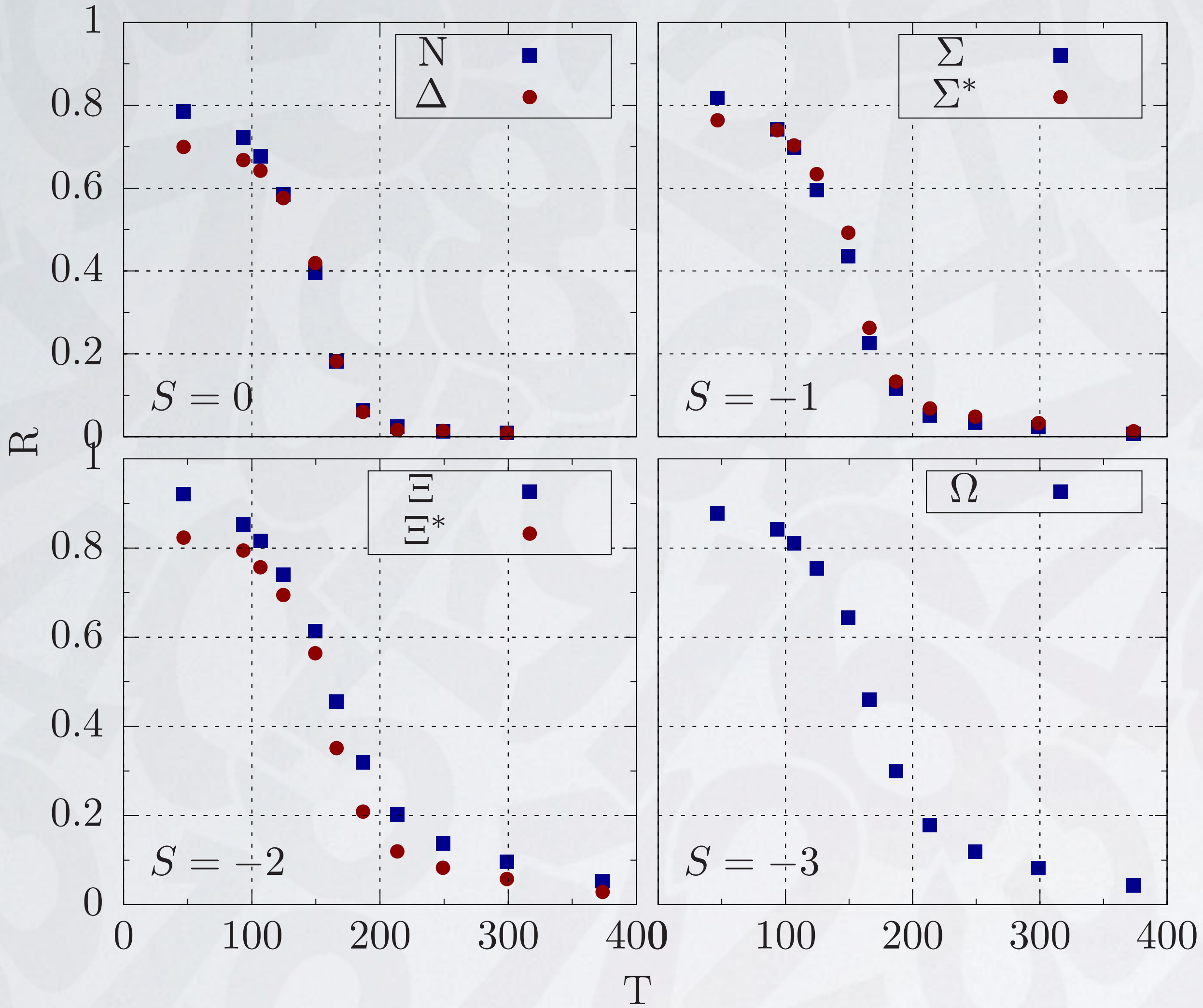
- Baryons are fermions with $T\ C_+(t) = C_-(N_t - t)$
  - Forward in time: Positive parity
  - Backwards in time: Negative parity

Baryons @ finite T



- Positive parity almost not affected by temperature
- Negative parity changes significantly with temperature

Baryons @ finite T



Define ratio

$$R(t) = \frac{C(t) - C(N_t - t)}{C(t) + C(N_t - t)}$$

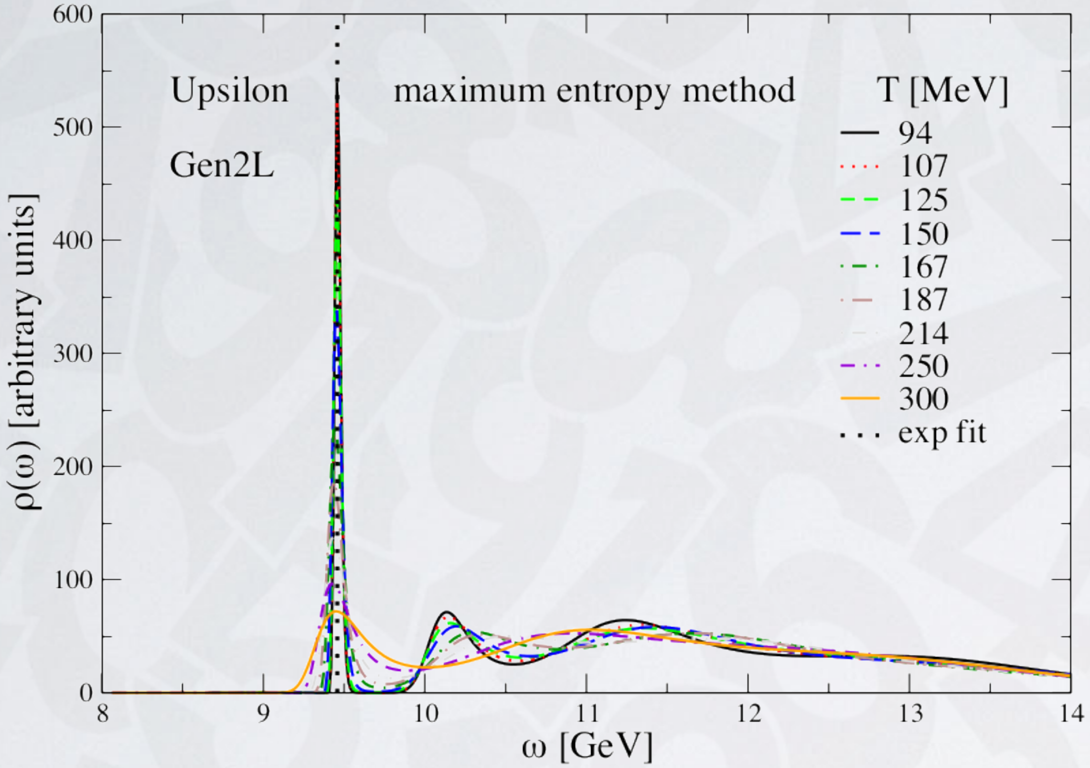
Summed ratio

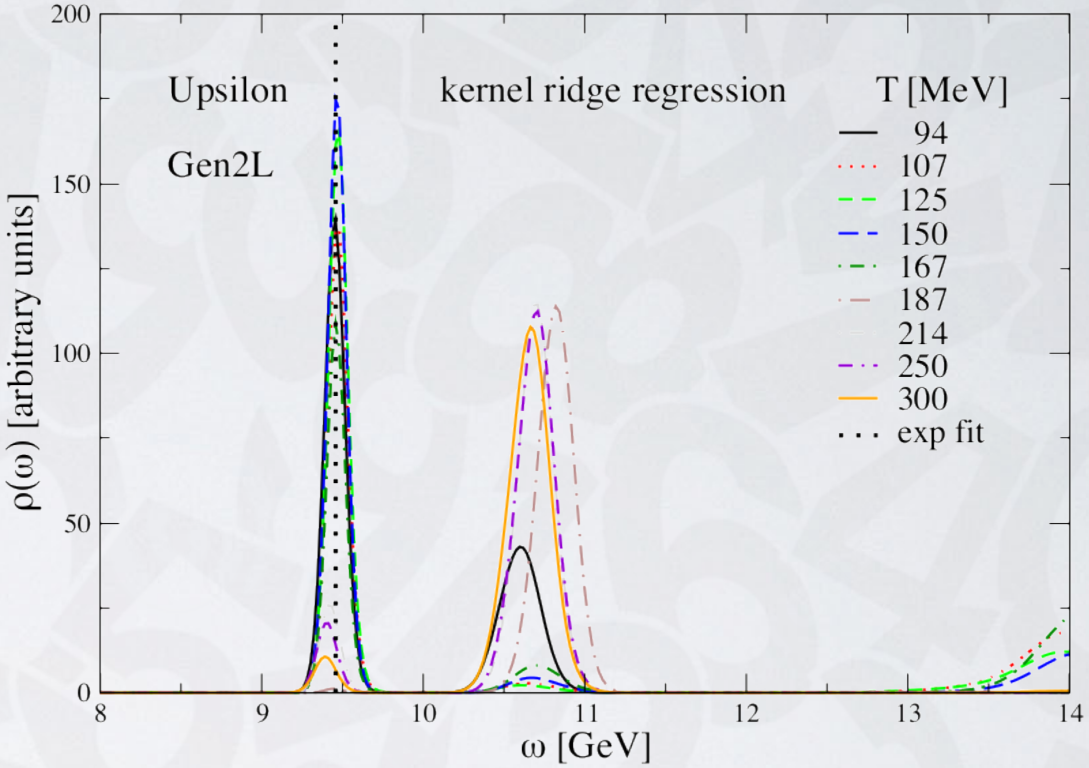
$$R = \sum_t \frac{R(t)/\sigma_t^2}{1/\sigma_t^2}$$

$$0 \leq R \leq 1$$

- If $C(t) = C(N_t - t)$ then $R \to 0$
- R is a measure of parity restoration, when $R \to 0$
- Can be used as a "thermometer"

Bottomonium



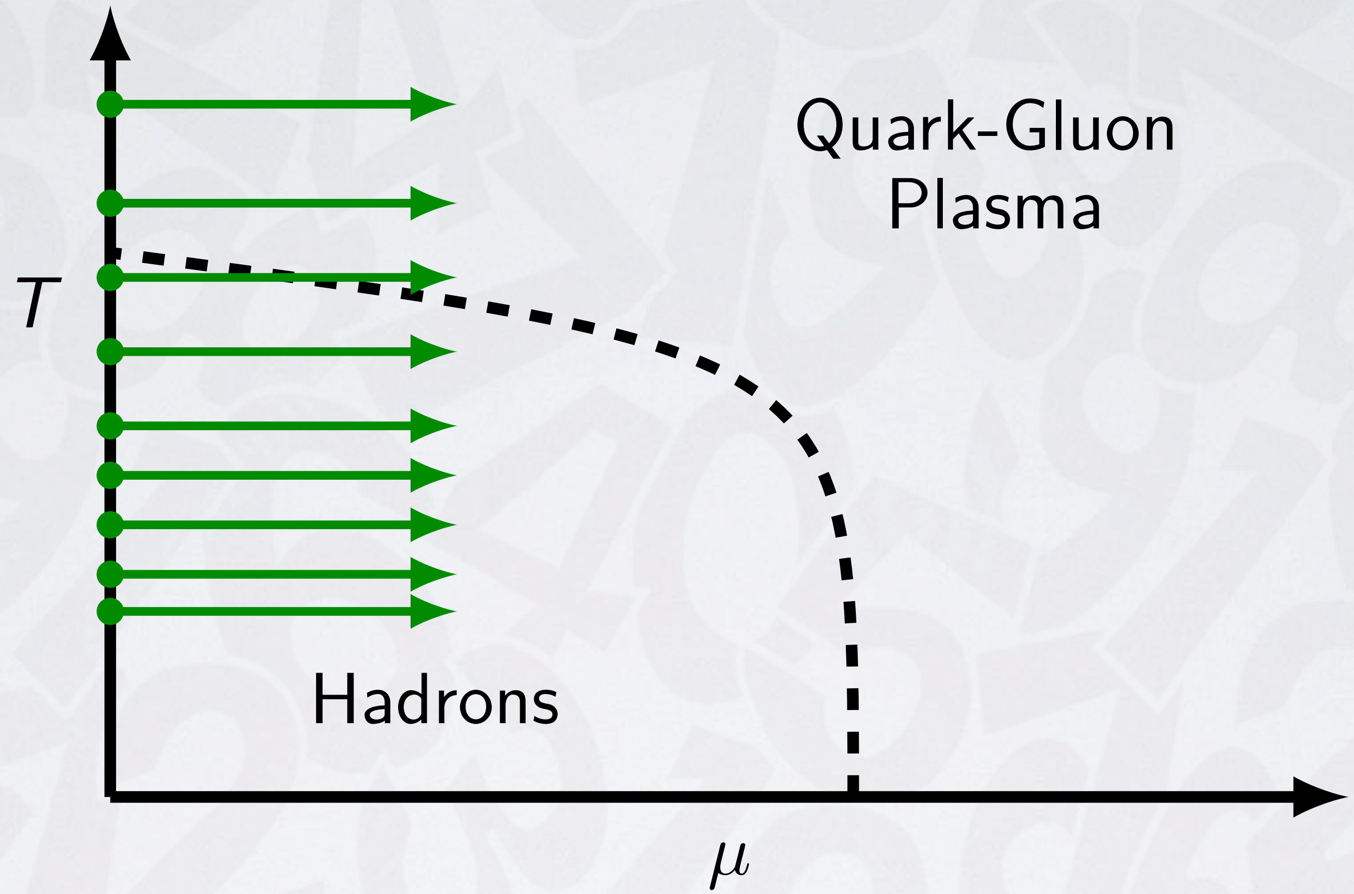


from 1912.12900

Spectral Reconstruction using ML

- MEM (Maximum Entropy Method) (left)
- KRR (Kernel Ridge Regression) (right)

Research Projects



Taylor Expansion

Taylor Expansion

Taylor expansion of observables

- Avoid sign problem by expanding from

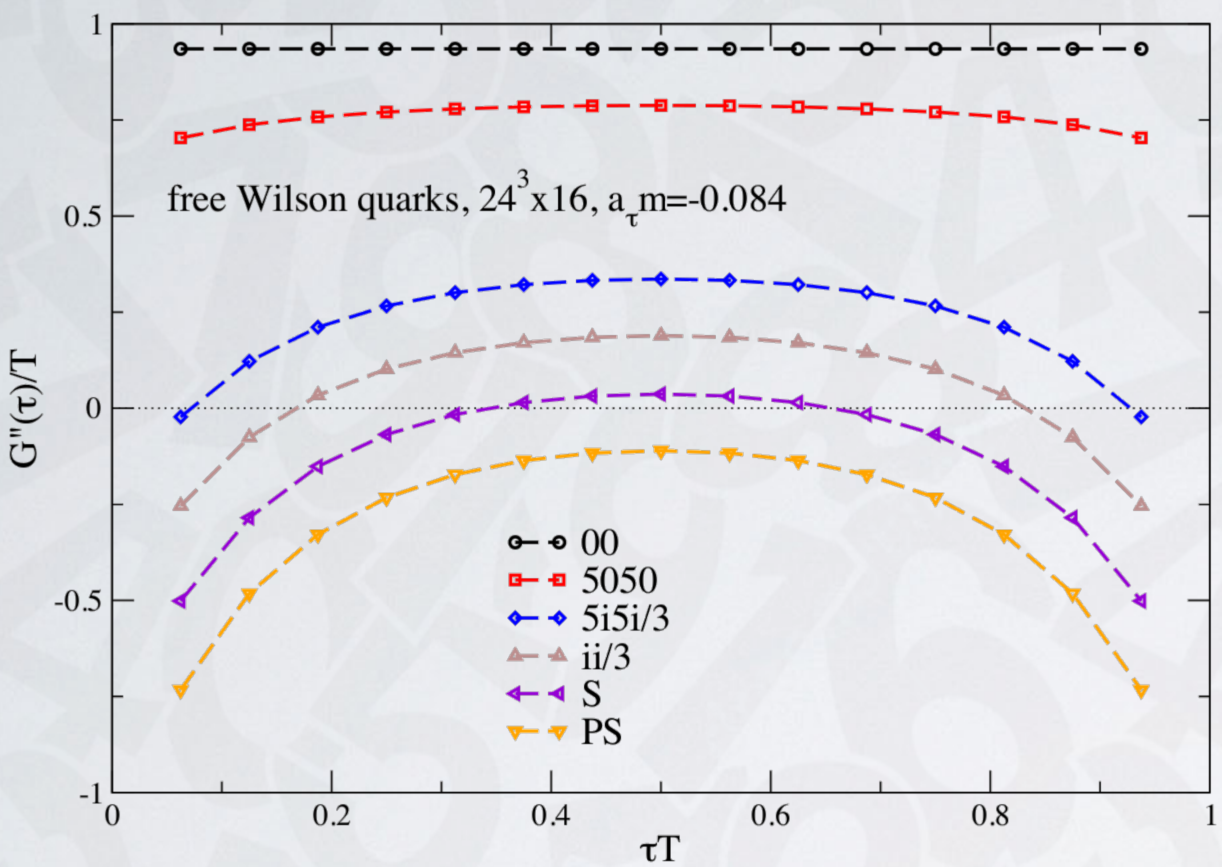
$$\frac{p}{T^4} = \sum_k c_k(T) \left(\frac{\mu}{T}\right)^k, \quad k = 0, 2, \ldots$$

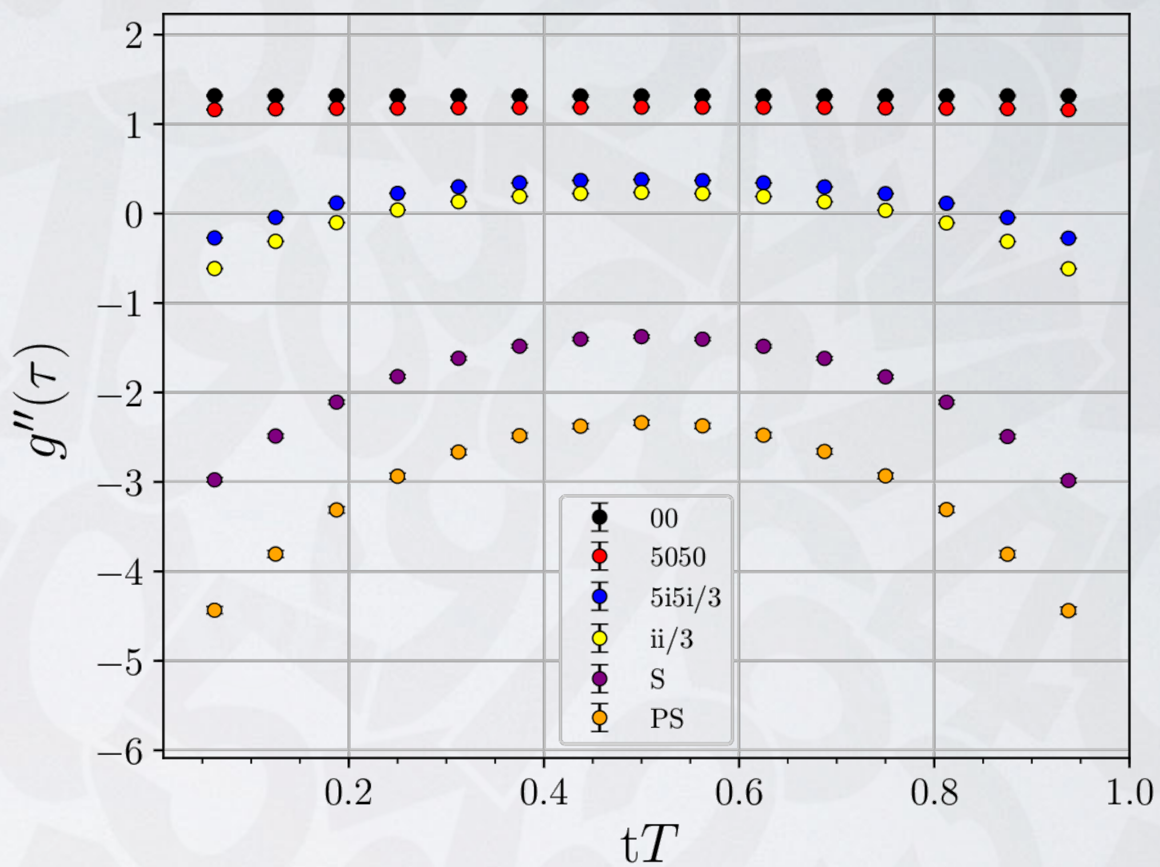
$$c_k = \frac{1}{n!\, VT^3} \left. \frac{\partial^k \log Z}{\partial\left(\mu/T\right)^k} \right|_{\mu=0}$$

- Typically these coefficients contain traces like

$$\mathrm{Tr}\left(M^{-a_1} \frac{\partial^{b_1} M}{\partial \mu^{b_1}} M^{-a_2} \frac{\partial^{b_2} M}{\partial \mu^{b_2}} \ldots\right)$$

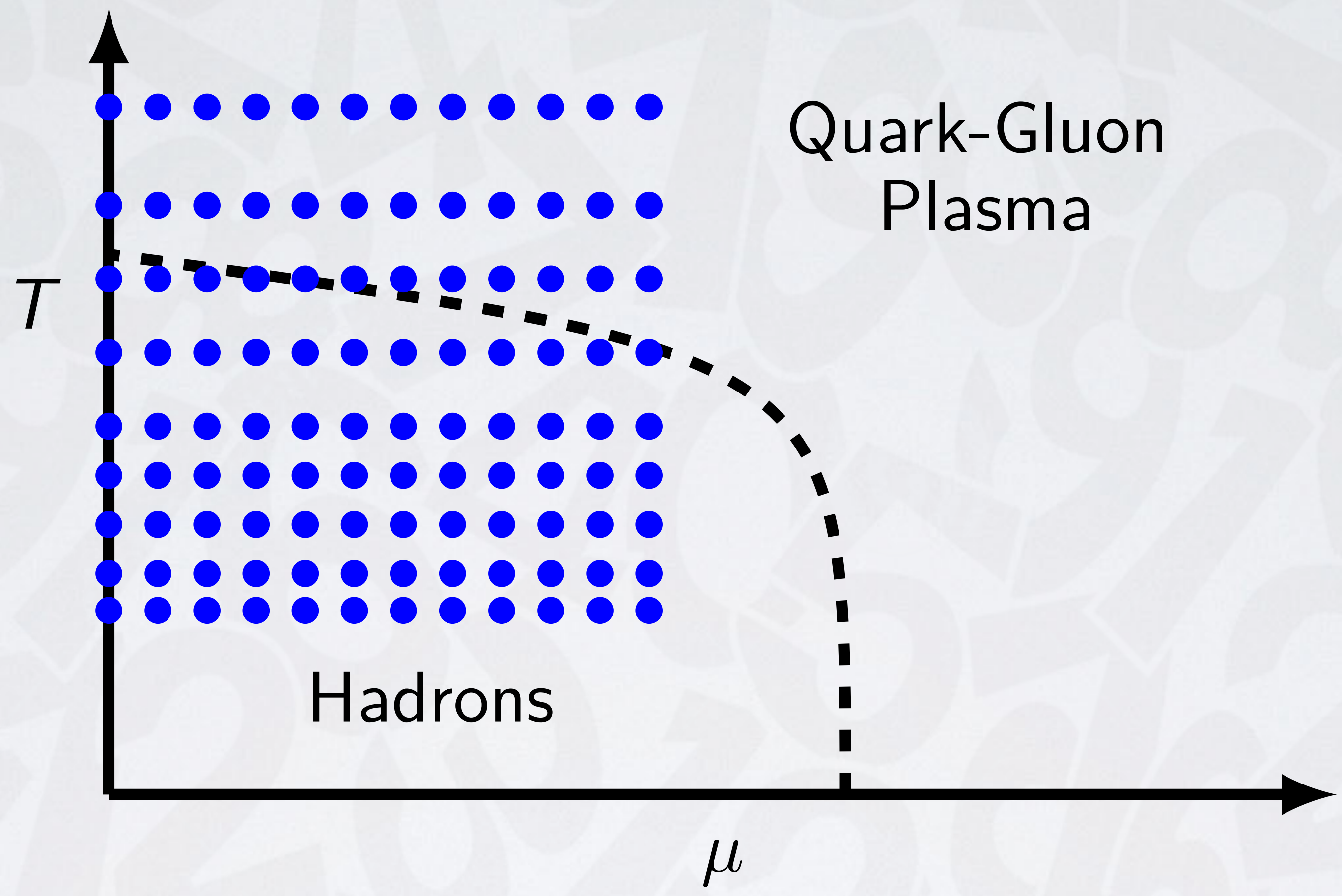
Taylor Expansion





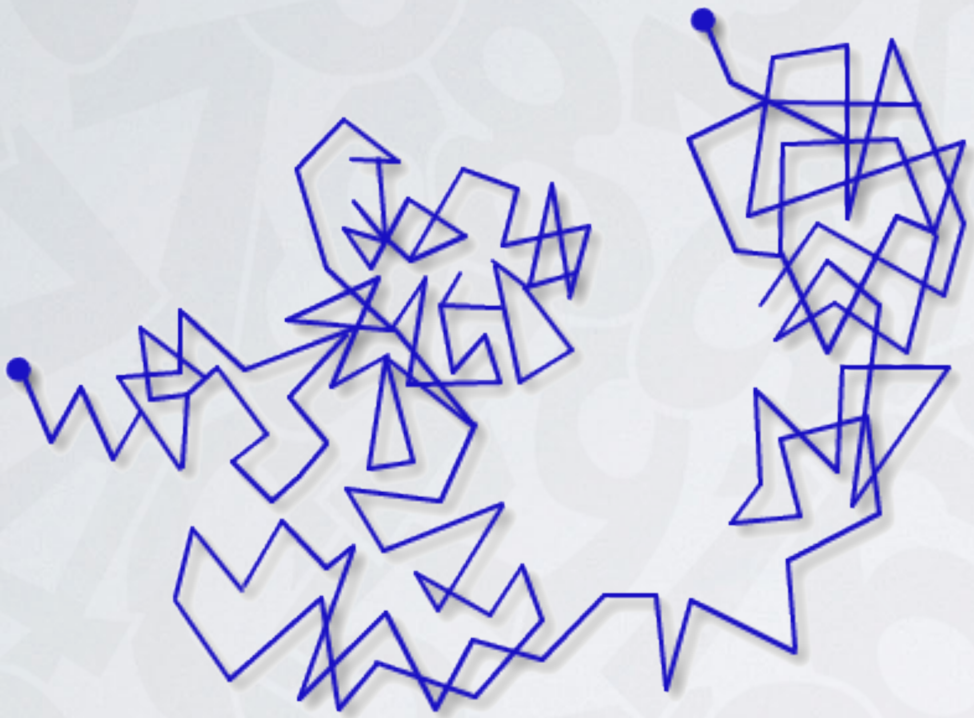
- Parts of the second coefficient on a Gen2 ensemble
- Comparison of free vs interacting scenario
- Qualitatively similar, details different

Research Projects



Complex Langevin

Complex Langevin



- Complexify degrees of freedom

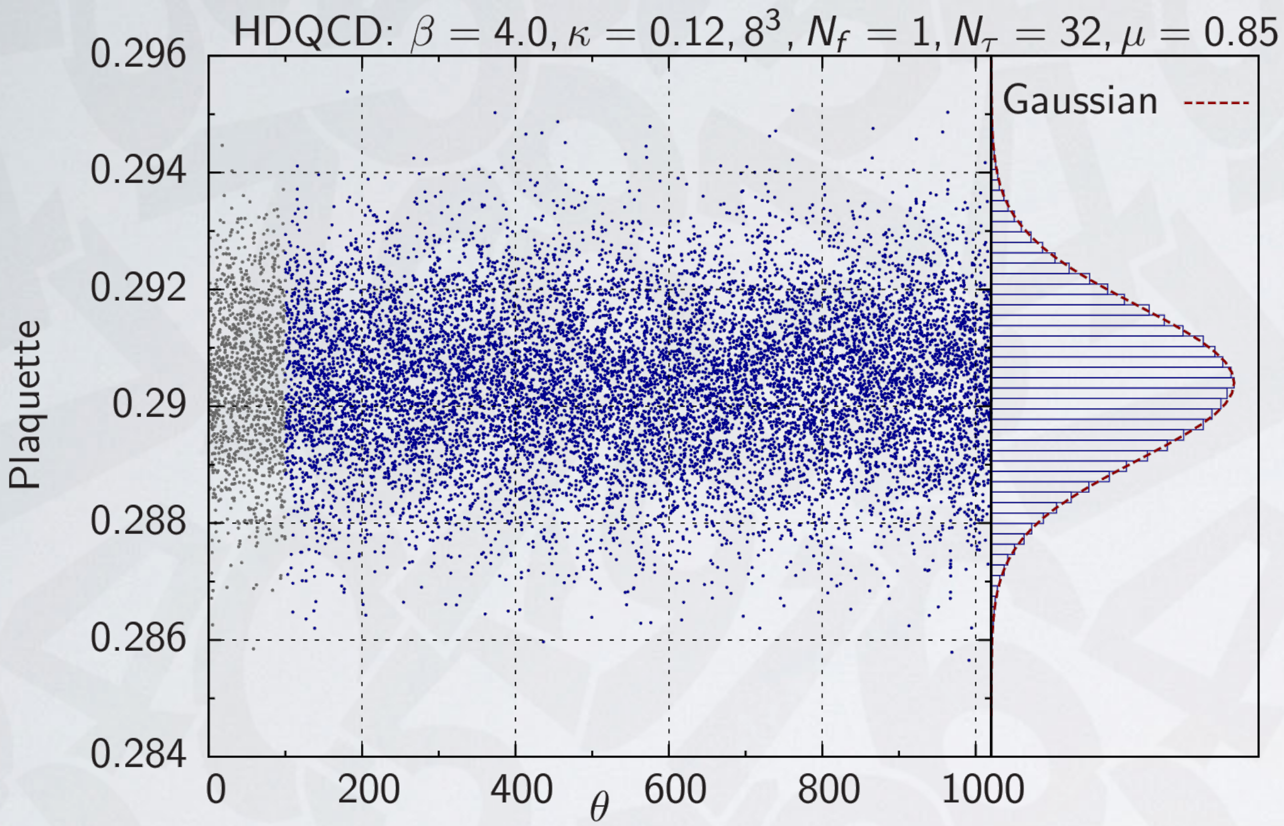
$$x \rightarrow z = x + \mathrm{i}\, y$$

- 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

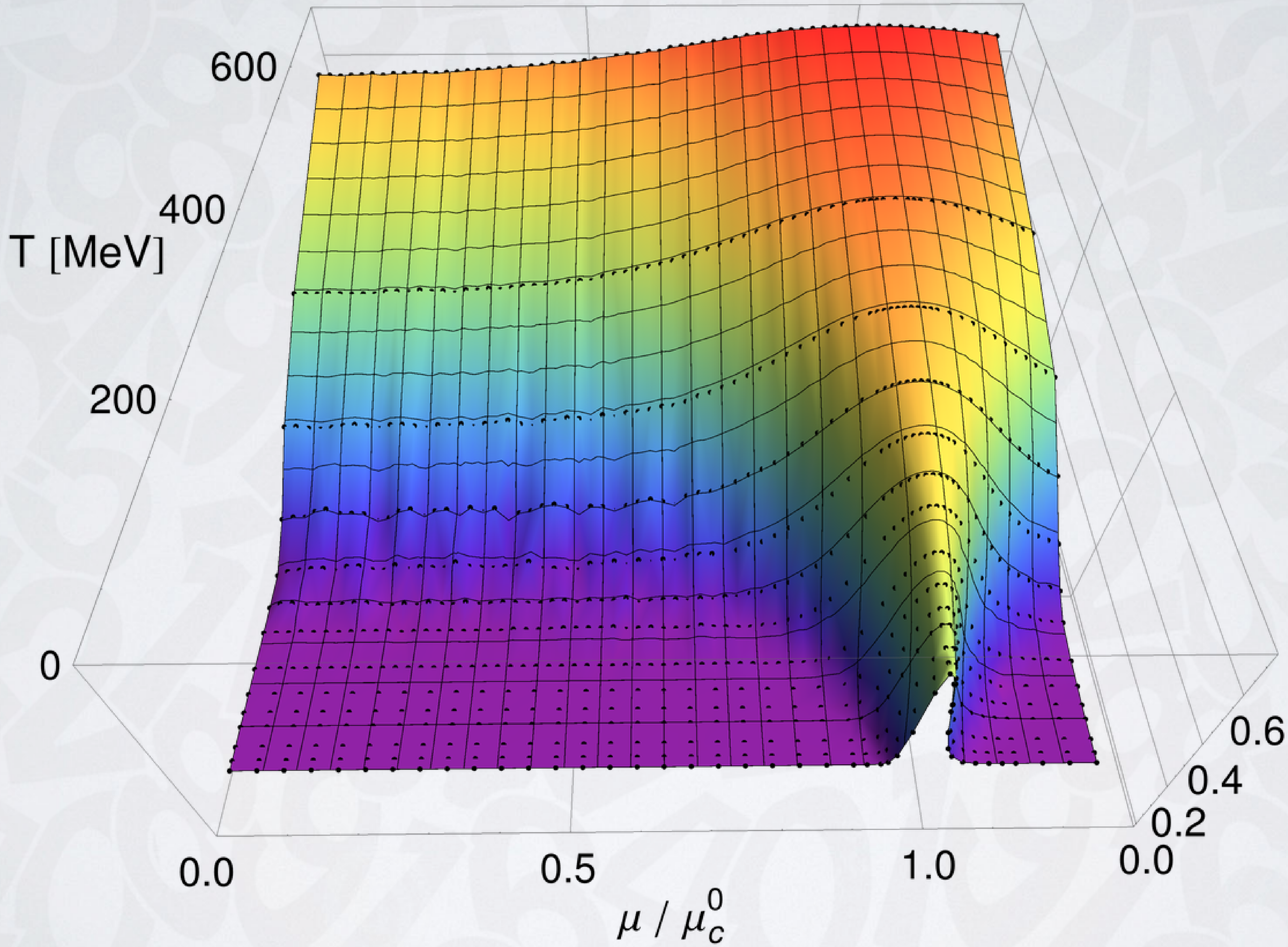
$$U_{x,\mu} = \exp\left[\mathrm{i}\, a\, \lambda_c \left(A^c_{x,\mu} + \mathrm{i} B^c_{x,\mu}\right)\right]$$

- Update scheme (First order discretisation)

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

- No accept-reject step necessary, but $\epsilon \to 0$
- Ito-calculus (stochastic differential equations)

Heavy Dense QCD



Full QCD

Volume	plaquette		$\bar{\psi}\psi$	
	HMC	CL	HMC	CL
6^4	0.58246(8)	0.582452(4)	0.1203(3)	0.12042(2)
8^4	0.58219(4)	0.582196(1)	0.1316(3)	0.1319(2)
10^4	0.58200(5)	0.58201(4)	0.1372(3)	0.1370(6)
12^4	0.58196(6)	0.58195(2)	0.1414(4)	0.1409(3)

- Full QCD @ $\mu = 0$
- Very good agreement between HMC and CL

Outlook

Thermodynamics

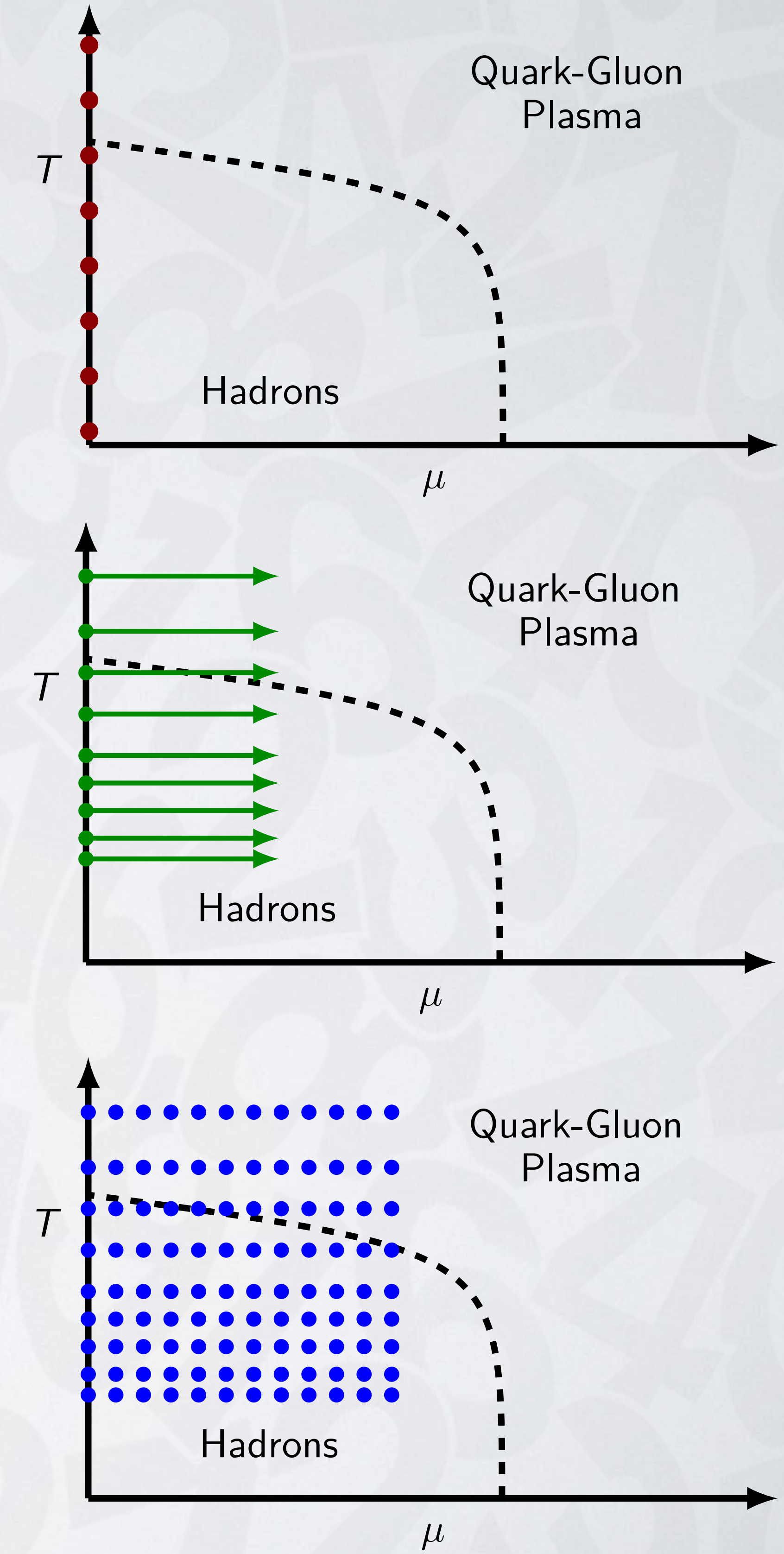
- New generations with physical quarks and higher anisotropy

Taylor expansion

- Start expanding into the QCD phase diagram

Complex Langevin

- Direct expiration of the phase diagram, especially at large T



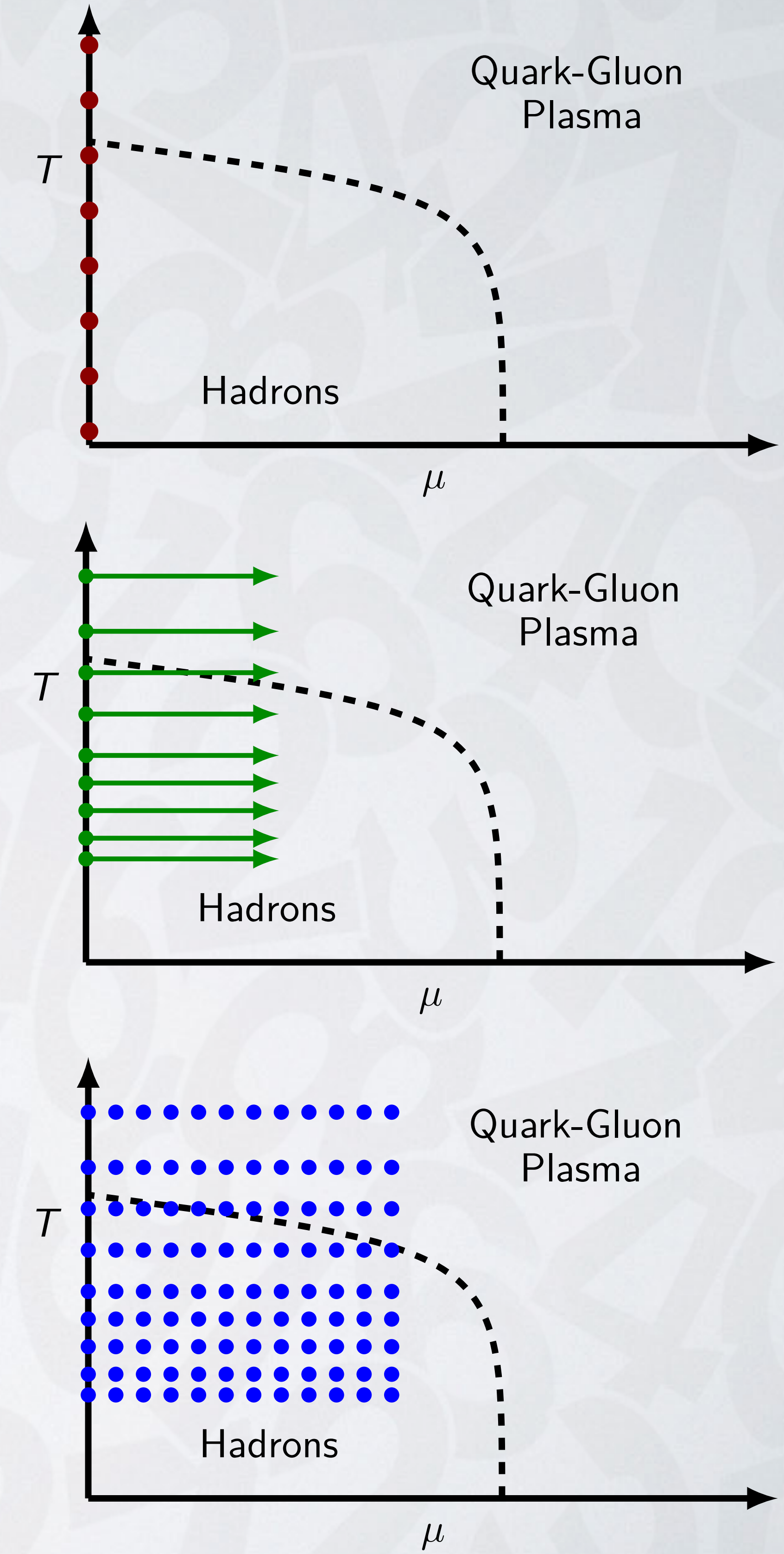
Codes

OpenQCD (based openQCD 1.6)

- Anisotropic
- Stout-Smearing
- AVX512 vectorisation

- http://fastsum.gitlab.io/
- (+ Inverter and 2pt mesons, baryons)

- Scales excellent on standard CPUs (Intel, AMD, BlueGene, Xeon Phi)



Computational needs

Strategies

1. continuum time limit $a_T \to 0$, a_s fixed, $\xi \to \infty$
2. continuum limit $a_s, a_T \to 0, \xi$ fixed
3. physical quarks $m_q \to m_{ud}, m_s$

Short-term plans

- Increase spatial volume $32^3 \to 48^3$ or 64^3
- More chiral
- Sufficient statistics (per-mille on correlator)

  - Gen2 $\to$ Gen2L $\to$ Gen2P
  - Gen2 $\to$ Gen3

Computational needs

Strategies

1. continuum time limit $a_T \to 0, a_s$ fixed, $\xi \to \infty$
2. continuum limit $a_s, a_T \to 0, \xi$ fixed
3. physical quarks $m_q \to m_{ud}, m_s$

Long-term plans

- New generations, i.e. finer spatial $a_s \to 0$
- At the physical point
- Sufficient statistics

Grants so far… (2011 - 2022)

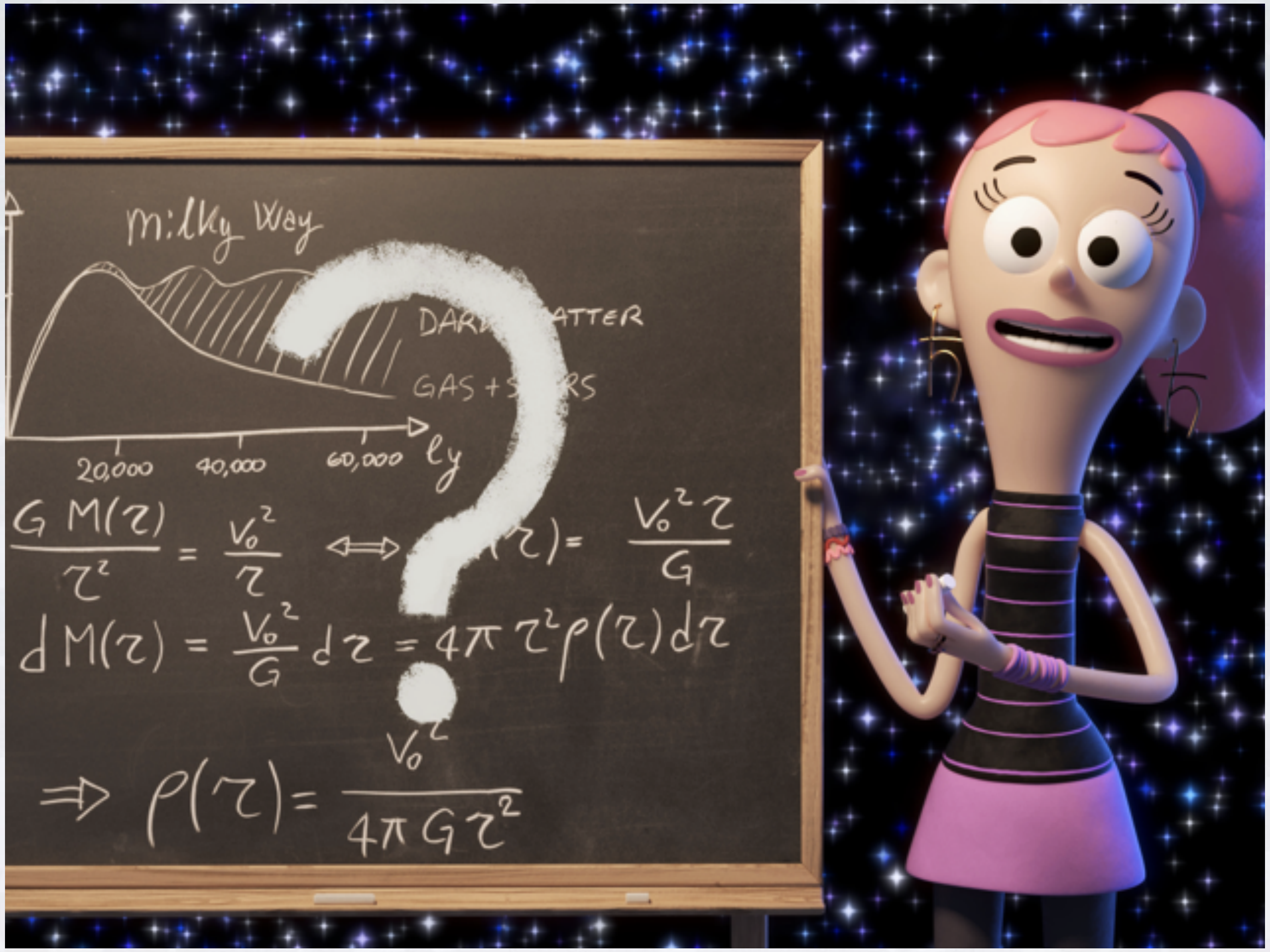
Prace

- 3rd 22M (BG/Q)
- 5th 32M (BG/Q)
- 12th 40M (BG/Q & KNL)
- 18th 30M (KNL; to be renewed)

DiRAC

- 1st: 200M (BG/Q)
- 7th: 400M (BG/Q)
- 10th: 30M (Tesseract)
- 11th: 300M (Tesseract)

Questions?



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