

THE QCD PHASE DIAGRAM: A (PHENO)THEORETICAL OVERVIEW

Johannes JAHAN, PhD Postdoc at University of Houston <u>jjahan@uh.edu</u>





OUTLINE

- 1. Phase diagram & thermodynamics
- 2. First-principle calculations
- 3. 1st-order phase transition & critical point
- 4. Constraints from the experiments
- 5. MUSES: one framework to unify them all

PHASE DIAGRAM OF NUCLEAR MATTER

• Representing different phases and transitions as a function of thermodynamic variables (temperature, pressure, entropy density...)

• What do we know about the nuclear phase diagram? (for sure, from observation)

- Atomic nuclei
- Hadron gas / nuclear liquid
- Quark-gluon plasma (QGP)

...and that's all.



HOW TO EXPLORE THE PHASE DIAGRAM?

Essentially 2 ways to learn about the structure of the phase diagram:

- Looking up at the sky
- Reproducing the evolution of the matter in the early Universe
- Study neutron star structure + mergers from gravitational waves
- Down on Earth, in colliders
 LHC @ CERN
- O RHIC @ BNL / SPS @ CERN
- $_{\odot}$ J-PARC @ Tokai / FAIR @ GSI



THERMODYNAMICS RELATIONS

To compute an **equation of state (EoS)**, one usually start by calculating one quantity as a function $\mathcal{H}(T, \mu//n)$ and derive all other quantities from there.

Basic thermodynamic relations, in the grand-canonical limit (from the partition function \mathscr{Z}):

 γ_1 (ρ_1)

Pressure:
$$P = -T \frac{\partial \ln(\mathscr{Z})}{\partial V}$$

Entropy density: $s = \left(\frac{\partial P}{\partial T}\right)_{\mu_i}$ Charge densities: $n_i = \left(\frac{\partial P}{\partial \mu_i}\right)_{T,\mu_{j\neq i}}$

Energy density:
$$\varepsilon = sT - P + \sum_{i} \mu_i . n_i$$

OUTLINE

1. Phase diagram & thermodynamics

2. First-principle calculations & baselines

- 3. 1st-order phase transition & critical point
- 4. Constraints from the experiments
- 5. MUSES: one framework to unify them all

THE RUNNING COUPLING CONSTANT OF QCD

- One fundamental property of QCD is the fact that its coupling α_s is changing magnitude depending on the energy involved in the process considered.
- Direct calculation of the pressure from QCD is only possible through perturbation methods for small α_s :





PERTURBATIVE QCD

- Perturbative calculation from Feynman diagrams are only possible at very high T/n_B
- In recent years, the approach have been generalized at NNLO to cover all T and n_B

Gorda et al., Phys.Rev.D 104 (2021) 7, 074015

- Only available for $n_B \ge 40 n_{sat}$ at low-T, pQCD helps to constrain the nuclear EoS through Bayesian analysis when considering:
 - Constraint from nuclear theory at low density
 - Imposing causal and stable EoS
 - Using known constraints from astronomical observations



Altiparmak, Eckert & Rezzolla, Astrophys. J.Lett. 939 (2022) 2, L34



NUCLEAR PHASE DIAGRAM

LATTICE QCD – QCD FROM FIRST PRINCIPLES

In the non-perturbative regime, no analytical solutions of QCD can be calculated.

<u>Solution</u>: discretizing space-time on a lattice and compute path integral using Monte-Carlo sampling for many configurations U

$$\left\langle \hat{O} \right\rangle = \frac{1}{Z} \int \mathcal{D}U \,\hat{O} \,\det M[U] \,e^{-S_G[U]}$$

for any observable \hat{O} .

Simulations achieved at different volumes V and different lattice spacings a to obtain in the end continuum limit results in an infinite volume.





Results at $\mu_{\rm B} = 0$ are consistent across different collaborations.

LATTICE QCD - THE SIGN PROBLEM

When using Monte-Carlo sampling:
$$\left<\hat{O}\right>=rac{1}{Z}\int\mathcal{D}U\,\hat{O}\det M[U]\,e^{-S_G[U]}$$

det $M[U] e^{-S[U]}$ is used as a statistical weight (least probable configurations U are ignored)

- <u>When $\mu_B^2 = 0$:</u> det $M[U] e^{-S[U]}$ is real
- <u>When $\mu_B^2 > 0$ </u>: det $M[U] e^{-S[U]}$ becomes complex and has highly oscillating phase

- Can't be interpreted as a statistical weight!



BUT! For purely imaginary μ_B (when $\mu_B^2 < 0$), det $M[U] e^{-S[U]}$ is real again: simulations possible...

LATTICE QCD — THE NATURE OF THE TRANSITION

If one considers the case where $m_u = m_d = 0$ (chiral limit), the **phase transition** is expected to be of **2nd order**.

However, in real-life QCD, $m_u \simeq m_d \neq 0$, and the chiral symmetry is broken.

→ smooth crossover from hadron gas to QGP (no discontinuity in 1st and 2nd order derivatives)



Hadrons basically melt like butter at room temperature





LATTICE QCD — THE NATURE OF THE TRANSITION

By extrapolating from complex μ_B lattice simulations to real μ_B , one can compute the shape of the transition line:

$$\frac{T_c(\mu_B)}{\mathbf{T_c}(\mu_B = \mathbf{0})} = 1 + \kappa_2 \left(\frac{\mu_B}{T_c(\mu_B)}\right)^2 + \kappa_4 \left(\frac{\mu_B}{T_c(\mu_B)}\right)^4 + \mathcal{O}(\mu_B^6)$$

(location, curvature, "hyper-curvature", ...)

Bazavov et al., PLB 795 (2019) 15-21

Most recent results:

 $T_c(\mu_B=0) = 158.0 \pm 0.6 \text{ MeV}$ $\kappa_2 = 0.0153 \pm 0.0018$ $\kappa_4 = 0.00032 \pm 0.00067$ Borsányi et al., PRL 125 (2020), 05 2001

Existence of a critical point excluded for $\mu_B < 300 \text{ MeV}$ by lattice QCD results.





NUCLEAR PHASE DIAGRAM

LATTICE QCD — GOING TO FINITE DENSITY

The sign problem in lattice QCD prevent from direct computation of thermodynamics at real finite $\mu_B \rightarrow$ need to employ expansion methods.

Taylor series expansion

$$\frac{\underline{P(T,\mu_B)}}{T^4} = \sum_i \frac{1}{i!} \chi_i^B(T,\mu_B=0) \left(\frac{\mu_B}{T}\right)^i$$

Allows to compute an EoS at finite density from expansion coefficients, called susceptibilities, computed at $\mu_{B/Q/S} = 0$ from lattice QCD.

$$\chi_i^B = \frac{\partial^i (P/T^4)}{\partial \hat{\mu}_B{}^i} \bigg|_{\hat{\mu}_B = 0}$$

Limitations:

- Expansion achieved at constant T, missing out curvature of transition line
- Large errors due to high-order terms leading at large $\mu_{\it i}/T$

 \rightarrow Expansion limited to $\mu_i/T \leq 2.5$



LATTICE QCD — GOING TO FINITE DENSITY

T-Expansion Scheme (TExS)

New method based on a resummation of Taylor expansion, defined from the following ansatz: $\frac{\chi_1^B(T, \hat{\mu}_B)}{\hat{\mu}_B} = \chi_2^B(T', 0)$

using a shifted temperature T' expanded in T and μ_B

$$T'(T,\mu_B) = T\left(1 + \kappa_2^{BB}(T)\hat{\mu}_B^2 + \kappa_4^{BB}(T)\hat{\mu}_B^4 \dots\right)$$

To compute the complete EoS, one has to integrate χ₁^B to get pressure
Separation in magnitude between expansion coefficients (related to χs) hints at better convergence than Taylor expansion

• Generalization to 4D (T, $\mu_{\rm B}$, $\mu_{\rm Q}$, $\mu_{\rm S}$) currently ongoing

 \rightarrow Trusted up to $\mu_{\rm B}/T$ = 3.5





NUCLEAR PHASE DIAGRAM

HADRON RESONANCE GAS MODEL

 Thermal model based on Fermi-Dirac & Bose-Einstein statistics, assuming a gas of interacting hadrons in their ground states can be modeled by a gas of non-interacting hadrons and resonances.

- Describes the hadronic phase only (blows up at the transition)
 → used as a reference for low-T QCD, as it matches with
 lattice QCD (which is too costly to compute below T~120 MeV)
- Can be improved by adding excluded volume correction and van der Waals attractive interaction
 - describes the nuclear liquid-gas phase transition





See <u>*QJavier Menéndez' talk</u> for discussion about description of nuclear*</u> matter at very low T (chiral EFT, many-body theories, etc.)

NUCLEAR PHASE DIAGRAM

 μ_B

000

Sep

OUTLINE

- 1. Phase diagram & thermodynamics
- 2. First-principle calculations
- 3. 1st-order phase transition & critical point
- 4. Constraints from the experiments
- **5.** MUSES: one framework to unify them all

QCD EFFECTIVE THEORIES

Several (radically) different **effective non-perturbative approaches to QCD** predict the **existence** of a **critical point** at finite baryon chemical potential, among which the most recent ones:



LOCATION OF A CRITICAL POINT FROM LATTICE QCD

Prediction of a critical point from lattice QCD

from simulations at imaginary baryon chemical potential, extrapolated to the real plane.



D.A. Clarke et al., arXiv:2405.10196

Compilation of predictions





See talk from <u>@Győző K.</u> on mean-field model EoS and <u>@Mathis H</u>. on behavior of the critical dynamics out-of-equil.

NUCLEAR Phase Diagram

OUTLINE

- 1. Phase diagram & thermodynamics
- 2. First-principle calculations
- 3. 1st-order phase transition & critical point
- 4. Constraints from the experiments
- 5. MUSES: one framework to unify them all

HOW TO LINK THEORY TO THE EXPERIMENTS?

The best way to confront theoretically calculated EoS with experimental results is to run simulations.

- Making data prediction/interpretation using pre-computed EoS
- Helps to constrain properties of the EoS by comparing to measurements

This is where FAIR enters the game!

Heavy-lon collisions

• EPOS4 HIJING

• Angantyr

• AMPT

UrQMD

SMASH

Microscopic transport

• Hadrons/quarks as d.o.fs



Relativistic hydrodynamics • Mesoscopic scale (using densities)



Neutron star mergers & Kilonovae



Relativistic Magnetohydrodynamics

(2015) 6. 064001

See talks from <u>@Christine C.</u>, @Aristeidis N., @Vimal V. & @Luke S.

FREEZE-OUT COORDINATES

Using the HRG model, one can extract information for temperature and chemical potentials at:

• <u>Chemical freeze-out:</u> when inelastic interactions cease, by fitting particle abundances through density

$$n_i^{\rm id}(T,\mu_i) = \frac{d_i}{2\pi^2} \int dm f_i(m) \int_0^\infty k^2 dk \left[\exp\left(\frac{\sqrt{k^2 + m^2} - \mu_i}{T}\right) + \eta_i \right]^2$$

• <u>Kinetic freeze-out</u>: when all interaction cease, by fitting the transvers momentum spectra

$$\frac{dN}{p_T \, dp_T} \propto \int_0^R r \, dr \, m_T I_0 \left(\frac{p_T \sinh \rho(r)}{T_{\rm kin}}\right) \times K_1 \left(\frac{m_T \cosh \rho(r)}{T_{\rm kin}}\right)$$

assuming a simple radial flow velocity profile $\beta = \beta_S (r/R)^n$



EXPERIMENTAL SEARCH OF THE CRITICAL POINT

Fluctuations of conserved charges

Cumulants of conserved charges are sensitive to the critical point $\kappa_n \propto$ (diverge in its vicinity, in theory)

$$\displaystyle < rac{\partial^n (\ln Z^{
m gce})}{\partial \mu^n}$$

→ using hadron species as proxies for conserved charges

- Differences between highly dynamic and short-lived HICs make comparison far from straight-forward:
 - choice of proxies
 - finite-volume effects
 - volume fluctuations
 - acceptance

...

See talks from @Rutik M., @Athira S., @Beatriz A.



INFERRING THE EOS FROM SPACE

Properties of neutron stars

Using the Tolman-Oppenheimer-Volkoff equation, one can compute (M,R) relations for a given nuclear EoS:

 $\frac{dP}{dr} = -\frac{G\epsilon(r)m(r)}{c^2r^2} \left[1 + \frac{P(r)}{\epsilon(r)}\right] \left[1 + \frac{4\pi r^3 P(r)}{m(r)c^2}\right] \left[1 - \frac{2Gm(r)}{c^2r}\right]^{-1}$

and confront the results to current measurements

+ other observables (tidal deformability, quad. moment...)



Tolos & Fabbietti, Prog.Part.Nucl.Phys. 112 (2020) 103770



Gravitational waves detection

GW signals detected from neutron star mergers can help to infer NS properties, as well as the nature of the composition, and hence of the transition type

TO LEARN EVEN MORE... ON THE MENU THIS WEEK

• Flow of dileptons

(probing chiral symmetry restoration, measuring T_{medium}, probing in medium interactions...)

See talks from @Sukyung K., @Pawan K.S., @Karina S. @Cornelius F.-R.

• Hyperon-nucleon/nucleon-nucleon interactions (to compute mean-field potentials, understand matter composition at high densities...)

See talks from @Snehankit P. @Konrad S., @Anna W., @Susanne G.

OUTLINE

- 1. Phase diagram & thermodynamics
- 2. First-principle calculations
- 3. 1st-order phase transition & critical point
- 4. Constraints from the experiments
- 5. MUSES: one framework to unify them all

Click here for more

Gathers physicists from heavy-ion, neutron star and low-energy nuclear physics and computer scientists

- Modular: different modules computing EoS for different regions of the nuclear phase diagram + associated observables
- **Unified:** modules are integrated in a single framework, to ensure
 - i. Maximum coverage of phase space
 - ii. Respect of their constraints



A.T. Manning, MUSES Collaboration Meeting 2023

Alpha release ongoing

(testing of the calculation engine by selected users)

PUBLIC RELEASE SOON!!! Stay tuned...

CONCLUSION

 Heavy-ion, low-energy nuclear physics and astro communities are working closer than ever to assess the structures of the phase diagram

FAIR will play an important role to explore the high-density
 & low-temperature region

 Collaboration efforts are being led to improve theoretical modeling and help bridging the gap with experimental results (*i.e.* <u>BEST</u>, <u>MUSES</u>, <u>ELEMENTS</u>...)

BACKUP

BACKUP SLIDES

- Limitation of Taylor expansion
- Other phase diagrams (eB / isospin)
- Bayesian analysis on EoS + UrQMD (Manjunath @ SQM)

LATTICE QCD HIGH-ORDER SUSCEPTIBILITIES

LATTICE QCD — THE NATURE OF THE TRANSITION

One can simulate lattice QCD at purely imaginary chemical potential, and determine the transition line by looking at:

• inflection point of the chiral condensate $\left< \bar{\psi}\psi \right> = \frac{T}{V} \frac{\partial \ln Z}{\partial m_{ud}}$

• peak of the chiral susceptibility $\chi = \frac{T}{V} \frac{\partial^2 \ln Z}{\partial m_{ud}^2}$





3

2D ISING-T.EX.S EQUATION OF STATE FROM L-QCD

Range: 30 MeV < T < 800 MeV $\,$; $\,\mu_{B/Q/S}\,{<}\,700$ MeV $\,$



one can thus redefine temperature and use an alternative expansion scheme:

$$T'(T, \hat{\mu}_B) = T\left(1 + \kappa_2^{BB}(T)\hat{\mu}_B^2 + \kappa_4^{BB}(T)\hat{\mu}_B^4 + \mathcal{O}(\hat{\mu}_B^6)\right)$$

with alternative expansion coefficients κ , related to susceptibilities:

$$\kappa_{2}^{BB}(T) = \frac{1}{6T} \frac{\chi_{4}^{B}(T)}{\chi_{2}^{B'}(T)} \qquad \kappa_{4}^{BB}(T) = \frac{1}{360\chi_{2}^{B'}(T)^{3}} \left(3\chi_{2}^{B'}(T)^{2}\chi_{6}^{B}(T) - 5\chi_{2}^{B''}(T)\chi_{4}^{B}(T)^{2}\right)$$

Empirical observation:

• all 1st order susceptibilities scale when defining a μ_B -dependent temperature $T'(T, \mu_B)$

μ_в)

•

scales like:

$$\frac{\chi_1^B(T,\hat{\mu}_B)}{\hat{\mu}_B} = \chi_2^B(T',0)$$

Main identity



2D ISING-T.EX.S EQUATION OF STATE FROM L-QCD



M. Kahangirwe, J.J., C. Ratti et al., PRD (2024); arXiv:2402.08636

4D-T.EX.S EQUATION OF STATE FROM L-QCD

Range: $T < 800 \; \text{MeV}$; $\mu_{B/Q/S} < ? \; 700 \; \text{MeV}$

• Generalization of the previous 2D T'-Expansion Scheme to 3 conserved charges by projecting the "cartesian" (μ_B , μ_Q , μ_S) coordinates to spherical ones

$$\hat{\mu} = \sqrt{\hat{\mu}_B^2 + \hat{\mu}_Q^2 + \hat{\mu}_S^2} \qquad \qquad \hat{\mu}_B = \hat{\mu} \cdot \cos(\theta) \\ \hat{\mu}_Q = \hat{\mu} \cdot \sin(\theta) \cos(\varphi) \\ \hat{\mu}_S = \hat{\mu} \cdot \sin(\theta) \sin(\varphi)$$

 \rightarrow still a 2D-TExS expansion, along a constant μ/T line

• Calculate expansion coefficient λ_2 based on so-called "generalized susceptibilities" $X_{2/4}$ (linear combinations of lattice QCD susceptibilities) + their Stefan-Boltzmann limits

$$\lambda_{2}^{\theta,\phi}(T) = \frac{1}{6T} \frac{1}{X_{2}^{\prime\,\theta,\phi}(T)} \times \left(X_{4}^{\theta,\phi}(T) - \frac{\overline{X}_{4}^{\theta,\phi}(0)}{\overline{X}_{2}^{\theta,\phi}(0)} X_{2}^{\theta,\phi}(T) \right) \qquad X_{2}^{\theta,\phi}(T) = c_{\theta}^{2} \cdot \chi_{2}^{B}(T) + s_{\theta}^{2} c_{\phi}^{2} \cdot \chi_{2}^{Q}(T) + s_{\theta}^{2} s_{\phi}^{2} \cdot \chi_{2}^{S}(T) + \dots + s_{\theta}^{2} \cdot \chi_{$$

4D-T.EX.S EQUATION OF STATE FROM L-QCD

Range: T < 800 MeV ; $\mu_{B/Q/S}$ <? 700 MeV

• Compute the "generalized charge density" X_1 along the projected line using the expanded temperature T' and the T.Ex.S main identity (modified to match with Stefan-Boltzmann limit at $T \rightarrow \infty$)

$$X_1^{\theta,\phi}(T,\hat{\mu}) = \frac{\overline{X}_1^{\theta,\phi}(\hat{\mu})}{\overline{X}_2^{\theta,\phi}(0)} \times X_2^{\theta,\phi}\left(T^{\prime\,\theta,\phi}(T,\hat{\mu}),0\right)$$

with
$$T^{\prime\,\theta,\phi}(T,\hat{\mu})=T\left(1+\lambda_2^{\theta,\phi}(T)\hat{\mu}_B^2
ight)$$

• Obtain pressure by integrating X_1 , allowing then to compute all thermodynamics

$$P^{\boldsymbol{\theta},\boldsymbol{\varphi}}(T,\hat{\boldsymbol{\mu}}) = P(T,0) + \int_0^{\hat{\boldsymbol{\mu}}} X_1^{\boldsymbol{\theta},\boldsymbol{\varphi}}(T,\hat{\boldsymbol{\mu}}') d\hat{\boldsymbol{\mu}}'$$



EQUATION OF STATE FROM HOLOGRAPHY

Range: 30 MeV < T < 400 MeV ; $\mu_{B} < 1100$ MeV

String theory/Classical gravity in 5D



By solving the equations of motion (EoM) for a 5D Einstein-Maxwell-Dilaton (EMD) model defined by the following action:

$$S = \frac{1}{2\kappa_5^2} \int_{\mathcal{M}_5} d^5 x \sqrt{-g} \left[R - \frac{(\partial_{\mu}\phi)^2}{2} - V(\phi) - \frac{f(\phi)F_{\mu\nu}^2}{4} \right]$$

in 4D

(simplest action reproducing a realistic 4D QCD EFT)

... one can obtain the following thermodynamic quantities by

- using the UV behavior of the EMD fields
- fixing free parameters Λ , κ_5 and the functional form of $V(\phi)$ and $f(\phi)$ by matching with IQCD results at $\mu_{\rm B} = 0$

$$T = \frac{1}{4\pi \phi_A^{1/\nu} \sqrt{h_0^{far}}} \Lambda \qquad s = \frac{2\pi}{\kappa_5^2 \phi_A^{3/\nu}} \Lambda^3$$
$$\mu_B = \frac{\Phi_0^{far}}{\phi_A^{1/\nu} \sqrt{h_0^{far}}} \Lambda \qquad \rho_B = -\frac{\Phi_2^{far}}{\kappa_5^2 \phi_A^{3/\nu} \sqrt{h_0^{far}}} \Lambda^3$$



TRAJECTORIES ACROSS THE PHASE DIAGRAM



Dore et al., J.Phys.Conf.Ser. 1602 (2020) 1, 012017

BAYESIAN INFERENCE OF THE EOS THROUGH HIC



Simulation achieved with UrQMD at different collision energies, using CMF equations of state.

WORKFLOWS IN MUSES

• Example of a typical workflow within MUSES, implying EOS generation + observable calculation





