

QCD Thermodynamics

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- Lecture I: QCD at finite temperature and density, continuum and lattice
- Lecture II: Applications of lattice thermodynamics
- Lecture III: Generalities on the phase diagram, the finite T transition, chemical potential
- Lecture IV: Towards the QCD phase diagram at finite density

Literature

- O.P., “Lattice QCD at non-zero temperature and density”, Les Houches lecture notes 2009, arxiv:1009.4089
- O.P., “The QCD equation of state from the lattice” Prog. Part. Nucl. Phys. 70 (2013) 55, arxiv:1207.5999

Proper references to covered material in those articles

Textbooks:

- Gale, Kapusta, “Finite temperature field theory: principles and applications”
- Montvay, Münster, “Quantum fields on a lattice”
- Gattringer, Lang, “Quantum chromodynamics on the lattice”

Units for these lectures

● Natural units:

$$\hbar = 1, c = 1$$

● Einstein sum convention:

$$a_i b_i \equiv \sum_i a_i b_i$$

Hopefully only in a few instances (not intentional):

● Small circle approximation:

$$\pi = 1$$

● Supra-natural approximations:

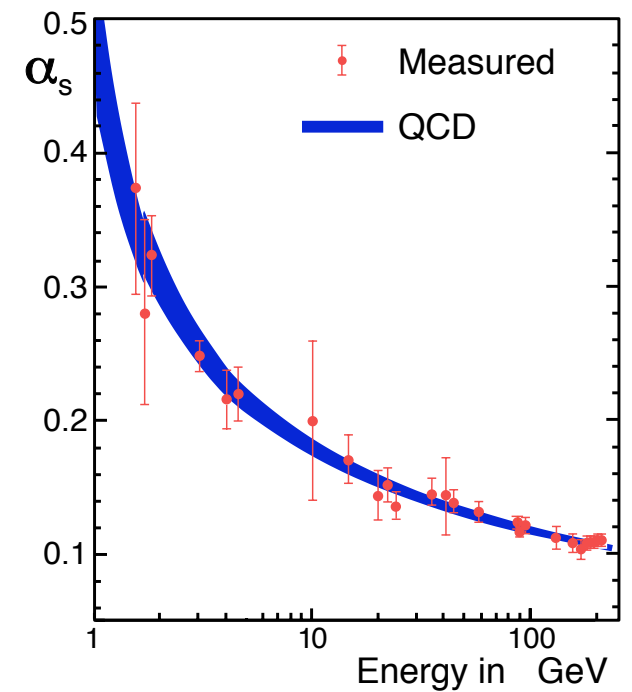
$$-1 = 1, i = 1$$

Lecture I: QCD at finite temperature and density

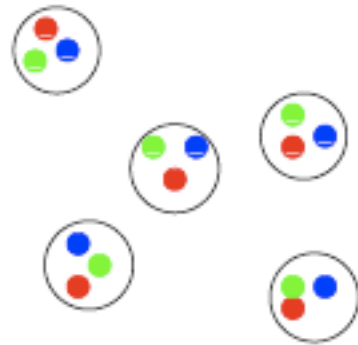
- Motivation: Why thermal QCD?
- The continuum formulation
- Differences and limitations of perturbation theory compared to $T=0$
- The lattice formulation

Why thermal QCD?

asymptotic freedom $\alpha_s(p \rightarrow \infty) \rightarrow 0$



T, μ_B



Hadrongas



Quark-Gluon-Plasma

Chiral symmetry:

broken

(nearly) restored

Order parameters:

$$\langle \bar{\psi}\psi \rangle, \langle \psi\psi \rangle$$

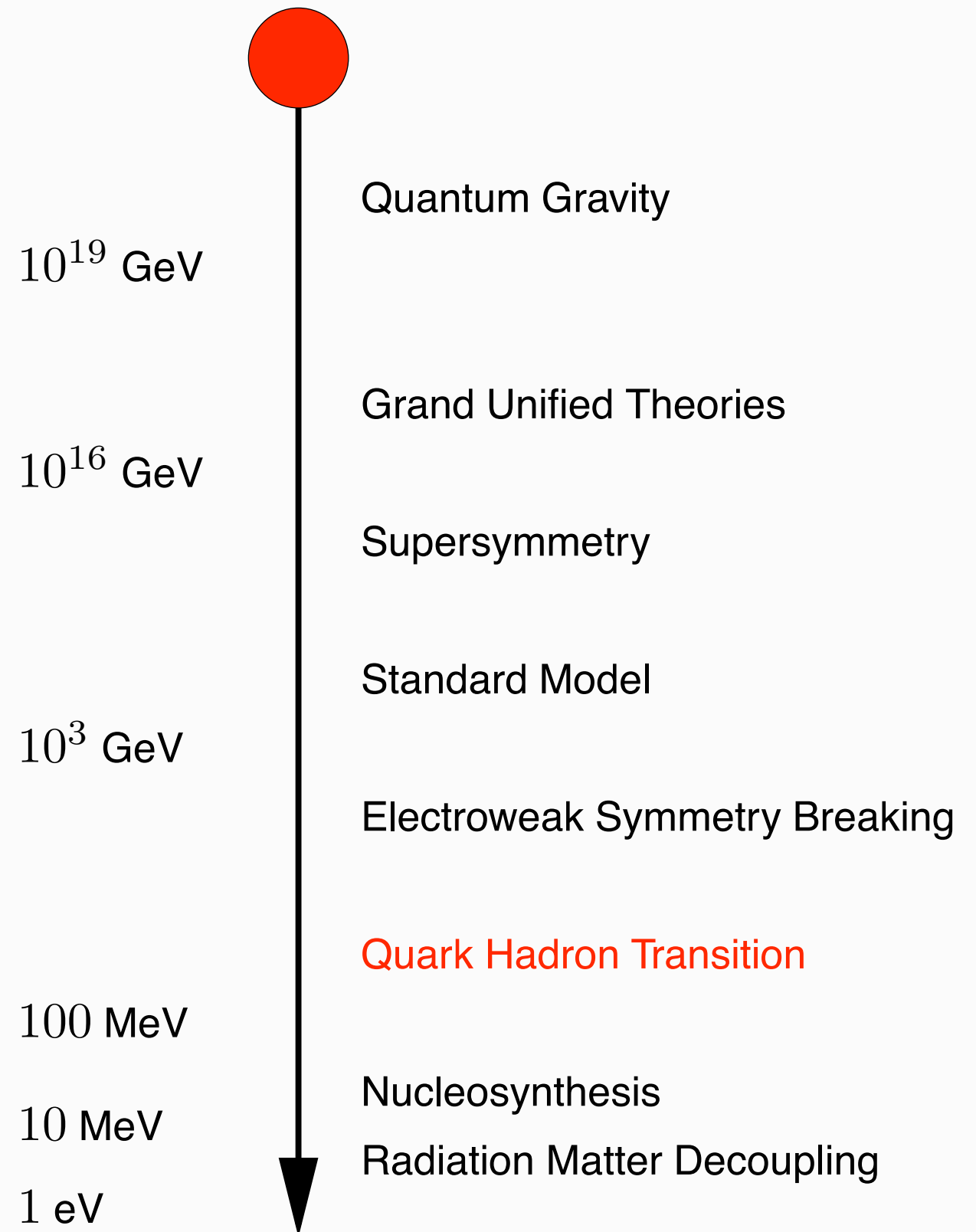
chiral condensate , Cooper pairs

Thermal QCD in nature

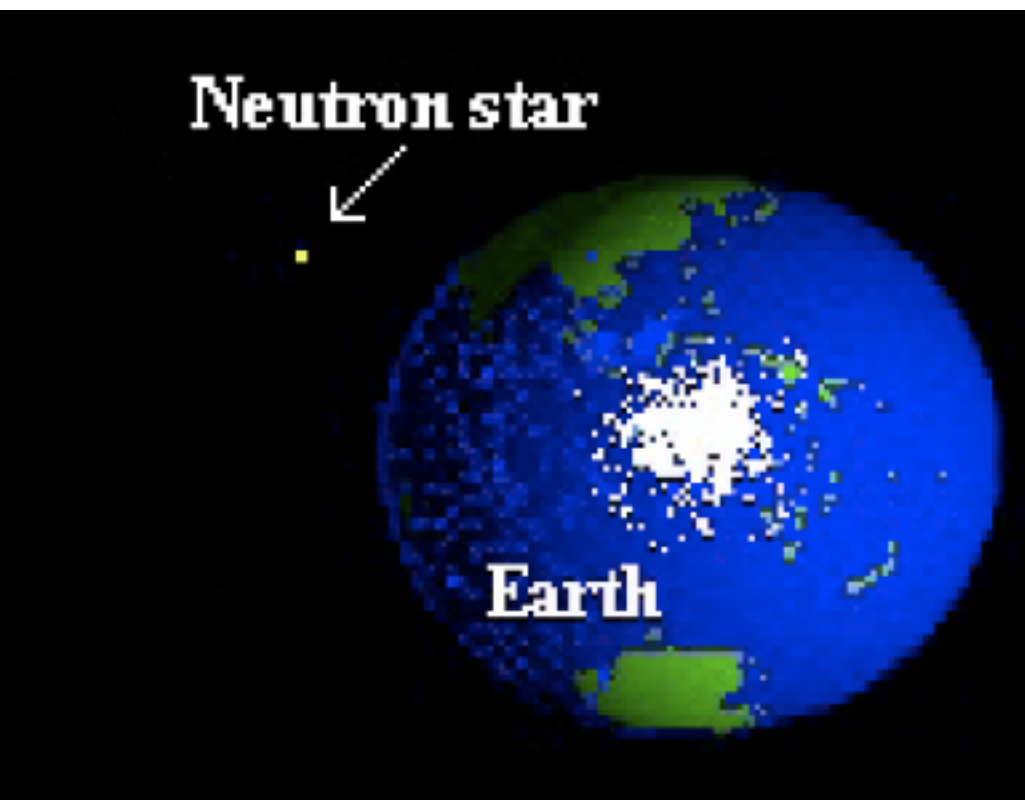
Physics of early universe:

non-abelian plasma physics
($\mu_B \approx 0$)

➔ QCD is prototype



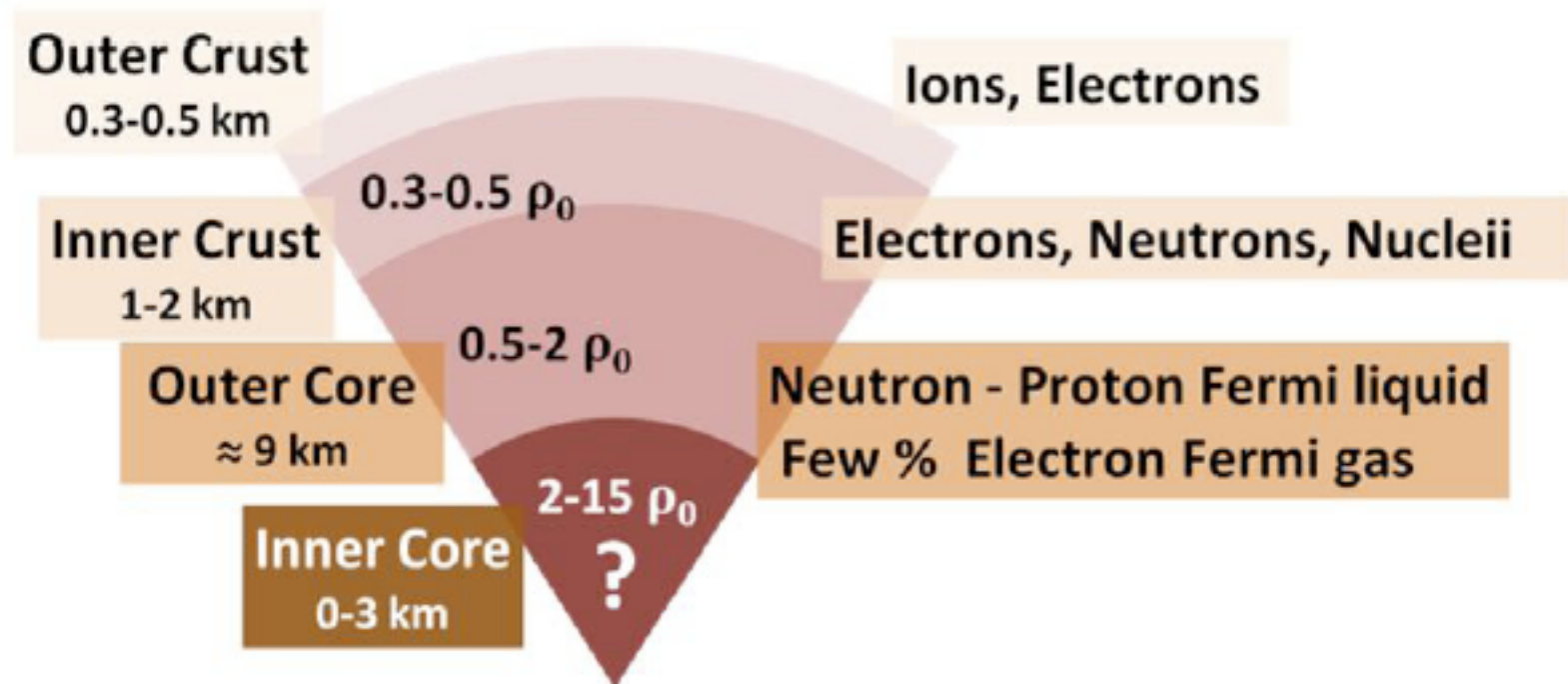
What are compact stars made of?



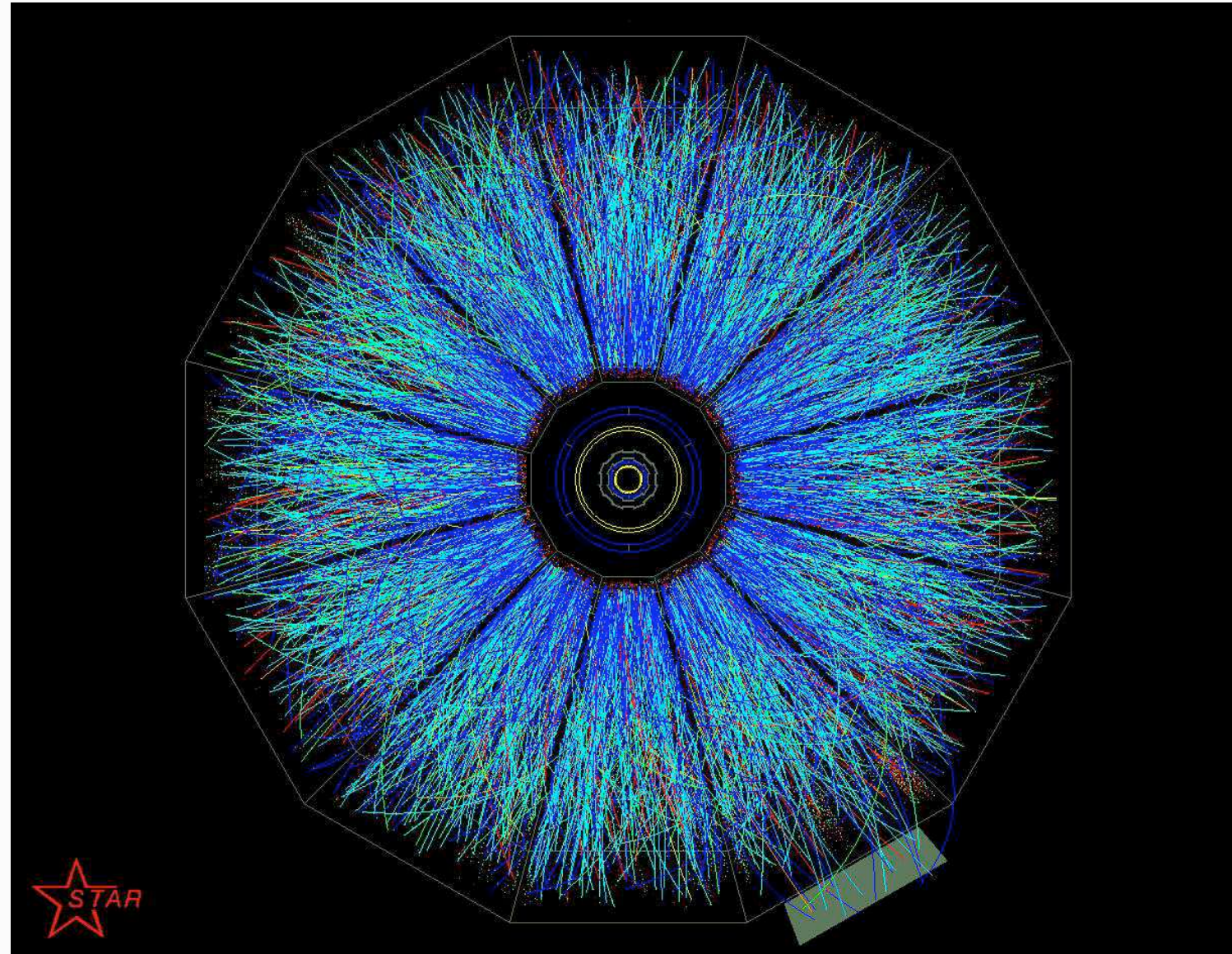
Radius $\sim 10\text{-}12$ km

Mass $\sim 1.2\text{-}2.2 \times$ Solar Mass

ρ_0 : nuclear density

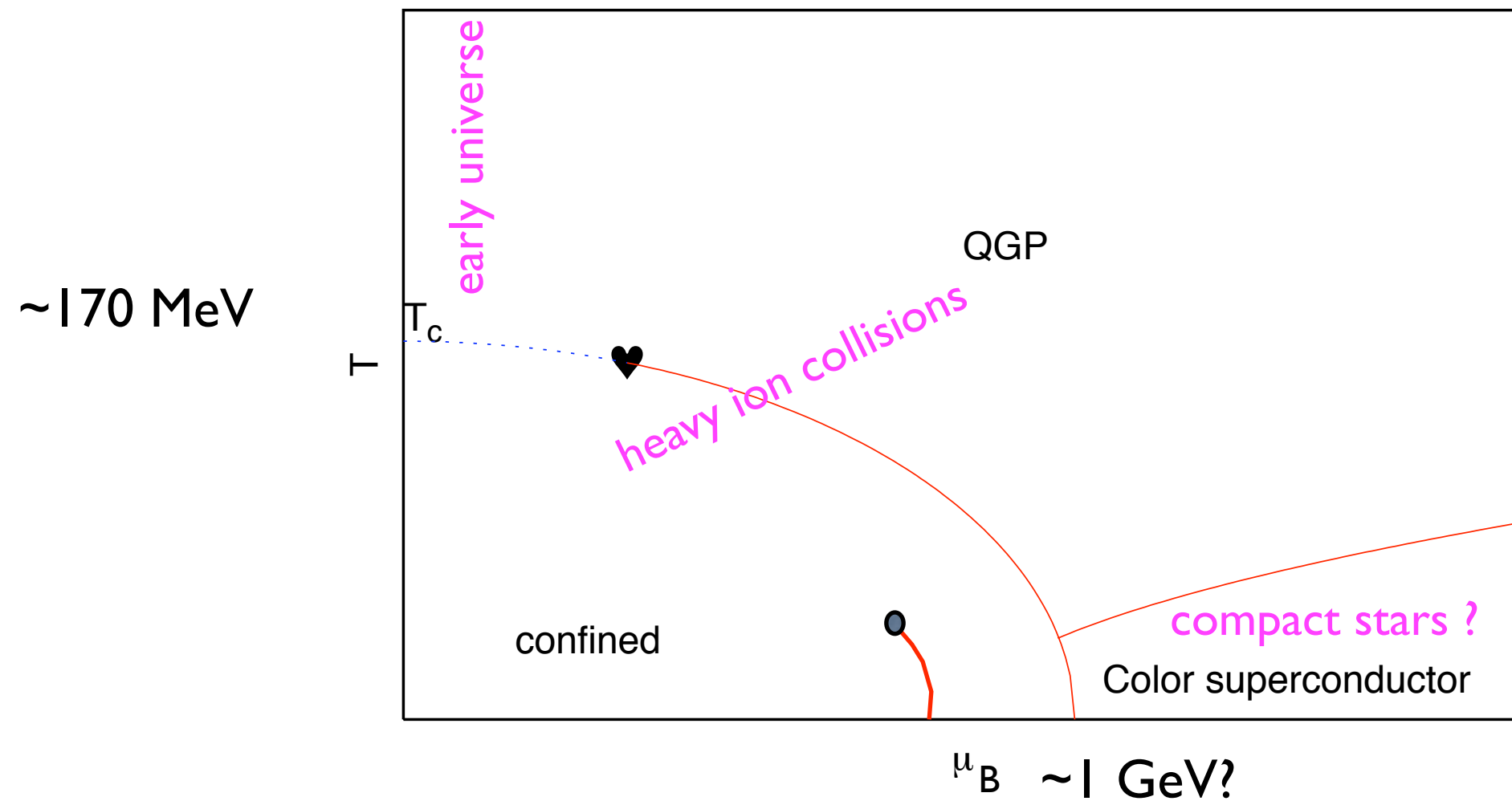


Thermal QCD in experiment



heavy ion collision experiments at RHIC, LHC, GSI....

QCD phase diagram: theorist's view (science fiction)

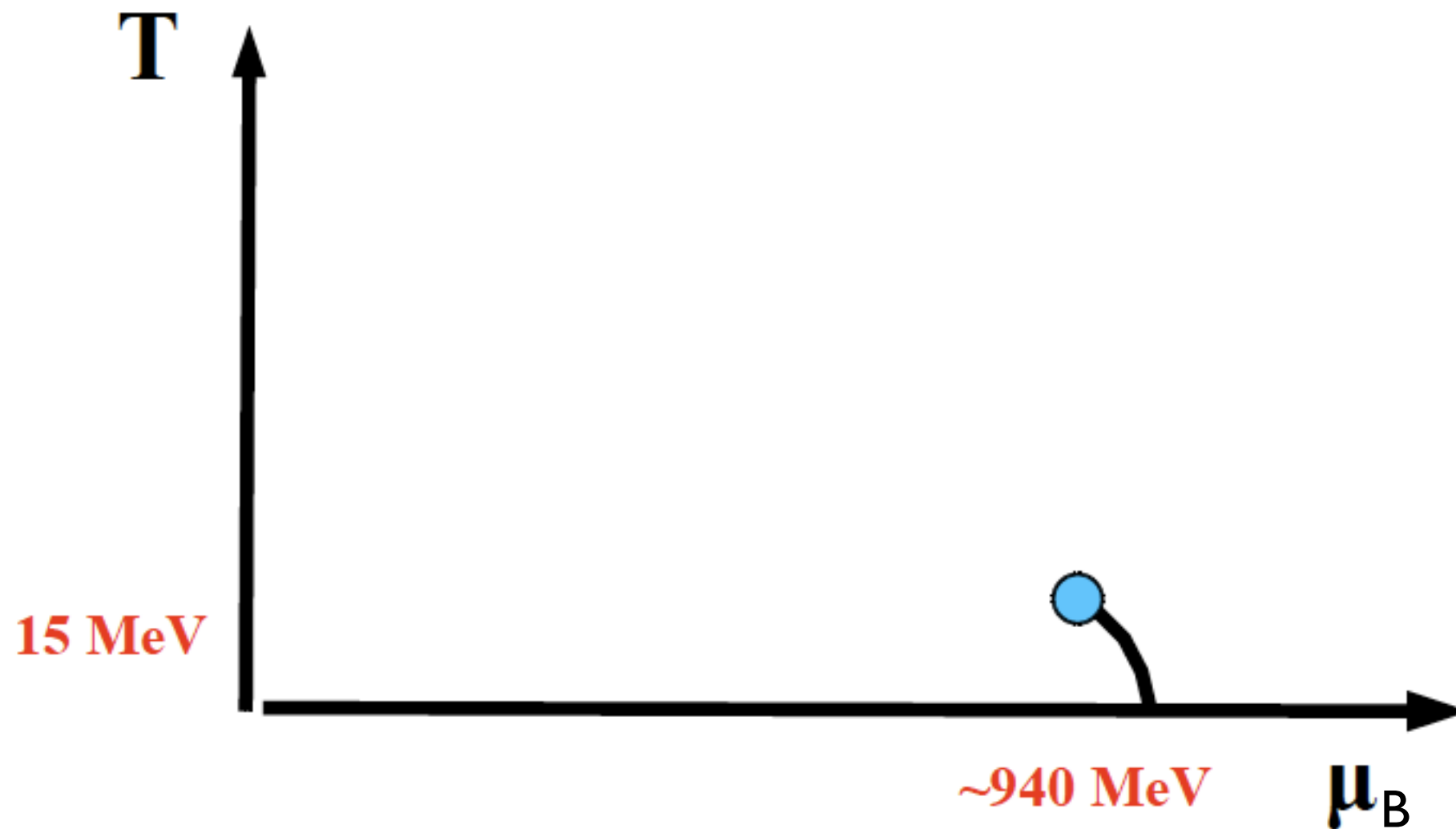


Until 2001: no finite density lattice calculations, **sign problem!**

Expectation based on simplifying models (NJL, linear sigma model, random matrix models, ...)

Check this from first principles QCD!

The QCD phase diagram established by experiment:



Nuclear liquid gas transition with critical end point

Statistical mechanics reminder

System of particles in volume V with conserved number operators, $N_i, i = 1, 2, \dots$
in thermal contact with heatbath at temperature T

Canonical ensemble: exchange of energy with bath, particle number fixed

Grand canonical ensemble: exchange of energy and particles with the bath

Density matrix,
Partition function:

$$\rho = e^{-\frac{1}{T}(H - \mu_i N_i)}, \quad Z = \hat{\text{Tr}}\rho, \quad \hat{\text{Tr}}(\dots) = \sum_n \langle n | (\dots) | n \rangle$$

Thermodynamics:

$$\begin{aligned} F &= -T \ln Z, & \bar{N}_i &= \frac{\partial(T \ln Z)}{\partial \mu_i}, \\ p &= \frac{\partial(T \ln Z)}{\partial V}, & E &= -pV + TS + \mu_i \bar{N}_i \\ S &= \frac{\partial(T \ln Z)}{\partial T}, \end{aligned}$$

Densities:

$$f = \frac{F}{V}, \quad p = -f, \quad s = \frac{S}{V}, \quad n_i = \frac{\bar{N}_i}{V}, \quad \epsilon = \frac{E}{V}$$

QCD at finite temperature and density

Grand canonical partition function

$$Z(V, T, \mu; g, N_f, m_f) = \text{Tr}(e^{-(H-\mu Q)/T}) = \int \mathcal{D}A \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{-S_g[A_\mu]} e^{-S_f[\bar{\psi}, \psi, A_\mu]}$$

Action

$$S_g[A_\mu] = \int_0^{1/T} d\tau \int_V d^3x \frac{1}{2} \text{Tr} F_{\mu\nu}(x) F_{\mu\nu}(x),$$

$$S_f[\bar{\psi}, \psi, A_\mu] = \int_0^{1/T} d\tau \int_V d^3x \sum_{f=1}^{N_f} \bar{\psi}_f(x) (\gamma_\mu D_\mu + m_f - \mu_f \gamma_0) \psi_f(x)$$

$$A_\mu(\tau, \mathbf{x}) = A_\mu(\tau + \frac{1}{T}, \mathbf{x}), \quad \psi_f(\tau, \mathbf{x}) = -\psi_f(\tau + \frac{1}{T}, \mathbf{x}) \quad \text{quark number} \quad N_q^f = \bar{\psi}_f \gamma_0 \psi_f$$

Parameters

$$g^2, m_u \sim 3\text{MeV}, m_d \sim 6\text{MeV}, m_s \sim 120\text{MeV}, V, T, \mu = \mu_B/3$$

$$N_f = 2 + 1 \quad \text{sufficient up to } T \sim 300\text{-}400 \text{ MeV}$$

Difference to $T=0$: compact, periodic time direction!

Fourier expansion of the fields: discrete Matsubara frequencies

$$A_\mu(\tau, \mathbf{x}) = \frac{1}{\sqrt{VT}} \sum_{n=-\infty}^{\infty} \sum_{\mathbf{p}} e^{i(\omega_n \tau + \mathbf{p} \cdot \mathbf{x})} A_{\mu,n}(p), \quad \omega_n = 2n\pi T, \quad p_i = (2\pi n_i)/L$$

$$\psi(\tau, \mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{n=-\infty}^{\infty} \sum_{\mathbf{p}} e^{i(\omega_n \tau + \mathbf{p} \cdot \mathbf{x})} \psi_n(p), \quad \omega_n = (2n+1)\pi T$$

Thermodynamic limit:

$$\frac{1}{V} \sum_{n_1, n_2, n_3} \xrightarrow{V \rightarrow \infty} \int \frac{d^3 p}{(2\pi)^3}$$

Modified Feynman rules:

Inverse (bosonic) free propagator:

$$\Delta^{-1} = p^2 + m^2 = \omega_n^2 + \mathbf{p}^2 + m^2 = (2n\pi T)^2 + \mathbf{p}^2 + m^2$$

Loop integration:

$$\sum_{n=-\infty}^{\infty} \int \frac{d^3 p}{(2\pi)^3}$$

Perturbation theory at finite T

Split action into free (Gaussian) and interacting part, expand in interactions

$$Z = N \int D\phi e^{-(S_0+S_i)} = N \int D\phi e^{-S_0} \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} S_i^l$$

$$\ln Z = \ln Z_0 + \ln Z_i = \ln \left(N \int D\phi e^{-S_0} \right) + \ln \left(1 + \sum_{l=1}^{\infty} \frac{(-1)^l}{l!} \frac{\int D\phi e^{-S_0} S_i^l}{\int D\phi e^{-S_0}} \right)$$

Renormalisation: Whatever renormalisation is necessary and sufficient at $T=0$ is also necessary and sufficient at finite temperature and density

UV behaviour: microscopic physics, depends on details of interactions

T, μ : macroscopic parameters, affect IR behaviour of the theory

Ideal gases from the Gaussian path integral

Important (sometimes unrealistic) model systems to (mis-)guide intuition

Real scalar field:

$$S_0 = \int_0^{\frac{1}{T}} d\tau \int d^3x \frac{1}{2} \phi(x) (-\partial_\mu \partial_\mu + m^2) \phi(x)$$

Fourier space:

$$S_0 = \frac{1}{2T^2} \sum_{n=-\infty}^{\infty} \sum_{\mathbf{p}} (\omega_n^2 + \omega^2) \phi_n(\mathbf{p}) \phi_n^*(\mathbf{p})$$

$$\omega = \sqrt{\mathbf{p}^2 + m^2} \quad \phi_n^*(\mathbf{p}) = \phi_{-n}(-\mathbf{p})$$

$$\begin{aligned} Z_0 &= N \prod_{\mathbf{p}} \int d\phi_0 \exp \left[-\frac{1}{2T^2} (\omega_0^2 + \omega^2) \phi_0^2(\mathbf{p}) \right] \\ &\quad \times \prod_{n>0} \int d\phi_n d\phi_n^* \exp \left[-\frac{1}{2T^2} (\omega_n^2 + \omega^2) \phi_n(\mathbf{p}) \phi_n^*(\mathbf{p}) \right] \\ &= N \prod_{\mathbf{p}} (2\pi)^{1/2} \left(\frac{\omega_0^2 + \omega^2}{T^2} \right)^{-\frac{1}{2}} \prod_{n>0} \int d|\phi_n| |\phi_n| \exp \left[-\frac{1}{2T^2} (\omega_n^2 + \omega^2) |\phi_n|^2 \right] \\ &= N \prod_{\mathbf{p}} (2\pi)^{1/2} \left(\frac{\omega_0^2 + \omega^2}{T^2} \right)^{-\frac{1}{2}} \prod_{n>0} \left(\frac{\omega_n^2 + \omega^2}{T^2} \right)^{-1} = N' \prod_{n=-\infty}^{\infty} \prod_{\mathbf{p}} \left(\frac{\omega_n^2 + \omega^2}{T^2} \right)^{-\frac{1}{2}} = N' (\det \Delta^{-1})^{-1/2} \end{aligned}$$

Note: T-independent constants may be dropped (no contribution to thermodynamics)

$$\ln Z_0 = -\frac{1}{2} \sum_{n=-\infty}^{\infty} \sum_{\mathbf{p}} \ln \frac{\omega_n^2 + \omega^2}{T^2}$$

For Matsubara sum:

$$\ln \left[(2\pi n)^2 + \frac{\omega^2}{T^2} \right] = \int_1^{\omega^2/T^2} \frac{d\theta^2}{\theta^2 + (2\pi n)^2} + \ln(1 + (2\pi n)^2)$$

$$\sum_{n=-\infty}^{\infty} \frac{1}{n^2 + (\frac{\theta}{2\pi})^2} = \frac{2\pi^2}{\theta} \left(1 + \frac{2}{e^\theta - 1} \right)$$

$$\begin{aligned} \ln Z_0 &= - \sum_{\mathbf{p}} \int_1^{\omega/T} d\theta \left(\frac{1}{2} + \frac{1}{e^\theta - 1} \right) + \text{T-indep.} \\ &\xrightarrow{V \rightarrow \infty} V \int \frac{d^3 p}{(2\pi)^3} \left[\frac{-\omega}{2T} - \ln \left(1 - e^{-\frac{\omega}{T}} \right) \right] . \end{aligned}$$

Vacuum energy, pressure: $E_0 = -\partial_{\frac{1}{T}} \ln Z_0 = \frac{V}{2} \int \frac{d^3 p}{(2\pi)^3} \omega$ $p_0 = T \partial_V \ln Z_0 = -\frac{E_0}{V}$

divergent, zero point energy!

Renormalisation:

$$p_{\text{phys}}(T) = p(T) - p(T = 0)$$

Final result:

$$\ln Z_0 = -V \int \frac{d^3p}{(2\pi)^3} \ln(1 - e^{-\frac{\omega}{T}})$$

$$m=0: \quad p = \frac{\pi^2}{90} T^4$$

Fermion fields (Grassmann!):

$$\ln Z_0 = 2V \int \frac{d^3p}{(2\pi)^3} \left[\ln\left(1 + e^{-\frac{\omega - \mu}{T}}\right) + \ln\left(1 + e^{-\frac{\omega + \mu}{T}}\right) \right]$$

↑
two spin components

← →
quarks and anti-quarks

$$m=0: \quad p = \frac{7}{8} \frac{\pi^2}{90} T^4$$

General one-particle (field) expression:

$$\ln Z_i^1(V, T) = \eta V \nu_i \int \frac{d^3p}{(2\pi)^3} \ln(1 + \eta e^{-(\omega_i - \mu_i)/T})$$

$\eta = -1$ for bosons ν_i : spin and internal d.o.f

$\eta = 1$ for fermions

Ideal gases in QCD

Free gas of quarks and gluons: valid at infinite temperature, weak coupling limit

$$\frac{p}{T^4} = \left(2(N^2 - 1) + 4N N_f \frac{7}{8} \right) \frac{\pi^2}{90}$$

2 gluon spin states gluon colours quark, anti-quark, each two spin states quark colours

Hadron resonance gas: at this point a model; later: strong coupling limit of full QCD

Quark-interactions “hidden” in hadrons; hadrons interact weakly

$$\ln Z(V, T) \approx \sum_i \ln Z_i^1(V, T) \quad i = \pi, \rho, K, p, n, \dots$$

IR-structure: divergences and mass scales

Inverse (bosonic) free propagator:

$$p^2 + m^2 = \omega_n^2 + \mathbf{p}^2 + m^2 = (2n\pi T)^2 + \mathbf{p}^2 + m^2$$

$\uparrow$
 effective thermal mass $\sim T$

n=0 mode: propagator of a 3d theory, divergent for $m=0$!

Corrections:



$$m_E^{LO} = \left(\frac{N}{3} + \frac{N_f}{6} \right)^{1/2} gT$$

electric or Debye screening mass

$$\langle A_0(\mathbf{x}) A_0(\mathbf{y}) \rangle$$

$$m_M^{LO} = 0, m_M \sim g^2 T \quad \text{from 2-loop}$$

magnetic screening mass

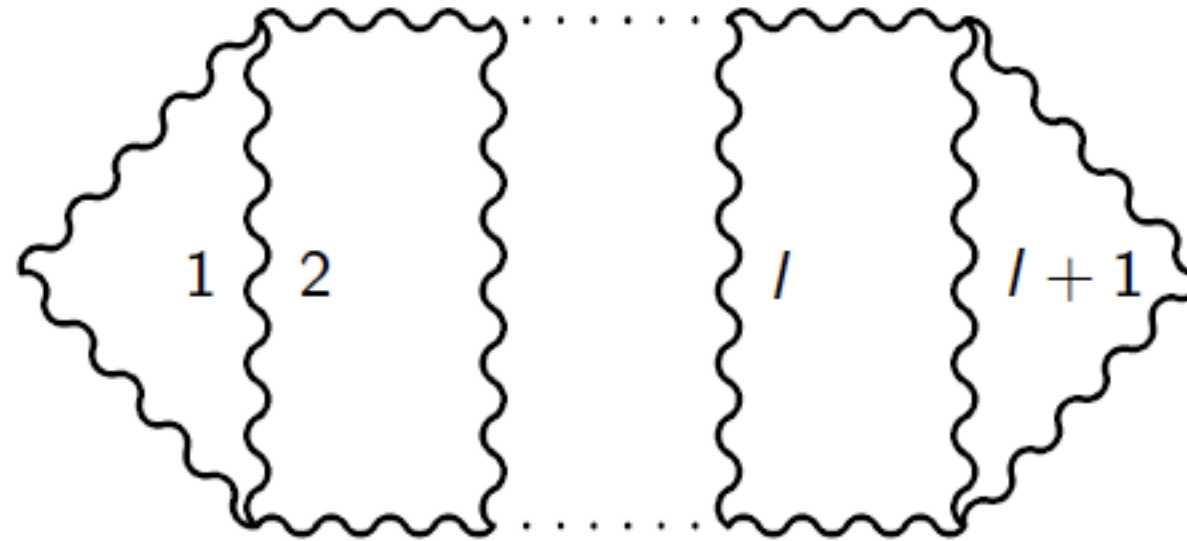
$$\langle A_i(\mathbf{x}) A_i(\mathbf{y}) \rangle$$

0-mode sector of 4d QCD at finite T contains 3d Yang-Mills theory with $g_3^2 \sim g^2 T$

Confining! Doom for perturbation theory....

The Linde problem of finite T QCD / 3d YM

- $(l + 1)$ -loop diagram contribution to pressure



contribution from
Matsubara 0-mode:

$$P \sim g^{2l} (T \int d^3 p)^{l+1} p^{2l} (p^2 + m^2)^{-3l}$$

$$\begin{aligned} & g^{2l} \quad \text{for } l = 1, 2 \\ & g^6 T^4 \ln(T/m) \quad \text{for } l = 3 \\ & g^6 T^4 (g^2 T/m)^{l-3} \quad \text{for } l > 3 \end{aligned}$$

magnetic mass $m_{mag} \sim g^2 T \Rightarrow$ **all loops** ($l > 3$) contribute to g^6

even for weak coupling!

Same problem for all observables!

Only the order to which it occurs is different:

E.g. for magnetic mass already at leading order (2-loop)

Perturbation theory at finite temperature works only up to a finite, observable-dependent order, no matter how weak the coupling!

Salvation comes as a lattice...



The lattice formulation at zero density

Hypercubic lattice: $N_s^3 \times N_\tau$, Lattice spacing a , Wilson's YM action:

$$S_g[U] = \sum_x \sum_{1 \leq \mu < \nu \leq 4} \beta \left(1 - \frac{1}{N} \text{ReTr} U_p \right)$$

Plaquette: $U_p = U_\mu(x) U_\nu(x + a\hat{\mu}) U_\mu^\dagger(x + a\hat{\nu}) U_\nu^\dagger(x)$ Lattice gauge coupling: $\beta = \frac{2N}{g^2}$

Periodic boundary conditions: $U_\mu(\tau, \mathbf{x}) = U_\mu(\tau + N_\tau, \mathbf{x}), U_\mu(\tau, \mathbf{x}) = U_\mu(\tau, \mathbf{x} + N_s)$

Transfer matrix formalism

Provides connection between path integral and Hamiltonian formalism

Rewrite action as sum over time slices:

$$S_g = \sum_{\tau} L[U_i(\tau + 1), U_0(\tau), U_i(\tau)],$$

$$L[U_i(\tau + 1), U_0(\tau), U_i(\tau)] = \frac{1}{2}L_1[U_i(\tau + 1)] + \frac{1}{2}L_1[U_i(\tau)] + L_2[U_i(\tau + 1), U_0(\tau), U_i(\tau)]$$

$$L_1[U_i(\tau)] = -\frac{\beta}{N} \sum_{p(\tau)} \text{ReTr} U_p, \quad \text{spatial plaquettes within one time slice}$$

$$L_2[U_i(\tau + 1), U_0(\tau), U_i(\tau)] = -\frac{\beta}{N} \sum_{p(\tau, \tau+1)} \text{ReTr} U_p, \quad \text{temporal plaquettes connecting slices}$$

Transfer matrix: operator acting on square-integrable functions $\psi[U]$

$$\text{Matrix elements: } T[U_i(\tau + 1), U_i(\tau)] = \int DU_0(\tau) \exp -L[U_i(\tau + 1), U_0(\tau), U_i(\tau)]$$

Translation of states by one time-slice: $|\psi[U_i(\tau + 1, \mathbf{x})]\rangle = T |\psi[U_i(\tau, \mathbf{x})]\rangle$

Identify: $T = e^{-aH}$

Rewrite partition function exactly:

$$Z = \int \prod_{\tau} (DU_i(\tau, \mathbf{x}) T[U_i(\tau + 1), U_i(\tau)]) = \hat{\text{Tr}}(T^{N_{\tau}}) = \hat{\text{Tr}}(e^{-N_{\tau} aH})$$

Identify: $\frac{1}{T} \equiv aN_{\tau}$ $H|n\rangle = E_n|n\rangle$

complete set of energy eigenstates

Thermal expectation value: $\langle O \rangle = Z^{-1} \hat{\text{Tr}}(e^{-\frac{H}{T}} O) = Z^{-1} \sum_n \langle n | T^{N_{\tau}} O | n \rangle = \frac{\sum_n \langle n | O | n \rangle e^{-aN_{\tau} E_n}}{\sum_n e^{-aN_{\tau} E_n}}$

Thermodynamic limit: $N_s \rightarrow \infty$ but keep T finite

Vacuum expectation value: $\langle 0 | O | 0 \rangle = \lim_{N_{\tau} \rightarrow \infty} \frac{\sum_n \langle n | O | n \rangle e^{-aN_{\tau} (E_n - E_0)}}{\sum_n e^{-aN_{\tau} (E_n - E_0)}}$

The space-wise transfer matrix

- Hamiltonian translates in time;
Spectrum: particle masses, from exp. decay of correlators in time
- May also define a Hamiltonian translating the system in space;
Spectrum: screening masses, from exp. decay of correlators in space

$$T[U(z+1), U(z)] \equiv e^{-aH_z}, \quad Z = \text{Tr}(e^{-aN_z H_z}) \quad U(z) : \{U_\mu(z) | \mu \neq 3\}$$

Vacuum physics: $N_{x,y,z,\tau} \rightarrow \infty$ H, H_z spectra identical

Thermal physics: $N_{x,y,z} \rightarrow \infty$ and keep N_τ

H_z acts on states defined on $N_{x,y,\tau}$ lattice;

spectrum of theory on torus with one side squeezed

Finite T physics = finite size effect of the shortened time direction!

Adding fermions

Pick a suitable fermion action:

$$S_f = \sum_{x,y} \bar{\psi}(x) M_{xy}(m_f) \psi(y)$$

Full QCD partition function:

$$Z(N_s, N_\tau; \beta, m_f) = \int DU \prod_f \det M(m_f) e^{-S_g[U]},$$

$$U_\mu(\tau, \mathbf{x}) = U_\mu(\tau + N_\tau, \mathbf{x}),$$

$$\psi(\tau, \mathbf{x}) = -\psi(\tau + N_\tau, \mathbf{x}).$$

Wilson fermions:

$$S_f^W = \frac{1}{2a} \sum_{x,\mu,f} a^4 \bar{\psi}_f(x) [(\gamma_\mu - r) U_\mu(x) \psi_f(x + \hat{\mu}) - (\gamma_\mu + r) U_\mu^\dagger(x - \hat{\mu}) \psi_f(x - \hat{\mu})]$$

$$+ (m + 4\frac{r}{a}) \sum_{x,f} a^4 \bar{\psi}_f(x) \psi_f(x)$$

pick your poison

- **Wilson fermions**
add irrelevant ops. (going away in CL) to make doublers very massive
breaks chiral symmetry for non-zero a
- **staggered (Kogut-Susskind) fermions**
distribute spinor components on different sites, reduces to 4 flavours
take 4th root of determinant to get to one flavour, keeps reduced chiral symm.
non-local operation, have to take CL before chiral limit, mixing of spin, flavour
- **domain wall fermions**
introduce 5th dimension, fermions massive in that dim. and chiral in the other
expensive
- **overlap fermions**
non-local formulation with modified chiral symmetry even for finite a
order: of magnitude more expensive than Wilson

Continuum limit

$$\frac{1}{T} \equiv aN_\tau$$

Fixed scale approach:

- For a given lattice spacing, N_τ controls temperature;
- Allows only discrete temperatures, too large for many applications;
- Continuum limit requires series of lattice spacings

Fixed N_τ approach:

- For a given N_τ , vary the lattice spacing via $\beta(a)$;
- Allows continuous temperatures, but each T value has different cut-off!
- Continuum limit requires series of N_τ

Lines of constant physics and setting the scale

- Compute observable for series of a, N_τ , $\langle O \rangle(\beta, m_f)$
- Tune bare parameters such that for each lattice spacing renormalised parameters are constant $m_f^R(am_{u,d}(\beta), am_s(\beta), \beta) = \text{const.}$
- More practical: keep physical quantities constant $O_i^{\text{phys}}(am_{u,d}(\beta), am_s(\beta), \beta) = \text{const}$
- Non-trivial because of cut-off effects:
Different for different quantities and actions $O^{\text{phys}}(a) = O^{\text{phys}} + c_1 a + c_2 a^2 + \dots$

Perturbative relation for $\beta(a)$: only good very close to continuum limit

$$\Lambda_{QCD} \text{ on lattice: } a\Lambda_L = \left(\frac{6b_0}{\beta}\right)^{-b_1/2b_0^2} e^{-\frac{\beta}{12b_0}},$$

$$b_0 = \frac{1}{16\pi^2} \left(11 - \frac{2}{3}N_f\right), \quad b_1 = \left(\frac{1}{16\pi^2}\right)^2 \left[102 - \left(10 + \frac{2}{3}\right)N_f\right]$$

Non-perturbatively: Express computed quantity in units of another known quantity

E.g. for the critical temperature of a phase transition:

$$\frac{T_c}{m_H} = \frac{1}{a_c m_H N_\tau} = \frac{1}{a(\beta_c) m_H N_\tau}$$

Compute hadron mass at the critical lattice spacing: $a^{-1} = \frac{m_H [\text{MeV}]}{(am_H)(\beta_c)}$

N.B.: Only possible when operating at physical quark masses!

For unphysical quark masses:

(out of computational limitations or interest in certain limits, mass dependence etc.)

Take quantity that depends only weakly on quark masses:

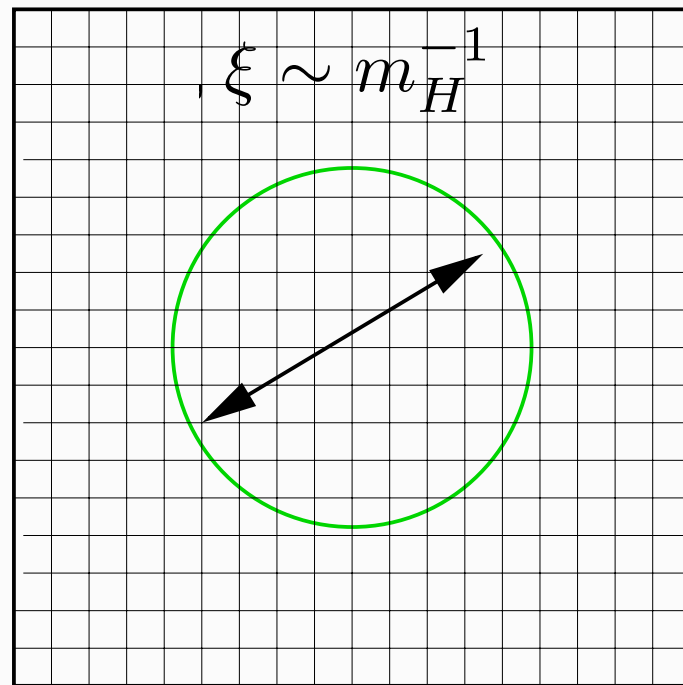
String tension, Sommer scale

$$\frac{T}{\sqrt{\sigma}} = \frac{1}{a\sqrt{\sigma}N_\tau}, \quad \sigma \approx 425 \text{ MeV}; \quad Tr_0 = \frac{r_0}{aN_\tau}, \quad r^2 \frac{dV(r)}{dr} = 1.65$$

Requirements for and constraints from the lattice:

correlation length ξ : lightest gauge invariant (hadronic?) mass scale

$$a \ll \xi \ll aL !$$



scale of interest:

$$T_c \sim 200\text{MeV} \sim (1\text{fm})^{-1}$$

feasible lattices:

$$32^3 \times 4, 16^3 \times 8$$

$$T = \frac{1}{aN_t}$$



$$N_t = 4, 8, 12 \text{ implies } a \approx 0.25, 0.125, 0.083 \text{ fm}$$



$$aL \sim 1.5 - 3\text{fm}$$

low T (confined) phase:

$$m_\pi \gtrsim 250\text{MeV}$$

lighter just beginning...

high T (deconfined) phase:

$$m_\pi \sim T, \xi \sim 1/T$$



$$\frac{1}{N_t} \ll 1 \ll \frac{L}{N_t}$$



$$T \lesssim 5T_c$$

Summary Lecture I

- Perturbation theory of finite T QCD in continuum has infrared problems
- Long wavelength modes of finite T QCD are always confining, even at high T
- Finite T on the lattice is a finite size effect
- For simulations with fixed Nt discretisation errors are T -dependent