Lattice QCD thermodynamics

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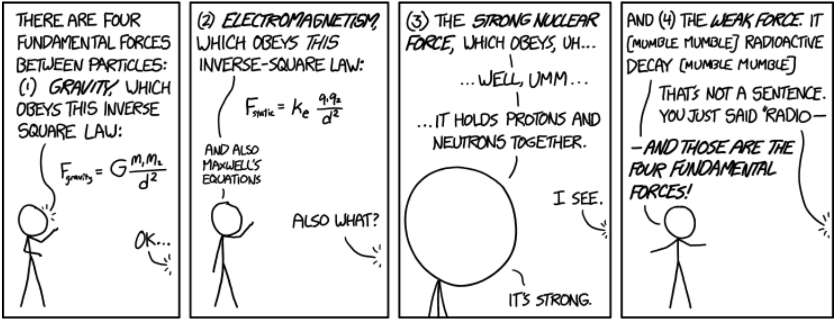
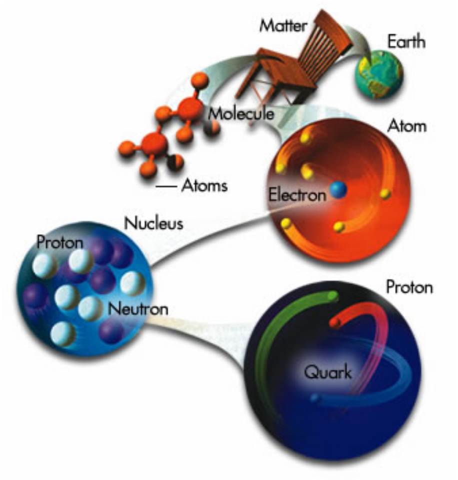


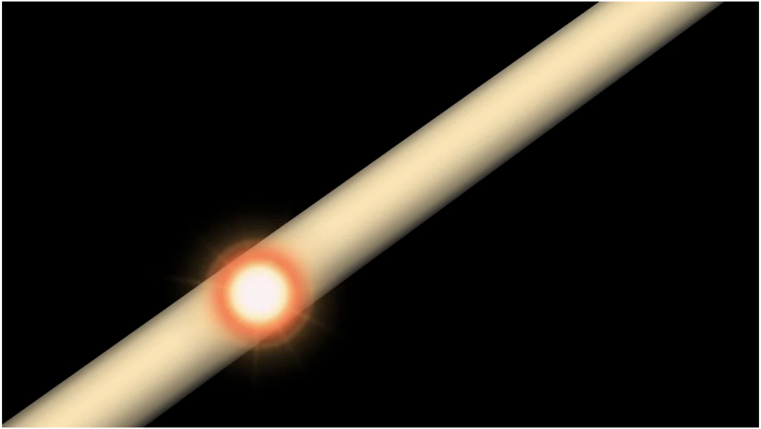
xkcd.com/1489

Strong force



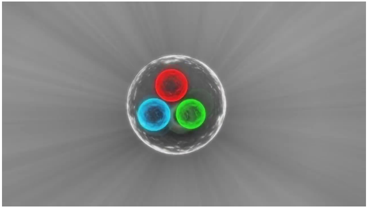
- quarks and gluons “confined” in the proton

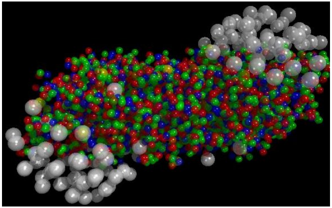
Collision experiments [CERN outreach]



Cold versus hot

- heavy ion collisions





- two distinct phases of matter

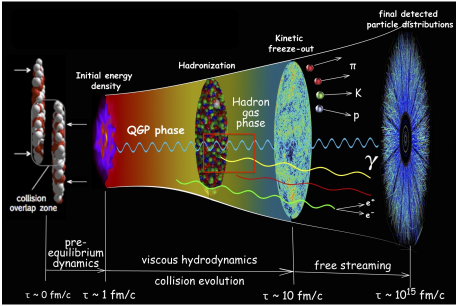
cold, confined	vs.	hot, deconfined
hadronic	vs.	quark-gluon plasma

- phase transition in between
- theory: QCD

what is the nature of these phases?
what is the reason behind confinement and deconfinement?

Strongly interacting matter in extreme conditions

- heavy ion collisions
  $T \lesssim 200$ MeV, $n \lesssim 0.12$ fm^{-3}, $Z/A \approx 0.4$



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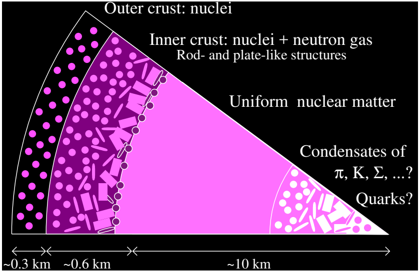
- neutron stars (mergers)
  $T \lesssim 1$ keV ($\lesssim 50$ MeV), $n \lesssim 2$ fm^{-3}, $Z/A \gtrsim 0.025$



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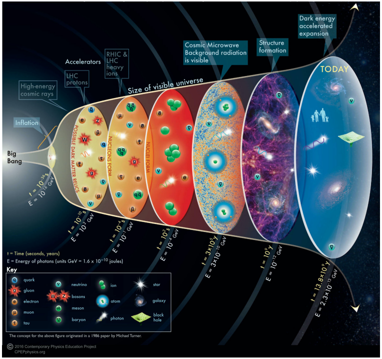
- eary universe, QCD epoch
  $T \lesssim 200$ MeV, $n_B/s \approx 10^{-11}$, $n_Q = 0$, $n_\ell/s \lesssim 0.01$

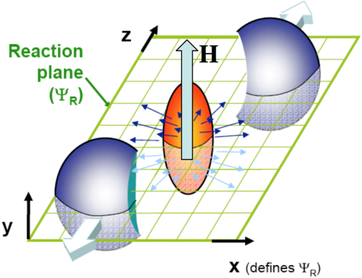


Magnetic fields

- off-central heavy-ion collisions Kharzeev, McLerran, Warringa '07

  impact: chiral magnetic effect, anisotropies, elliptic flow ...

  Fukushima '12 Kharzeev, Landsteiner, Schmitt, Yee '14



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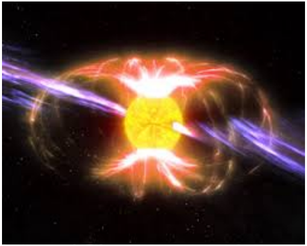

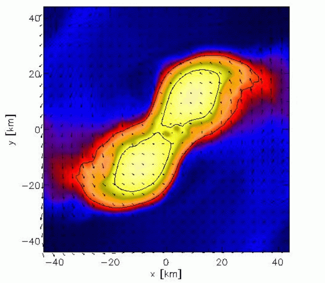

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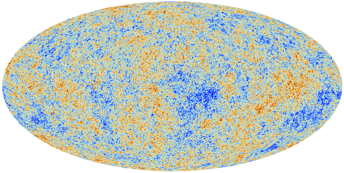

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- strength: $B \approx 10^{15}$ T $\approx 10^{20} B_{\mathrm{earth}} \approx 5 m_\pi^2$
  $\rightsquigarrow$ competition between strong force and electromagnetism

Outline

Outline overall

- lecture 1: introduction to QCD and thermodynamics
- lecture 2: hot Yang-Mills theory on the lattice
- lecture 3: hot QCD on the lattice
- lecture 4: QCD in extreme conditions on the lattice

Literature

- introduction to lattice
  - Gattringer, Lang Lect. Notes Phys. '10
  - Rothe '05
- finite temperature field theory
  - Laine, Vuorinen Lect. Notes Phys. '16
  - Kapusta, Gale '06
- numerical methods
  - DeGrand, DeTar '06
  - Newman, Barkema '99

Outline lecture 1

- QCD, path integral and stochastic integration
- phase transitions and the Ising model
- finite temperature QFT

QCD and the path integral

QCD

- quark field

$$\psi_{f,\alpha,c}$$

- gluon field

$$A_\mu = A_\mu^a T^a$$

- Euclidean Lagrangian

$$\mathcal{L}_{\mathrm{QCD}} = \frac{1}{4}\,\mathrm{Tr}\,F_{\mu\nu}F_{\mu\nu} + \bar{\psi}[\gamma_\mu(\partial_\mu + ig_s A_\mu) + m]\psi$$

- field strength

$$F_{\mu\nu} = F_{\mu\nu}^a T^a, \qquad F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + g_s f^{abc} A_\mu^b A_\nu^c$$

Path integral

- weak, electrodynamic interactions: $g, g_W \ll 1$:
  perturbation theory applicable
- strong interactions $g_s \sim 1$:
  need a *nonperturbative* approach
- path integral Feynman Rev. Mod. Phys. '48

$$\mathcal{Z} = \int \mathcal{D}\bar{\psi}\,\mathcal{D}\psi\,\mathcal{D}A_\mu\ \exp(-S[\bar{\psi},\psi,A_\mu])$$

- with the action

$$S = \int \mathrm{d}^4x\,\mathcal{L}(\bar{\psi},\psi,A_\mu)$$

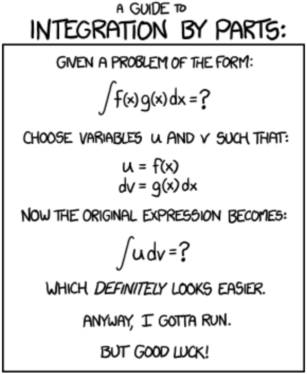
- largest weight $\leftrightarrow$ minimum of action (equations of motion)

Stochastic integration

Numerical integration

- we want to calculate the integral

$$F = \int_0^1 \mathrm{d}x \, P(x) \, f(x), \qquad \int_0^1 P(x) = 1$$



xkcd.com/1201

Stochastic integration

- uniform sampling:
  generate $x_n \in [0,1]$ uniform random variables

$$F = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} P(x_n)\, f(x_n)$$

```
endrodi@pcend:~$ od -N2 -An < /dev/random
 046620
```

Importance sampling

- importance sampling:
  generate x_n with probability $P(x_n)$

$$F = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} f(x_n)$$

$\rightarrow$ animation

Markov chains

- what if we cannot generate x_n according to P?
- Markov chain

$$x_0 \to x_1 \to x_2 \to x_3 \to \dots$$

$$F = \lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} f(x_n)$$

$\to$ animation

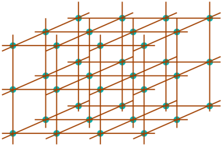
Path integral

- same kinds of integrals, but in ∞ dimensions:

$$\langle F \rangle = \int \mathcal{D}\phi \, P[\phi] \, f[\phi]$$

x point $\leftrightarrow$ $\phi = \phi(x, y, z, t)$ field configuration

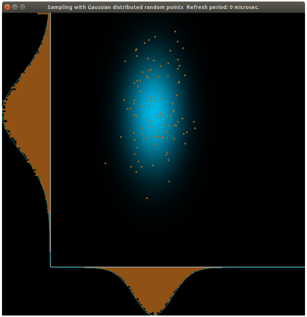
- $P[\phi] = \exp(-S[\phi])$
- discretize space and time Wilson PRD '74



- 10^9-dimensional integrals $\rightsquigarrow$ high-performance computing

QCD vacuum

- how do the relevant field configurations look like?



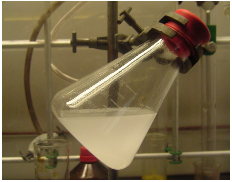
$\rightsquigarrow$

animation courtesy D. Leinweber

Phase transitions

Types of transitions

- 2^{nd} order phase transitions: opalescence



web.mst.edu

- 1^{st} order phase transitions: bubbles

- crossover transition: no singularity

Types of phase transitions

- Ehrenfest classification:

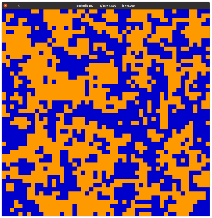
$$n\text{-th order phase transition} \\ \Leftrightarrow \\ n\text{-th derivative of } \log \mathcal{Z} \text{ is discontinuous}$$

- partition function is analytic in finite volume
  $\rightsquigarrow$ singularities only arise in $\log \mathcal{Z}$ as $V \to \infty$
  (practically: V macroscopic)

Ising model

2D Ising model

- two-dimensional lattice $i \in \mathbb{Z}^2$
  degrees of freedom $s_i = \pm 1$
  exact solution Onsager Phys. Rev. '44
  numerical analysis Newman, Barkema



- Hamiltonian with nearest-neigbor $\langle i, j \rangle$ interaction and magnetic field h

$$H[s] = -\sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i$$

- partition function

$$\mathcal{Z} = \operatorname{tr} e^{-H/T} = \sum_{\{s\}} e^{-H[s]/T}$$

- expectation values

$$\langle A \rangle = \frac{1}{V} \frac{1}{\mathcal{Z}} \sum_{\{s\}} A[s]\, e^{-H[s]/T}$$

Spontaneous symmetry breaking

- Hamiltonian

$$H[s] = \overbrace{-\sum_{\langle i,j \rangle} s_i s_j}^{H_0[s]} - h \overbrace{\sum_i s_i}^{M[s]}$$

- at $h = 0$, system is invariant under parity

$$\mathcal{P} s_i = -s_i \qquad H_0[\mathcal{P} s] = H_0[s]$$

- but dominant configurations are not invariant at low T

$$M[\mathcal{P} s] = -M[s]$$

- parity symmetry restored at high T
- phase transition at $T = T_c$

  $\rightarrow$ animation

Explicit symmetry breaking

- Hamiltonian

$$H[s] = \overbrace{-\sum_{\langle i,j \rangle} s_i s_j}^{H_0[s]} - h \overbrace{\sum_i s_i}^{M[s]}$$

- at $h \neq 0$ parity invariance is lost

$$\mathcal{P} s_i = -s_i \qquad H[\mathcal{P}s] \neq H[s]$$

- magnetization always aligned with h

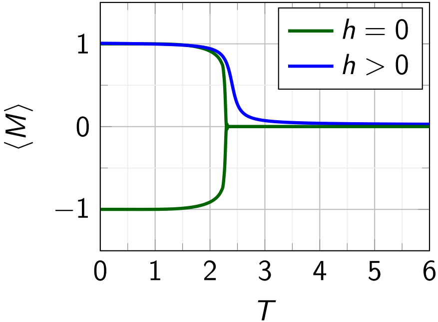
$$hM[s] > 0$$

- transition smoothed out

  $\rightarrow$ animation

Magnetization

- sketch of results in infinite volume

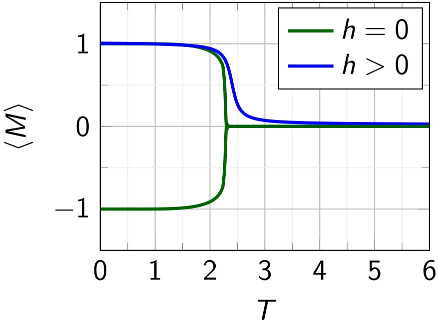


- magnetization as derivative

$$\langle M \rangle = \frac{1}{V}\frac{1}{\mathcal{Z}}\sum_{\{s\}} M[s]\, e^{-H[s]/T} = \frac{1}{V}\frac{\partial \log \mathcal{Z}}{\partial h}$$

Magnetization

- sketch of results in infinite volume



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$$\langle M \rangle = \frac{1}{V} \frac{1}{\mathcal{Z}} \sum_{\{s\}} M[s]\, e^{-H[s]/T} = \frac{1}{V} \frac{\partial \log \mathcal{Z}}{\partial h}$$

- Ehrenfest: $\langle M \rangle$ continuous, $\partial \langle M \rangle / \partial T$ discontinuous
  $\rightsquigarrow$ second order phase transition

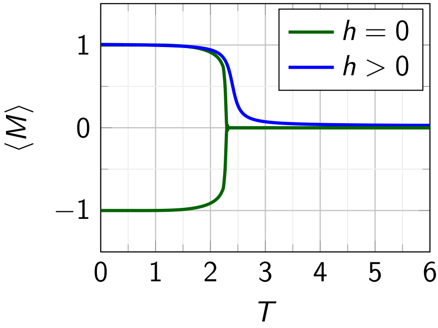
Order parameter

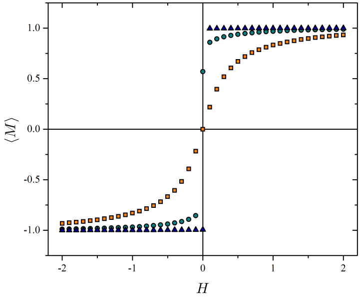
- how to define spontaneous symmetry breaking in terms of an expectation value?

$$h = 0 \quad V < \infty : \quad \langle M \rangle = 0 \qquad \forall T$$

- spontaneous breaking by explicit breaking

$$\lim_{h \to 0^\pm} \lim_{V \to \infty} \langle M \rangle \gtrless 0 \qquad T < T_c$$

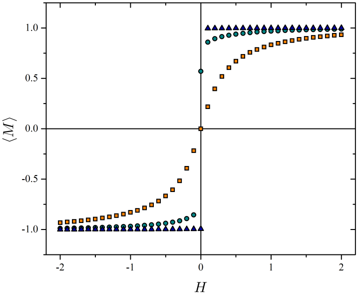


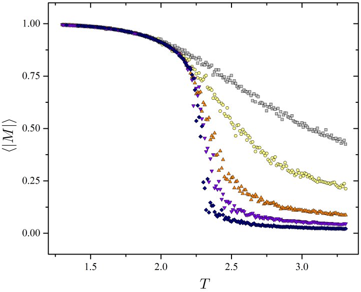


Ibarra-García-Padilla et al. EJP '16

Order parameter

- a little cheating: instead of $\lim_{h\to 0^+} \lim_{V\to\infty} \langle M \rangle$
  use $\lim_{V\to\infty} \langle |M| \rangle$ at $h = 0$





Ibarra-García-Padilla et al. EJP '16

- critical behavior is the same for both observables

Newman, Barkema

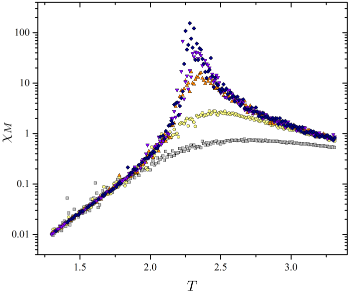
Susceptibility

- magnetization

$$\langle M \rangle = \frac{1}{V}\frac{1}{\mathcal{Z}}\sum_{\{s\}} M[s]\, e^{-H[s]/T} = \frac{1}{V}\frac{\partial \log \mathcal{Z}}{\partial h}$$

- susceptibility

$$\chi_M = \frac{\partial \langle M \rangle}{\partial h} = V\left[\langle M^2 \rangle - \langle M \rangle^2\right]$$



Ibarra-García-Padilla et al. EJP '16

Critical behavior in the thermodynamic limit

- second order phase transition: correlation length ξ diverges
- critical exponents (valid at $V \to \infty$)

$$\xi \propto |T - T_c|^{-\nu}$$

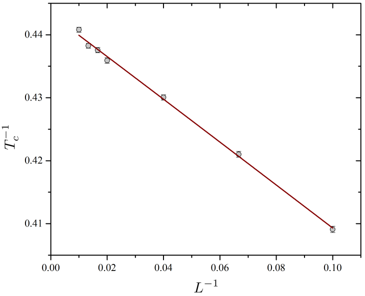
$$\langle |M| \rangle \propto |T - T_c|^{\beta} \qquad \chi_M \propto |T - T_c|^{-\gamma} \qquad \langle |M| \rangle_{T=T_c} \propto h^{1/\delta}$$

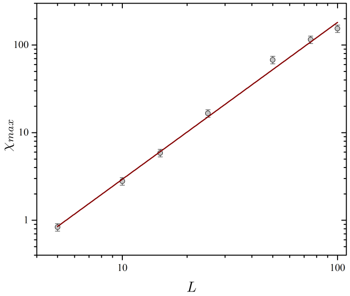
- universality: symmetries and system dimension set the exponents

Critical behavior towards the thermodynamic limit

- how to measure these in finite volume?
- in finite volume, system becomes ordered already when $\xi \approx L$ (Fisher scaling hypothesis)

$L \propto |T_c(L) - T_c|^{-\nu}$ $\qquad T_c(L) - T_c \propto L^{-1/\nu}$ $\qquad \boxed{\chi_M(L, T_c(L)) \propto L^{\gamma/\nu}}$





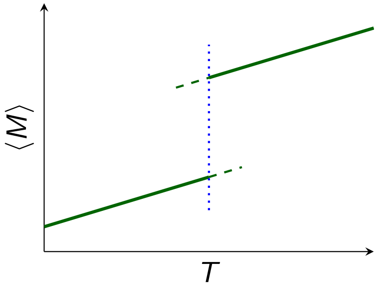
🔗 Ibarra-García-Padilla et al. EJP '16

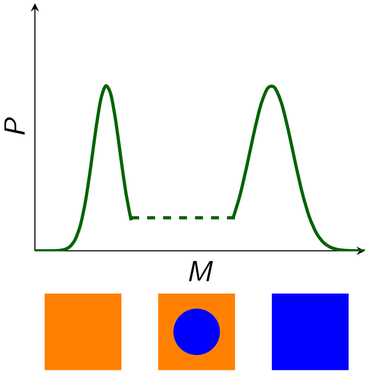
- slope gives critical exponents $\gamma/\nu = 7/4$

First-order phase transitions

First-order phase transitions

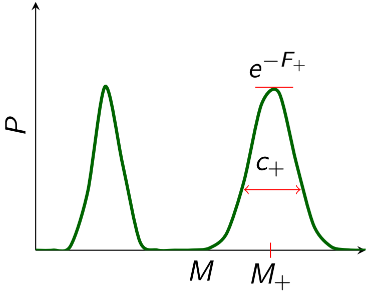
- latent heat and metastability
- distribution at $T = T_c$ and bubbles





First-order phase transitions

- for large volumes



$$P(M) \approx \exp\left[-F_+ - \frac{(M - M_+)^2}{2c_+^2}\right] + \exp\left[-F_- - \frac{(M - M_-)^2}{2c_-^2}\right]$$

Ukawa '93

Finite size scaling

- partition function

$$\mathcal{Z} = \int \mathrm{d}M \, P(M)$$

- susceptibility

$$\chi_M = V \left[\langle M^2 \rangle - \langle M \rangle \right]$$

- close to T_c

$$F_{\pm} = F_0 \mp f \cdot (T - T_c)$$

- susceptibility for large volumes

$$\chi_M = V \frac{c_+ c_-}{(e^{f(T-T_c)} c_+ + e^{-f(T-T_c)} c_-)^2} (M_+ - M_-)^2$$

peak at $T_c + \mathcal{O}(1/V)$, height $\mathcal{O}(V)$ and width $\mathcal{O}(1/V)$

$$\boxed{\chi_M(L, T_c(L)) \propto L^d}$$

Crossovers

Crossover

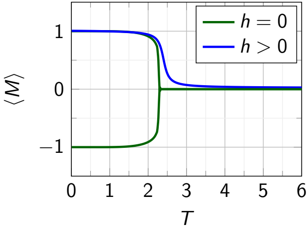
- distribution changes smoothly

$$P(M) \approx \exp\left[-F_1 - \frac{(M - M_1)^2}{2c_1^2}\right]$$

as $M_1(T)$ passes from one value to another

$$\boxed{\chi_M(L, T_c(L)) \propto L^0}$$

- example for crossover: Ising model at $h \neq 0$



Susceptibility at a phase transition: summary

- susceptibility χ of order parameter
- finite size scaling

$$\chi(L, T_c(L)) \propto L^{\rho}$$

ρ	transition type
0	crossover
γ/ν	second order
d	first order

- transition strength

$$d > \gamma/\nu > 0 \qquad 1^{\text{st}} > 2^{\text{nd}} > \text{crossover}$$

Finite temperature field theory

Equation of state

- free energy (density)

$$F = -T \log \mathcal{Z} \qquad f = \frac{F}{V}$$

- entropy density

$$s = -\frac{1}{V}\frac{\partial F}{\partial T}$$

- pressure

$$p = -\frac{\partial F}{\partial V} \xrightarrow{V\to\infty} -f$$

- energy density

$$\epsilon = -\frac{1}{V}\frac{\partial \log \mathcal{Z}}{\partial (1/T)} = f + Ts$$

- interaction measure

$$I = \mathrm{tr}\, T_{\mu\nu} = \epsilon - 3p$$

- all we need is $\log \mathcal{Z}$

Quantum mechanics

- reminder: QM path integral for transition amplitude $x(t)$

$$\langle x_f | e^{-i\hat{H}t} | x_i \rangle = \int_{\substack{x(0)=x_i \\ x(t)=x_f}} \mathcal{D}x \, e^{iS_M[x]}$$

implying (usually used for $t \to \infty$)

$$\int \mathrm{d}x \langle x | e^{-i\hat{H}t} | x \rangle = \int_{x(0)=x(t)} \mathcal{D}x \, e^{iS_M[x]}$$

- similarly, finite T partition function $x(\tau)$

$$\mathcal{Z} = \operatorname{tr} e^{-\hat{H}/T} = \int_{x(0)=x(1/T)} \mathcal{D}x \, e^{-S[x]}$$

- differences
  - argument of x: imaginary time τ
  - over compact interval $0 \le \tau \le 1/T$
  - Euclidean action $S = -S_M(t \to \tau = it)$ all terms in it positive!

Scalar quantum field theory

- partition function for real scalars

$$\mathcal{Z} = \int_{\phi(x,0)=\phi(x,1/T)} \mathcal{D}\phi \, e^{-S[\phi]}$$

  over commuting numbers $\phi(x,\tau)$

- partition function for complex scalars

$$\mathcal{Z} = \int_{\substack{\phi(x,0)=\phi(x,1/T) \\ \phi^*(x,0)=\phi^*(x,1/T)}} \mathcal{D}\phi^* \, \mathcal{D}\phi \, e^{-S[\phi^*,\phi]}$$

- for quadratic actions (free case)

$$\int \mathcal{D}\phi \, e^{-\frac{1}{2}\phi M \phi} = C \cdot [\det(M)]^{-1/2}$$

$$\int \mathcal{D}\phi^* \mathcal{D}\phi \, e^{-\phi^* M \phi} = C' \cdot [\det(M)]^{-1}$$

Fermionic quantum field theory

- partition function for fermions

$$\mathcal{Z} = \int_{\psi(x,0)=-\psi(x,1/T)} \mathcal{D}\bar{\psi}\,\mathcal{D}\psi\, e^{-S[\bar{\psi},\psi]}$$

  over Grassmann numbers $\psi(x,\tau)$
- for bilinear actions (not just free case!)

$$\int \mathcal{D}\bar{\psi}\,\mathcal{D}\psi\, e^{-\bar{\psi}M\psi} = C'' \cdot \det(M)$$

- Euclidean Dirac operator

$$M = \partial\!\!\!/ + m = \gamma_\mu \partial_\mu + m \qquad \{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$$