Outline

- Lattice field theory:
  - Quantum Mechanics with Path Integral (demo)
  - Lattice ϕ^4
  - Scalar QED $\rightarrow$ QCD
- → Monte Carlo
- Finite temperature: Y-M deconfinement transition
- Fermions:
  - Continuum symmetries
  - Species doubling
  - Numerical simulation
  - Finite temperature
- Finite chemical potential:
  - Expectations
  - Sign problem
  - Imaginary chemical potential

Why Monte Carlo?

- To compute: $Z = \int \prod_N dx_i \exp[-S(\{x_i\})], \quad \langle W \rangle = \frac{1}{Z} \int \prod_N dx_i \, W(\{x_i\}) \exp[-S(\{x_i\})]$

  ie. [ratios of] high-dimensional integrals

- Simpson's (trapezoidal) rule: *systematic* error $\mathcal{O}(h^3), h \sim n^{-1/d}, n \sim$ CPU, ie. error $\sim \mathrm{CPU}^{-3/d}$

  Also: trapezoidal rule in high-dimension? nb. points per dim. < 2 ?

- Stochastic method:
  - unbiased estimator (systematic error = 0)
  - statistical error $\sim \frac{1}{\sqrt{\mathrm{CPU}}}$ in any dimension d

  } beats Simpson's rule when $\mathbf{d > 6}$

- How to sample $Z = \sum_{\text{states}} \exp[-S(\text{state})]$?

- Random sampling: Pick states with *uniform* probability, give them weight $\exp(-S)$

- **Importance** sampling: Pick states with probability $\exp(-S)$, give them *uniform* weight

$$Z \approx \sum_{\text{sampled states}}^{n} 1, \quad \langle W \rangle \approx \frac{1}{n} W_i$$

Monte Carlo error $\sim 1/\sqrt{\text{CPU}}$

- Monte Carlo error: $\epsilon \equiv \frac{1}{n}\sum_n W_i - \langle W \rangle; \quad \epsilon_i = W_i - \langle W \rangle; \quad \epsilon = \frac{1}{n}\sum_n \epsilon_i$

- Moments of the error:

  - error is *unbiased:* $\langle \epsilon \rangle = 0$

  - $\langle \epsilon^2 \rangle = \left(\frac{1}{n} \sum_n \epsilon_i \right)^2 = \frac{1}{n^2} \sum_{i,j} \epsilon_i \epsilon_j \underset{\substack{\text{uncorrelated} \\ \text{measurements}}}{=} \frac{1}{n^2} \sum_i \epsilon_i^2 = \frac{1}{n} \left(\langle W^2 \rangle - \langle W \rangle^2 \right)$

- Cf. central limit theorem:

$$\frac{1}{n}\sum_n W_i = \langle W \rangle + \mathcal{O}\left(\sqrt{\frac{\langle W^2 \rangle - \langle W \rangle^2}{n}} \right)$$

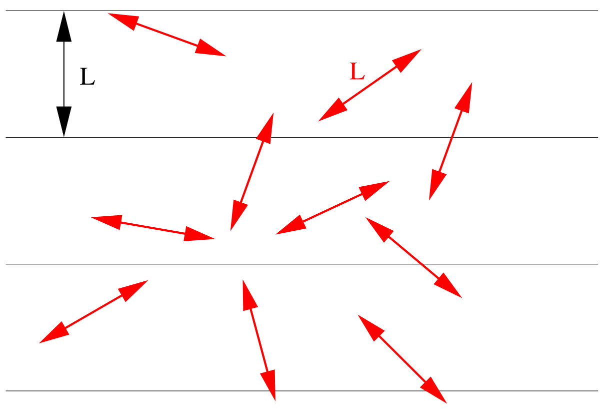
Pre-history of Monte Carlo

- **Pascal** $\longrightarrow$ Fermat , 1654: "Problem of Points" (cf. Chevalier de Méré, gambler)

  Pascal triangle

- **Buffon**: 1777, Buffon' needle problem $\mathrm{Prob(intersect)} = \frac{2}{\pi}$

  (also "noodle problem")



- **Bayes**: 1763, statistical inference

- **Laplace**: 1812, "Théorie analytique des probabilités"

- **Brown**: 1828, pollen grains on water

- **Manhattan project**: 1942-46, "neutron transport" (scattering, absorbtion, fission)

APS News

July 1654: Pascal's Letters to Fermat on the "Problem of Points"

Games of chance are as ancient as human history, with archaeologists unearthing evidence of them on prehistory digs. Gambling also led, indirectly, to the birth of probability theory, as players sought to better understand the odds. In the mid-17th century, an exchange of letters between two prominent mathematicians–Blaise Pascal and Pierre de Fermat–laid the foundation for probability, thereby changing the way scientists and mathematicians viewed uncertainty and risk.

Born in 1623 in Clermont-Ferrand, France, Pascal was a child prodigy largely educated by his father, Etienne, a local magistrate who was also well-connected with some of the most famous intellectuals of that era, including Rene Descartes and Pierre de Fermat. As a result, young Blaise was privileged to sit in on salon-style meetings of some of the greatest minds in Europe. At age 11, he wrote an essay on the sounds of vibrating bodies; the following year, he devised his own proof that the sum of the angles of a triangle equals two right angles.

By the time he was 16, Pascal had progressed sufficiently in his mathematical studies to write a treatise on conic sections, giving rise to what we now call Pascal's Theorem, which states that if a hexagon is inscribed in a conic section, then the three intersection points of opposite sides lie on a straight line. One indication of how impressive this achievement was is the fact that Descartes, when shown the paper, initially did not believe the young teenager had written it.

When Pascal's father became king's commissioner of taxes in Rouen and was struggling with endless calculations and re-calculations, Pascal–not yet 19–invented a mechanical calculator for adding and subtracting to ease his father's task, which became known as the Pascaline. By 1646, he had become interested in Evangelista Torricelli's experimentation on barometers, performing definitive experiments to demonstrate the existence of a vacuum. The SI unit of pressure is the pascal, in his honor.

In 1654, a French essayist and amateur mathematician named Antoine Gombaud, who was fond of gambling, found himself pondering what is known as "the problem of points." It was first proposed in 1494 by an Italian monk named Luca Paccioli in his treatise *Summa de Arithmetica, Geometrica, Proportioni et Proportionalita.* In the game of balla, for example, six goals are needed to win the game. The question posed by Paccioli was how one should divide the winnings if the game is interrupted when one player has five goals and the other has three goals? The player with five goals should have a larger share, but how much larger should his share be?

Gombaud turned to Pascal, who had taken up gambling when his doctors advised him to abandon mental exertions for the sake of his health. The year before, Pascal had worked out the principles of "Pascal's Triangle," a method for determining the binomial coefficients for a given value of $(a+b)^n$–similar to a method devised some 400 years earlier by Chinese mathematician Yang Hui.

Intrigued, Pascal realized he would need to invent a new method of analysis to solve the puzzle, since the solution would need to reflect each player's chances of victory given the score at the time the game was interrupted. Thus began his legendary correspondence with fellow mathematician Pierre de Fermat that, over the course, of several weeks, laid the foundation for modern probability theory. Their respective methods involved listing all the possibilities, and then determining the proportion of time that each player would win, in order to solve it.

Fermat's approach rested on a complete enumeration of the possible outcomes. For example, if the winner of a coin toss game needs to win the best of five tosses, and one player is ahead 2 to 1 when the game is interrupted, Fermat reasoned there would be four possible outcomes had the game continued. Three of those four favor the player with the edge; ergo, he should win three-fourths of the pot. A sticking point is a counter-argument using a different scheme of counting that only finds three possible outcomes instead of four.

Pascal's approach sidestepped this issue by devising an algorithm employing what is now known as induction and incursion. It involves a logical cycle of playing out each possible outcome for each successive round, starting from the point where the game was interrupted. Once the end state is reached, it is then possible to work backward through the intermediate steps and assign a number to the probability of winning for each player at the point when the game was interrupted, and the pot would be divided accordingly.

Pascal's analysis stopped short of considering less idealized situations where a finite number of equally likely possible outcomes could not be listed, such as the weather, or the stock market. By the early 18th century, Jakob Bernoulli had devised the law of large numbers in an attempt to provide a formal proof that uncertainty decreases as the sample size increases for problems with an infinite number of outcomes. Other developments by leading scientists and mathematicians followed, ultimately transforming economics, actuarial science, and the social sciences.

A few weeks after his last correspondence with Fermat, Pascal narrowly escaped death when his carriage nearly ran off a bridge, prompting a religious conversion. He switched his focus from math and science to philosophical and religious treatises, and renounced games of chance. He did an occasional bit of math: between 1658 and 1659 he explored the cycloid and how it might be used to calculate the volume of solids, for example.

His early work on probability seeped into his philosophical work as well, most notably the famous "Pascal's Wager," wherein he reasoned that the odds favor belief in God, even though God's existence cannot be definitively proven. Pascal died of a brain hemorrhage on August 19, 1662, just before his 39th birthday. History has yet to record the outcome of his wager.

Parallel histories

Theoretical

Path integral: Feynman 1948

Imaginary time: Wick 1954

Renormalization: 60's -- 70's

Asymptotic freedom: Gross & Wilczek, Politzer 1973

Lattice gauge theory: Wilson 1974

Simulations

Manhattan project: 1942-1946

Von Neumann, Ulam, Metropolis, Fermi

Fermiac (dedicated MC analog computer): 1947

(Eniac, Maniac, Illiac,...)

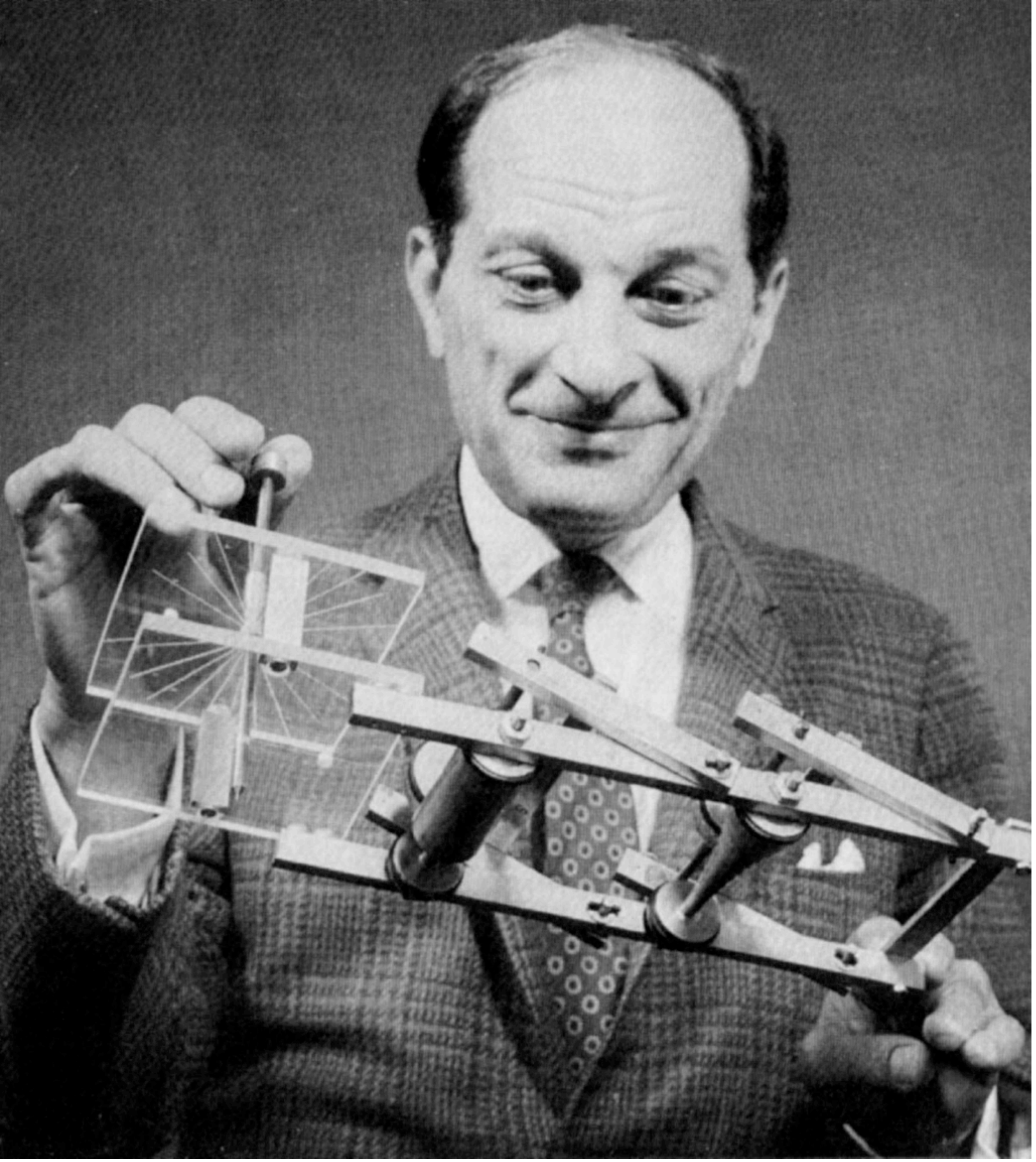
First Monte Carlo symposium: 1949 (pub. 1951)

Metropolis algorithm: 1953

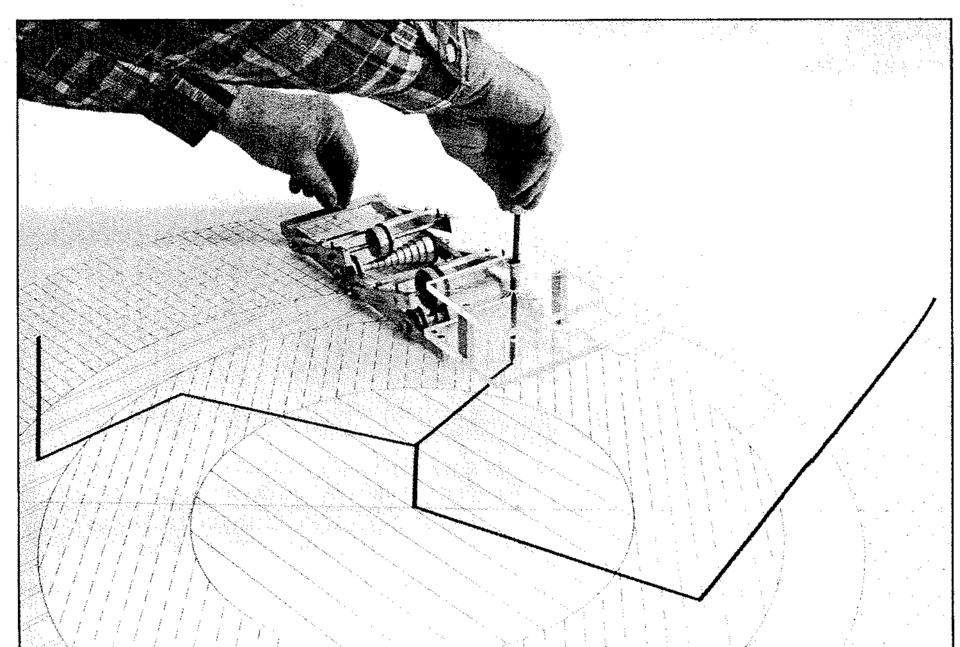
Lattice Monte Carlo study of $SU(2)$: Creutz 1980

Hybrid Monte Carlo (quarks) : Duane et al. 1987

Nowadays: collaboration LQCD $\longleftrightarrow$ industry (IBM/Columbia U. ; Fujitsu/JLQCD)



Stanislaw Ulam with FERMIAC



THE FERMIAC

The Monte Carlo trolley, or FERMIAC, was invented by Enrico Fermi and constructed by Percy King. The drums on the trolley were set according to the material being traversed and a random choice between fast and slow neutrons. Another random digit was used to determine the direction of motion, and a third was selected to give the distance to the next collision. The trolley was then operated by moving it across a two-dimensional scale drawing of the nuclear device or reactor assembly being studied. The trolley drew a path as it rolled, stopping for changes in drum settings whenever a material boundary was crossed. This infant computer was used for about two years to determine, among other things, the change in neutron population with time in numerous types of nuclear systems.

ABC of MC

- Construct **Markov chain:**

  At each Monte Carlo step, Prob(next state) depends on current state only (not on past history)

- Take finite Hilbert space (size $\mathcal{N}$) for simplicity

  After Monte Carlo step k, $\text{Prob}(\text{state } i,\ i = 1..\mathcal{N})$ forms vector $v^k = \begin{pmatrix} v_1^k = \text{Prob}(\text{state } 1) \\ v_2^k = \text{Prob}(\text{state } 2) \\ \dots \end{pmatrix}$

- v^{k+1} is obtained from v^k by application of *Markov matrix* M : $M_{ij} \equiv \text{Prob}(\text{state } i \to \text{state } j)$

$$v_i^{k+1} = \sum_j v_j^k \ \text{Prob}(\text{state } j \to \text{state } i) \implies \mathbf{v^{k+1} = M^T v^k}$$

- Properties of [non-symmetric] Markov matrix: $M_{ij} \geq 0$

  $\sum_j M_{ij} = 1 \ \forall i$ (from i , one always goes somewhere) $\Rightarrow$ $\text{eigenvalues } |\lambda| \leq 1$ (Frobenius)

$$M \begin{pmatrix} 1 \\ 1 \\ \dots \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ \dots \end{pmatrix} \quad \Rightarrow \quad M$$ has at least one eigenvalue $\lambda = 1$

Convergence of Markov chain

- M has at least one eigenvalue $\lambda = 1$ $\Rightarrow$ Every Markov chain has a stationary prob. distribution

  ie. $\exists\, v^\infty$ such that $M^T v^\infty = v^\infty$: $\forall i, \sum_j \mathrm{Prob}(\mathrm{state}\ j \to \mathrm{state}\ i)\ v_j^\infty = v_i^\infty$ "balance eq."

- $v^{k+1} = M^T v^k$ is *contracting map* for eigenmodes with $|\lambda| < 1$

  IF $\lambda = 1$ is the only magnitude-1 eigenvalue, THEN $v^k \xrightarrow[k\to\infty]{} v^\infty$ such that $M^T v^\infty = v^\infty$

- Necessary and sufficient conditions:

  - ergodicity (well-known): $\forall i, j,\ \exists k$ such that $(M^k)_{ij} > 0$

    No two states are unreachable from each other

  - regularity (not well-known): $\exists k$ such that $\forall i, j,\ (M^k)_{ij} > 0$ (*example*)

- Rate of convergence to stationary distribution v^∞ : second largest eigenvalue λ_1 of M

  Damping of associated eigenmode after k steps: $\lambda_1^k = \exp(k \log \lambda_1) = \exp(-k/\tau_{\exp})$

  $\tau_{\exp} = -1/\log \lambda_1$ is "exponential autocorrelation time" (cf. thermalization time)

Detailed balance and Metropolis algorithm

- In practice, v^∞ is given (Boltzmann weight). How to design Markov matrix M ?

  Sufficient condition: "detailed balance", ie. $\forall i, j, \; \frac{M_{ij}}{M_{ji}} = \frac{v_j^\infty}{v_i^\infty}$

- Detailed balance $\Longrightarrow$ balance (+ *assume* ergodicity & regularity)

$$\frac{M_{ij}}{M_{ji}} = \frac{v_j^\infty}{v_i^\infty} \Rightarrow M_{ij} v_i^\infty = M_{ji} v_j^\infty \underset{\sum_i}{\Rightarrow} \sum_i M^T_{ji} v_i^\infty = \underbrace{(\sum_i M_{ji})}_{1} v_j^\infty$$

- **Metropolis** algorithm satisfies detailed balance:

$$\left.\begin{aligned} M_{ij} &= \text{Prob}(\text{candidate } j|i) \times \underbrace{\text{Prob}(\text{accept } j)}_{\min(1, v_j^\infty / v_i^\infty)} \\ M_{ji} &= \text{Prob}(\text{candidate } i|j) \times \underbrace{\text{Prob}(\text{accept } i)}_{\min(1, v_i^\infty / v_j^\infty)} \end{aligned}\right\} \Rightarrow \frac{M_{ij}}{M_{ji}} = \mathbf{1} \times \frac{v_j^\infty}{v_i^\infty}$$

- Normalization $1/Z$ of v^∞ not needed

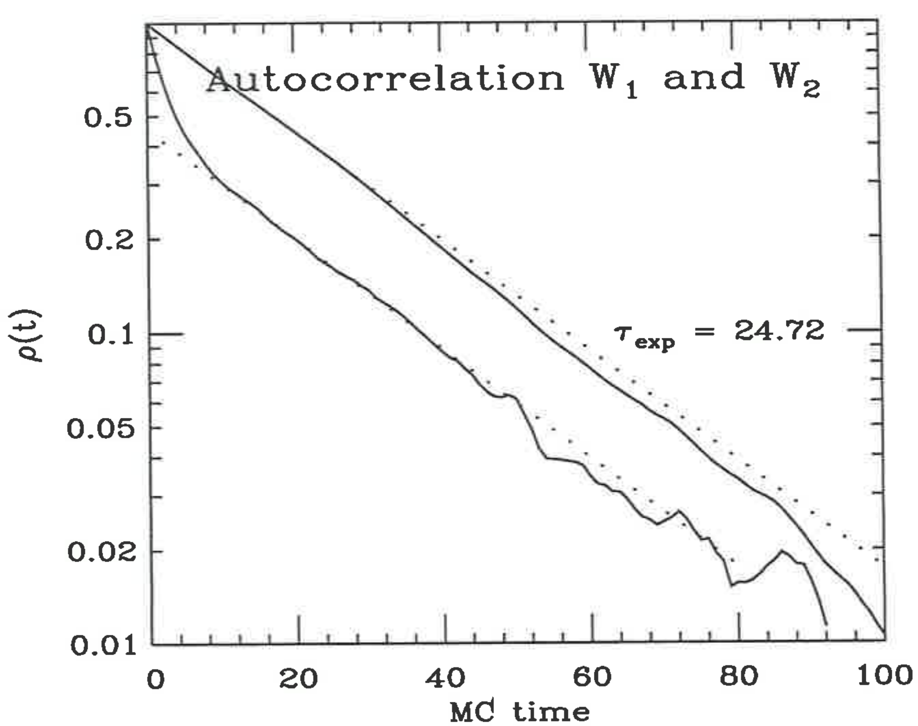
- With $j = T_{\text{rand}} \circ i, \; i = T_{\text{rand}}^{-1} \circ j,$ need $\text{Prob}(T_{\text{rand}}) = \text{Prob}(T_{\text{rand}}^{-1})$

Example: 3 states; $V^{\infty} = \begin{pmatrix} 1/6 \\ 1/3 \\ 1/2 \end{pmatrix}$

Detailed balance $\rightarrow P = \begin{pmatrix} 1-2a-3b & 2a & 3b \\ a & 1-a-\frac{3}{2}c & \frac{3}{2}c \\ b & c & 1-b-c \end{pmatrix}$

eg. $a = 0.1, b = c = 0.01 \rightarrow \lambda_1 = 0.96035, \tau_{exp} = -1/\ln\lambda_1 = 24.72$

Observables: $W_1 \equiv \delta(x,3) \quad (\langle W_1 \rangle = \frac{1}{2});$
$W_2 \equiv 3\delta(x,1) - \delta(x,3) \quad (\langle W_2 \rangle = 0)$



$$C(t) \equiv \langle W(s)\ W(s+t) \rangle_s - \langle W \rangle^2$$

Normalized: $\rho(t) \equiv \frac{C(t)}{C(0)}$ in $[-1, +1]$

$$\rho(t) \underset{t \to \infty}{\sim} \exp(-t/\tau_{exp})$$

Integrated autocorrelation time $\tau_{int}(W)$:

time necessary between $\sim$ independent measurements

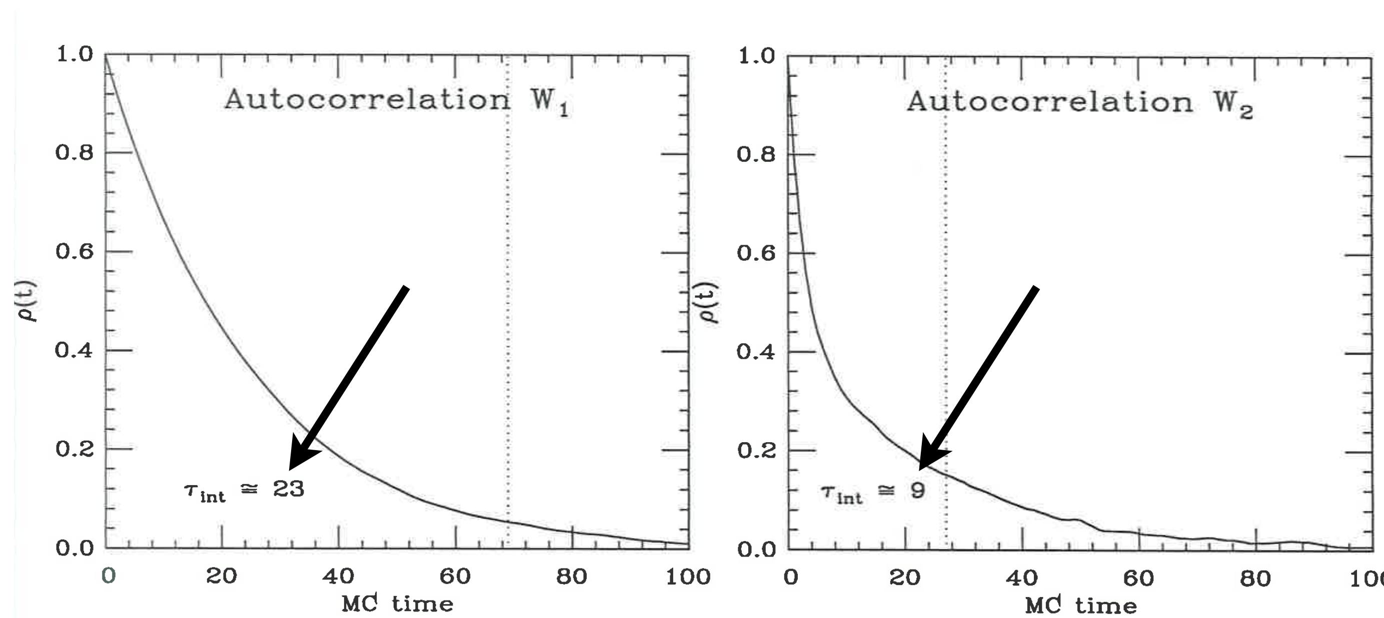
- Definition: $\tau_{int} \equiv \frac{1}{2} + \sum_{t=1}^{\infty} \rho(t)$ -- *depends on observable*

- If $\rho(t) \approx e^{-t/\tau}$, then $\int_0^\infty dt\ \rho(t) = \tau = \tau_{int} = \tau_{exp}$

- Typically, $\rho(t)$ decreases quickly at small t, and has long noisy tail

$\longrightarrow$ truncate $\sum_{t=1}^{\infty}$: $\tau_{int} \sim \frac{1}{2} + \sum_{t=1}^{M} \rho(t)$, self-consistency: $M > 3\tau_{int}$

$W_1 \equiv \delta(x,3)\ \ (\langle W_1 \rangle = \frac{1}{2})$;
$W_2 \equiv 3\delta(x,1) - \delta(x,3)\ \ (\langle W_2 \rangle = 0)$



Example: 3 states; $V^\infty = \begin{pmatrix} 1/6 \\ 1/3 \\ 1/2 \end{pmatrix}$ Again

Detailed balance $\rightarrow P = \begin{pmatrix} 1-2a-3b & 2a & 3b \\ a & 1-a-\frac{3}{2}c & \frac{3}{2}c \\ b & c & 1-b-c \end{pmatrix}$

eg. $a = 0.1, b = c = 0.01 \rightarrow \lambda_1 = 0.96035, \tau_{exp} = -1/\ln\lambda_1 = 24.72$

Increase hopping prob. a, b, c to decrease $\tau_{exp,int}$

Limiting case: $a = 0, b = 1/3, c = 2/3 \rightarrow P = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1/3 & 2/3 & 0 \end{pmatrix}$

Lose convergence: still ergodic but not regular

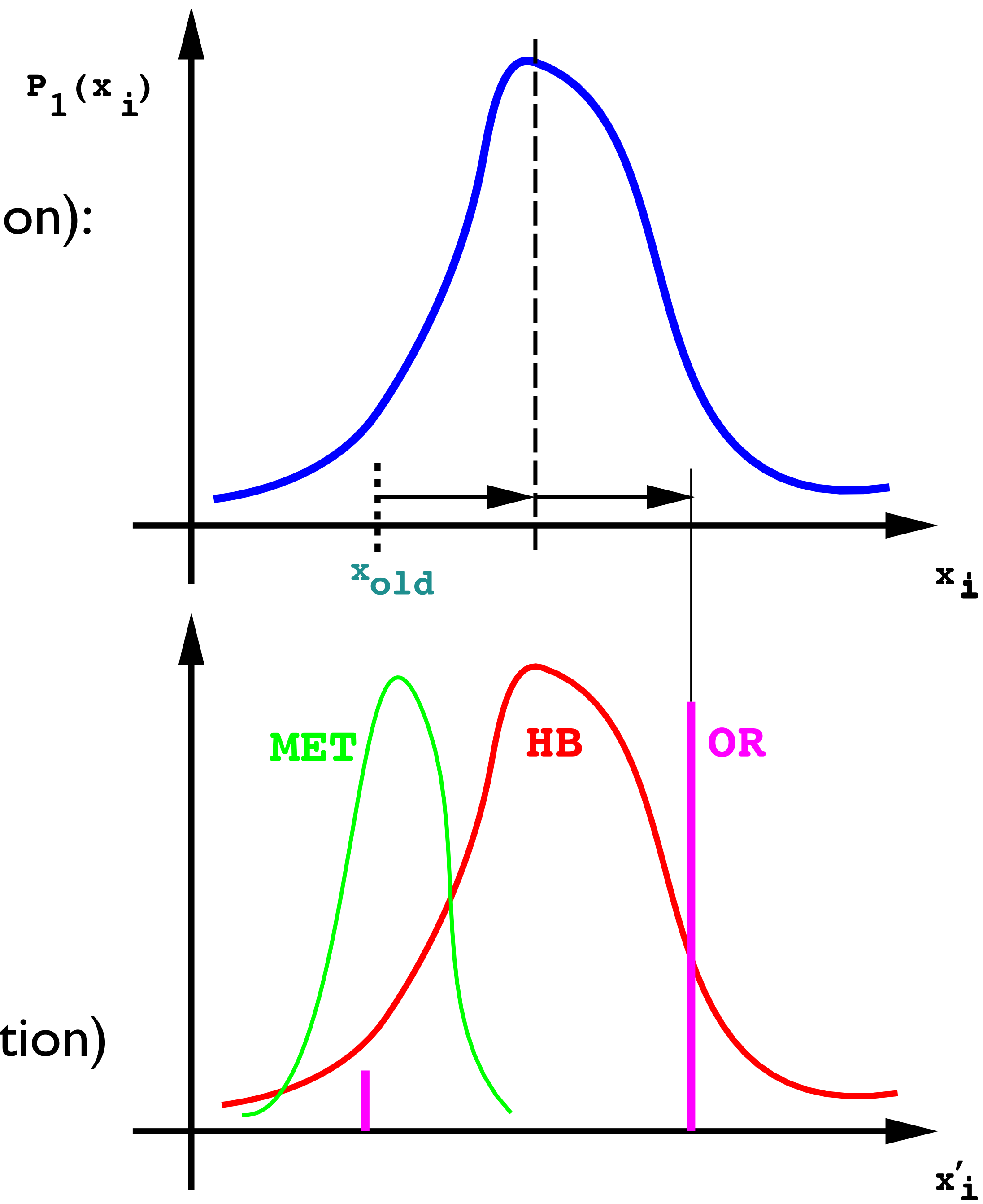
$(s\ even \rightarrow (P^s)_{13} = 0; s\ odd \rightarrow (P^s)_{11} = 0)$, Eigenvalues $\{1, -1, 0\}$

Local updates: Metropolis and alternatives

- Monte Carlo program: perform many "sweeps"

  - Each sweep: loop over all degrees of freedom (eg. $\phi(x),\ U_\mu(x)$) and update one at a time

  - Measure observables after fixed number of sweeps



- Update algorithms (can/should mix for better decorrelation):

  - Metropolis (can perform several "hits" on each d.o.f.)

  - Heatbath: $\mathrm{Prob}(i \to j) = v_j^\infty$

    - Old state i is forgotten $\longrightarrow$ better decorrelation (cf. Metropolis with $\mathrm{nhits} = \infty$)

    - Feasible for simple distributions v^∞ only: Gaussian, exponential, uniform,...

  - Over-relaxation: Metropolis with *deterministic* $j = T \circ i,\ T^2 = 1$(ie. reflection)

    - Excellent when feasible (v_i^∞ almost Gaussian)

- Consider the possibility of subgroup update (esp. $SU(2) \subset SU(3)$)

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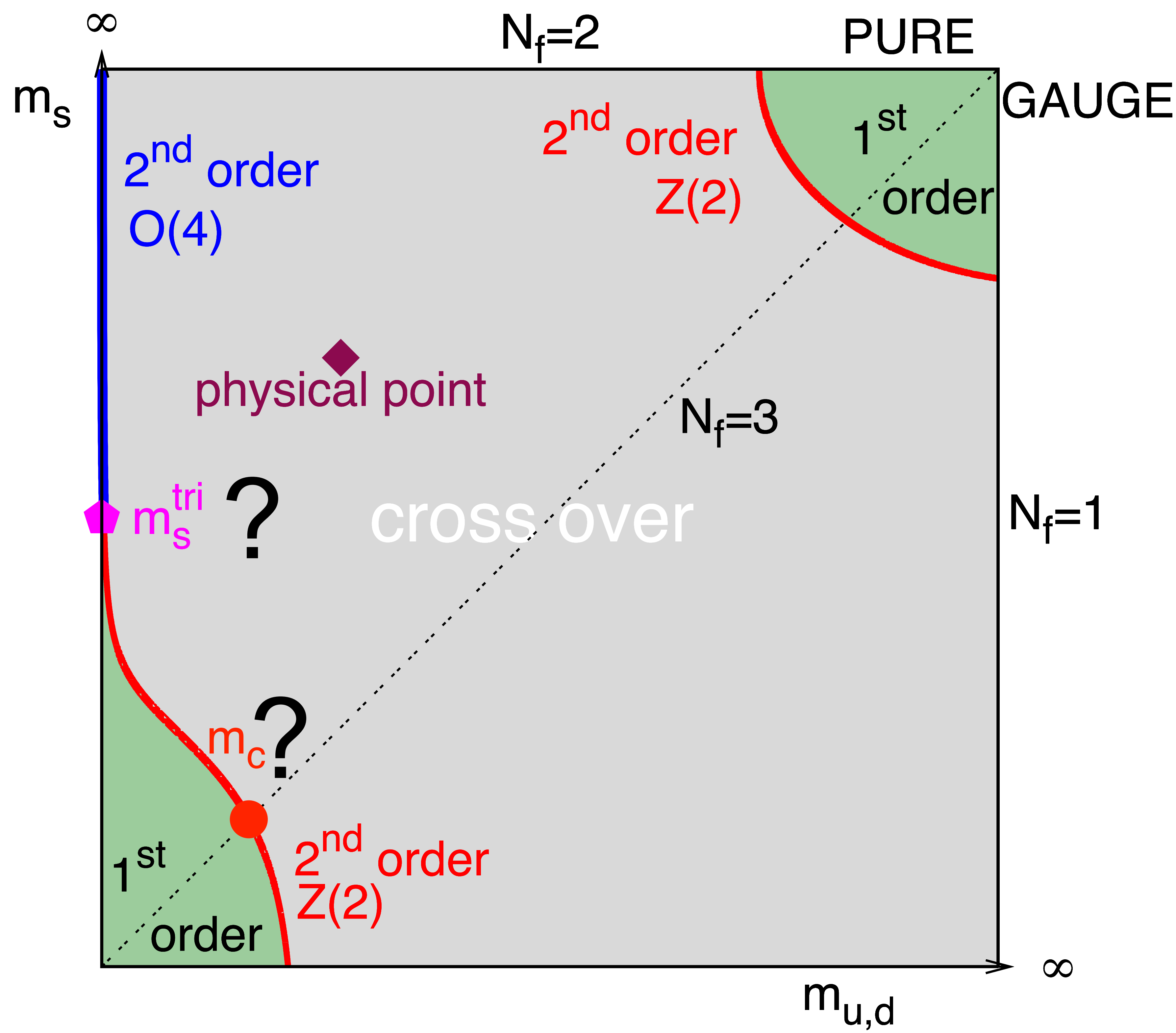
Finite temperature: the Columbia plot



Projection of $(m_u = m_d, m_s, T)$ phase diagram of QCD

Finite temperature: pure gauge $SU(3)$

- Physical expectations:

  - At low T quarks are confined. Excitations are color-singlet bound-states of quarks and gluons

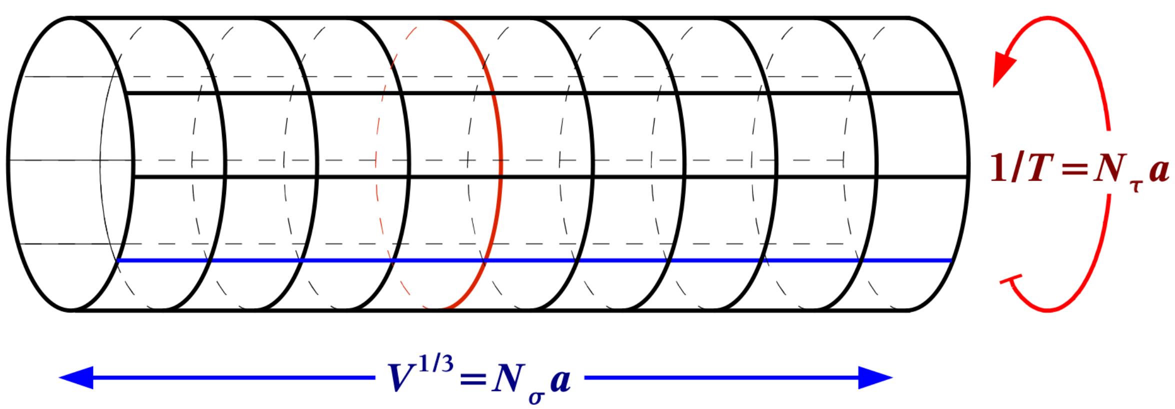
  - At high T typical scattering energy is $\sim T$. By asymptotic freedom, $g(T) \underset{T\to\infty}{\to} 0$

Expect qualitative change ("deconfinement") at high enough T

- Recall thermal boundary conditions:

  - Euclidean time is compact: $\tau \in [0, \beta = 1/T]$

  - Bosonic fields are periodic: $\phi(x,\beta) = \phi(x,0)$



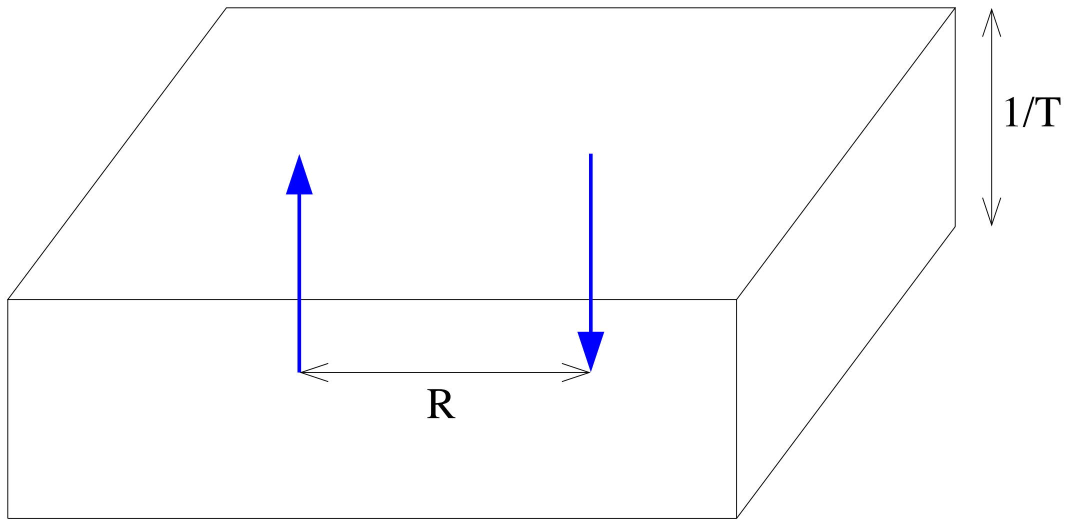
$\Rightarrow$ New closed loop: Polyakov loop (Wilson line) $L(x) \equiv \prod_{\tau=1,N_\tau} U_4(x,\tau) \; = \exp(ig \int_0^\beta d\tau A_0(x,\tau))$

$\mathrm{Tr} L(x)$ is gauge-invariant (and independent of starting τ)

Physical meaning: $L(x)$ is worldline of static color charge (cf. quark)

Order parameter for confinement

- Compare system containing charge-anticharge with empty system: $\frac{Z_{q\bar{q}}}{Z_0} = \exp\left(-\frac{1}{T}F_{q\bar{q}}(R)\right)$



- Express ratio as expectation value:

$$\exp\left(-\frac{1}{T}F_{q\bar{q}}(R)\right) = \frac{\int \mathcal{D}U \ \mathrm{Tr}L(0) \ \mathrm{Tr}L(R)^\dagger \ \exp(-S_{YM}(U))}{\int \mathcal{D}U \ \exp(-S_{YM}(U))}$$

$$= \langle \mathrm{Tr}L(0) \ \mathrm{Tr}^* L(R) \rangle_{Z_0} \ \underset{R\to\infty}{\to} \ |\langle \mathrm{Tr}L \rangle|^2$$

- If $\langle \mathrm{Tr}L \rangle = 0,$ then $F_{q\bar{q}}(R) \underset{R\to\infty}{\to} +\infty,$ ie. confinement
- If $\langle \mathrm{Tr}L \rangle \neq 0,$ then $F_{q\bar{q}}(R) \underset{R\to\infty}{\to} \text{finite},$ ie. deconfinement

$\langle \mathrm{Tr}L \rangle$ is Order Parameter for confinement in Yang-Mills

Deconfinement transition

- When $T = 0, \ \langle \mathrm{Tr} L \rangle = 0$ (confinement).

  When $T \to \infty, \ g(T) \to 0 \ \Rightarrow |\langle \mathrm{Tr} L \rangle| \to 1$ (free theory)

Plausible: $\exists \ T_c$ such that $|\langle \mathrm{Tr} L \rangle|_{T<T_c} = 0, \ \ |\langle \mathrm{Tr} L \rangle|_{T>T_c} > 0$, ie. deconfinement transition

- Phase transition is found:
  - second-order (ξ infinite) for $SU(2)$ Yang-Mills
  - first-order (ξ finite) for $SU(N), \ N > 2$

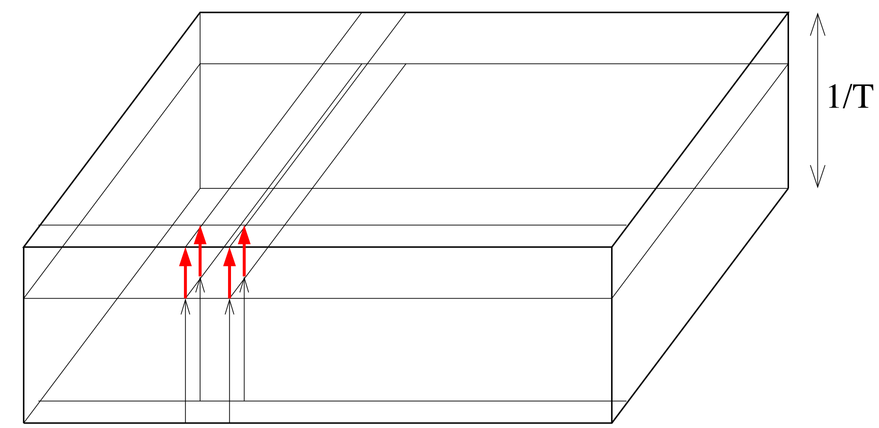
- Hand-waving explanation: entropy mismatch at $T_c \longrightarrow$ first-order
  - low T : spectrum consists of $\mathcal{O}(N^0)$ color singlet glueballs
  - high T : spectrum consists of $(N^2 - 1)$ gluons

Is the phase transition associated with spontaneous symm. breaking?

Center symmetry

- Consider "center transformation" ("large gauge transformation" in continuum):

$$U_4(x,\tau_0) \;\to\; \underbrace{\exp\left(i\frac{2\pi}{N}k\right)}_{z_k \in \mathbf{Z_N}} U_4(x,\tau_0) \quad \forall x; \quad \tau_0 \quad \text{fixed}$$



- space-like plaquettes unaffected

- time-like plaquettes at $\tau = \tau_0$ multiplied by $z_k \times z_k^\dagger = 1$ (z_k commutes with all links)

Action $S_L = \beta \sum_{\Box} \frac{1}{N} \mathrm{ReTr}\, \Box$ invariant

- But Polyakov loop rotated: $L(x) \to z_k L(x)\ \forall x$, ie. $\langle \mathrm{Tr} L \rangle \longrightarrow z_k \langle \mathrm{Tr} L \rangle$

- Center symmetry realized $\Longrightarrow \langle \mathrm{Tr} L \rangle = 0$, ie. confinement
- Center symmetry spontaneously broken $\Longrightarrow \langle \mathrm{Tr} L \rangle \neq 0$, ie. deconfinement

Note: "inverse" symmetry breaking, ie. at *high* temperature (YM: less disorder at high T)

Svetitsky-Yaffe conjecture: any gauge group, in $(d+1)$ dimensions

- *Suppose transition is second-order* ($\xi \to \infty$):

  - Long-range physics dominated by fluctuations of order parameter $\mathrm{Tr} L$

  - If effective Hamiltionian for $\mathrm{Tr} L$ is short-range, then only symmetry group and dimension matter

Universality class is that of dim-d Z_N−symmetric scalar field theory

- Consequences: IF second-order transition, THEN

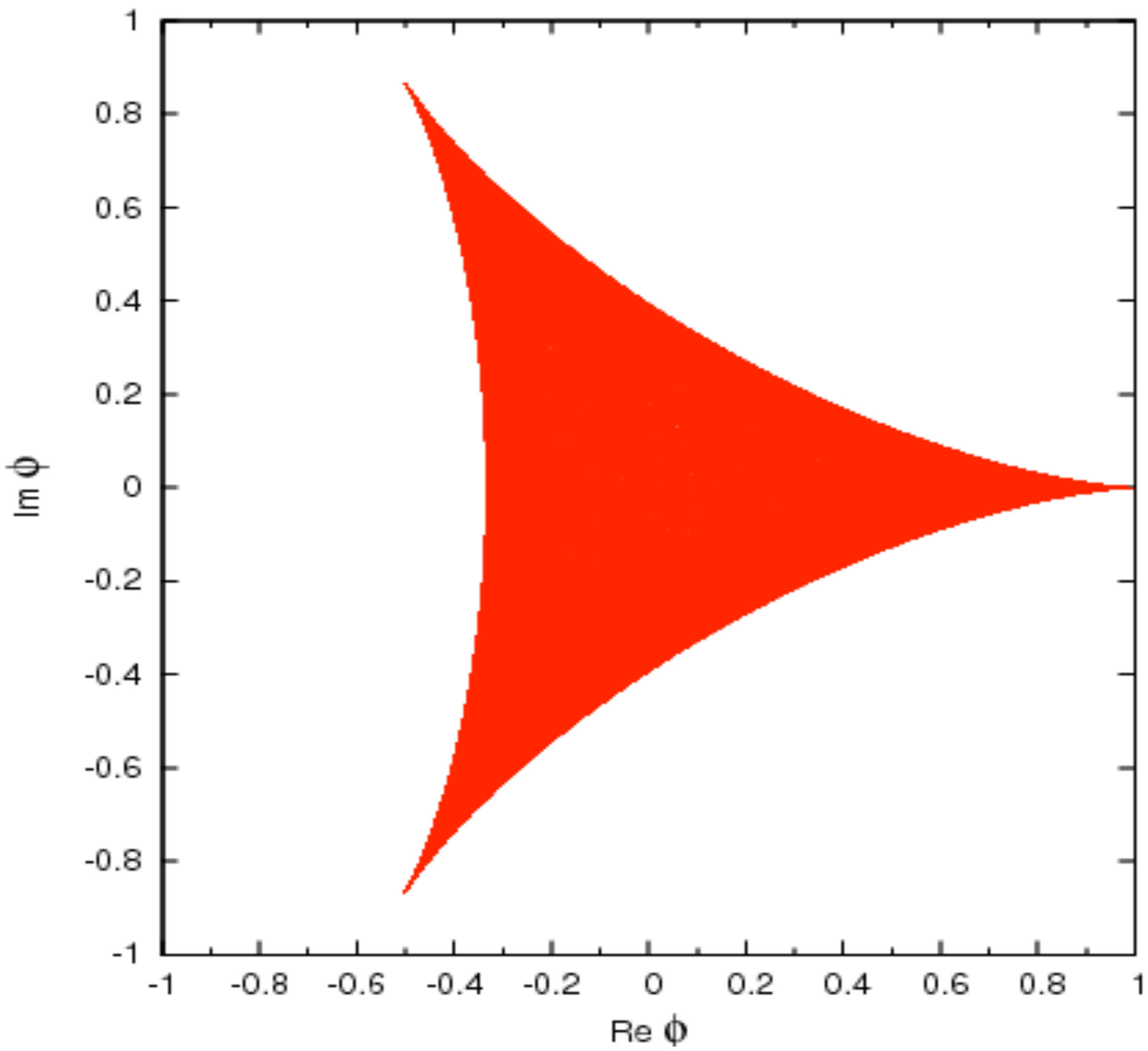
  $SU(2) \sim 3d$ Ising True

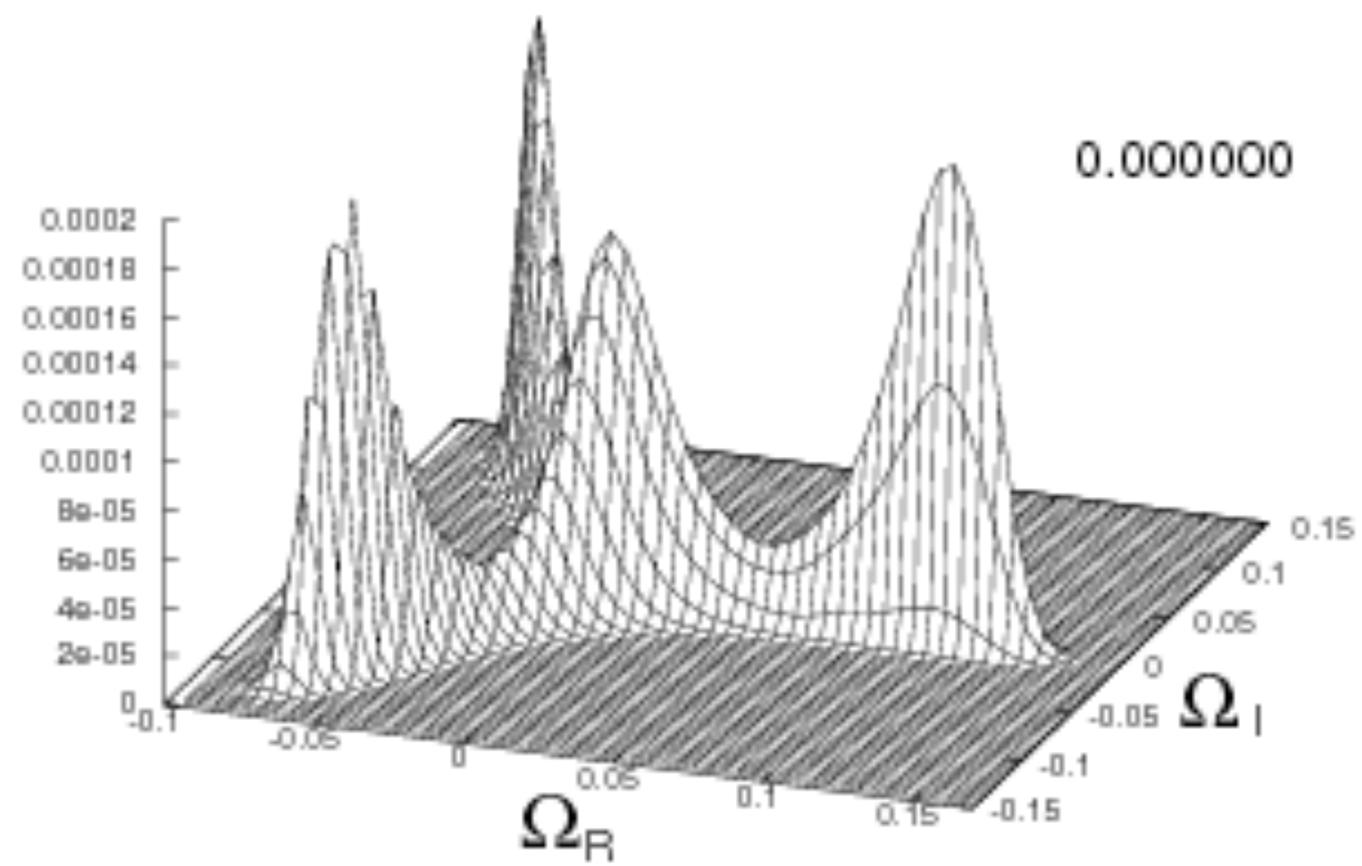
  $SU(3) \sim 3d\ Z_3$?? no known such universality class $\longrightarrow$ first-order? **True**

  $Sp(2) \sim 3d$ Ising ? **NO**: first-order hep-lat/0312022

Svetitsky-Yaffe does NOT predict the order of the phase transition

$SU(3)$ Yang-Mills deconfinement transition is first-order

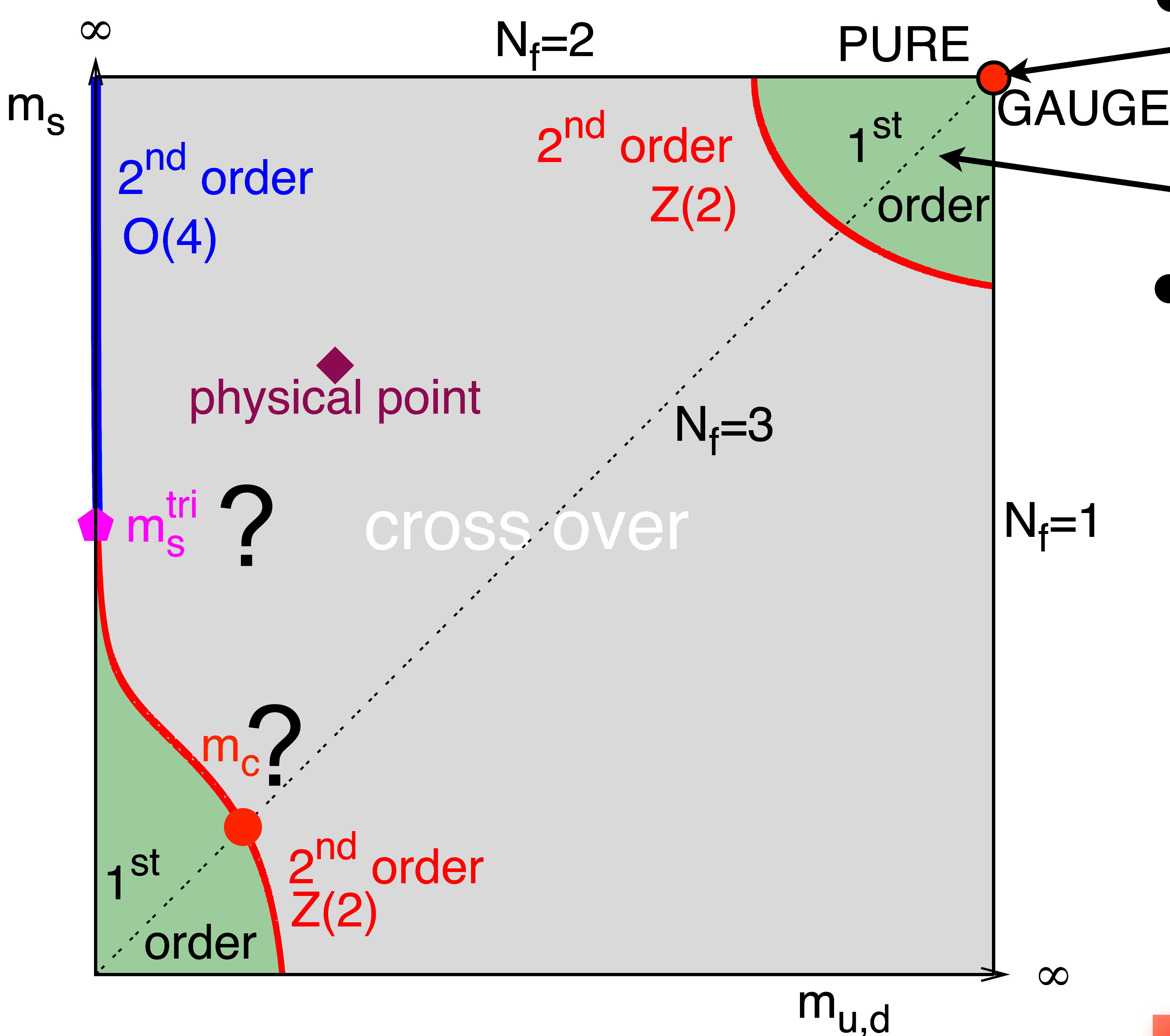




Distribution of $\mathrm{Tr}L$ in complex plane at T_c

Allowed domain in complex plane for $\mathrm{Tr}L,\ L \in SU(3)$

Upper right corner of Columbia plot: first-order



- $SU(3)$ Yang-Mills $\longrightarrow$ first-order

  $T_c \approx 270$ MeV

- First-order transition robust against small changes of parameters (latent heat does not vanish instantly)

Effects of fermions ?