Simulating lattice QCD at finite baryon density

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Lattice QCD



 $-V^{1/3} = N_{\sigma} a$

Scope of lattice QCD simulations: Physics of color singlets

* "One-body" physics: confinement hadron masses form factors, etc..





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Scope of lattice QCD simulations: Physics of color singlets













*** Many-body physics: nuclear matter phase diagram vs (temperature T, density $\leftrightarrow \mu_B$)

Finite μ : why is it important?



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Finite μ : why is it important?



Finite μ : what is known?

Equilibrium w.r.t. weak interactions (β -eq.) + electric neutrality \rightarrow single μ



Commonly believed "minimal" phase diagram ("conventional fiction")

Finite μ : what is known?



Minimal, possible phase diagram

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Finite μ : what is known?



Analogy with water



• quarks anti-commute \rightarrow integrate analytically: det $(\not D (U) + m + \mu \gamma_0)$ $\gamma_5(i\not p + m + \mu \gamma_0)\gamma_5 = (-i\not p + m - \mu \gamma_0) = (i\not p + m - \mu^* \gamma_0)^{\dagger}$

det real only if $\mu = 0$ (or $i\mu_i$), otherwise can/will be complex

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- Measure $d\varpi \sim \det p$ must be complex to get correct physics:

$$\langle \text{Tr Polyakov} \rangle = \exp(-\frac{1}{T}F_q) = \int \text{Re Pol} \times \text{Re } d\varpi - \text{Im Pol} \times \text{Im } d\varpi$$



$$\langle \text{Tr Polyakov}^* \rangle = \exp(-\frac{1}{T}F_{\bar{\mathbf{q}}}) = \int \text{Re Pol} \times \text{Re } d\varpi + \text{Im Pol} \times \text{Im } d\varpi$$

 $\mu \neq 0 \Rightarrow F_{\bar{\mathbf{q}}} \neq F_{\bar{\mathbf{q}}} \Rightarrow \text{Im}d\varpi \neq 0$

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$$\langle \text{Tr Polyakov}^* \rangle = \exp(-\frac{1}{7}F_{\bar{\mathbf{q}}}) = \int \text{Re Pol} \times \text{Re } d\varpi + \text{Im Pol} \times \text{Im } d\varpi$$
$$\mu \neq 0 \Rightarrow F_a \neq F_{\bar{a}} \Rightarrow \text{Im} d\varpi \neq 0$$

• Origin: $\mu \neq 0$ breaks charge conj. symm., ie. usually complex conj.

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Sampling oscillatory integrands

• Example: $Z(\lambda) = \int dx \exp(-x^2 + \mathbf{i}\lambda \mathbf{x})$ lambda= 0 lambda=20 integrand -3 0 з • $Z(\lambda)/Z(0) = \exp(-\lambda^2/4)$: exponential cancellations \rightarrow truncating deep in the tail at $x \sim \lambda$ gives $\mathcal{O}(100\%)$ error "Every x is important" \leftrightarrow How to sample?

Reweighting and optimal sampling of oscillatory integrand

• To "sample": $Z_f \equiv \int dx \ f(x)$, $f(x) \in \mathbf{R}$, with f(x) sometimes negative

Sample w.r.t. auxiliary partition function $Z_g \equiv \int dx \ g(x), \ g(x) \ge 0 \ \forall x$ $\langle W \rangle_f = \frac{\int dx \ W(x)f(x)}{\int dx \ f(x)} = \frac{\int dx \ W(x)\frac{f(x)}{g(x)}g(x)}{\int dx \ \frac{f(x)}{g(x)}g(x)} = \boxed{\frac{\langle W\frac{f}{g} \rangle_g}{\langle \frac{f}{g} \rangle_g}}$ Reweighting, a.k.a. "put sign in observable"

 $\frac{f}{g}$ is the "reweighting factor", $\langle \frac{f}{g} \rangle_g = \frac{Z_f}{Z_g}$ is the "average sign"

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Statistical error on average sign (^f/_g)_g propagates to any observable W optimal sampling → minimize its relative variance ((f/g)²)_g - (f/g)²_g/(f/g)²_g)
 Solution when av. sign → 0: g(x) = |f(x)| , ie. f/g = sign(f) hep-lat/0209126

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• Generically, average sign is exponentially small: $\langle \frac{f}{g} \rangle_g = \frac{Z_f}{Z_g} = \exp(-\frac{V}{T} \Delta f(\mu^2, T))$ Each meas. of $\frac{f}{g}$ gives value $\mathcal{O}(1) \Longrightarrow \operatorname{error} \approx \frac{1}{\sqrt{\# \operatorname{meas.}}}$ Constant rel. accuracy \Longrightarrow need statistics $\propto \exp(+2\frac{V}{T}\Delta f)$

Large V, low T inaccessible

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• av. sign =
$$\frac{Z_{\text{QCD}}(\mu)}{Z_{|\text{QCD}|}(\mu)} = e^{-\frac{V}{T}(f(\mu_u = +\mu, \mu_d = +\mu) - f(\mu_u = +\mu, \mu_d = -\mu))}$$
 (for $N_f = 2$)
• $\sqrt{\pi^2 + 0}$ (for $N_f = 2$)
• $\Delta f(\mu^2, T)$ large in the Bose phase \rightarrow "severe" sign pb.

• av. sign =
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For $T, \mu \ll m_{\rho}$, analytic results via RMT/ χ PT Splittorff, Verbaarschot et al.
• Can improve by incorporating baryons via HRG \rightarrow Prediction: 1005.0539
sign $\geq 0.1 \Leftrightarrow \mathcal{O}(10)$ baryons max. at $T \lesssim T_c$ (less as $T \searrow$, hardly more as $V \nearrow$)

Reweighting strategies

• Sample isospin- μ ensemble + reweight with $e^{i\theta} \rightarrow$ only 0711.0023, 1111.6363

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Reweighting strategies

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- Further danger: "overlap pb." between sampled and reweighted ensembles \rightarrow WRONG estimates in reweighted ensemble for finite statistics

• Example: sample
$$\exp(-\frac{x^2}{2})$$
, reweight to $\exp(-\frac{(x-x_0)^2}{2}) \rightarrow \langle x \rangle = x_0$?





Insufficient overlap ($x_0 = 5$)



Very non-Gaussian distribution of reweighting factor Log-normal Kaplan et al.

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Reweighting from $\mu = 0$: Glasgow and multi-parameter

- "Glasgow": β fixed, reweight with $\frac{\det(\mu)}{\det(\mu=0)} \rightarrow \text{overlap pb.}$
- Fodor & Katz: sample $(\mu = 0, \beta = \beta_c)$ and reweight with $\frac{\det(\mu)}{\det(\mu=0)} \times e^{-\Delta\beta S_{YM}}$ along pseudo-critical line $T_c(\mu)$
 - less fluctuations in reweighting factor
 - improved (ensured?) overlap: both phases sampled



hep-lat/0402006 (physical quark masses, $N_t = 4$) $\rightarrow (\mu_E^q, T_E) = (120(13), 162(2)) \text{MeV}$

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- Abrupt qualitative change near μ_E : abrupt change of physics or breakdown of reweighting ?
- Revival (esp. Wilson fermions): Ukawa et al., Nakamura et al., Fodor & Katz

Alternative at $T \approx 0$: $\mu = 0 + baryonic sources/sinks$



• Mitigated with variational baryon ops. $\rightarrow m_{eff}$ plateau for 3 or 4 baryons ? Savage et al., 1004.2935 At least 2 baryons \rightarrow nuclear potential Aoki, Hatsuda et al., eg. 1007.3559

 Beautiful results with up to 12→72 pions or kaons Detmold et al., eg. 0803.2728 (cf. isospin-µ: no sign pb.)

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Change of strategy

Reweighting gives exact answer in small volumes (work $\sim \exp(V)$)

Try instead: approximate answer in large volume ?

Improvement: reliability hard to assess \rightarrow full confidence?

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Consider expansion parameter $\frac{\mu}{T} \lesssim 1$:

- Taylor expansion about $\mu = 0$
- Imaginary μ + polynomial fit + analytic continuation

Taylor expansion

$$P(T,\mu) = \underbrace{P(T,\mu=0)}_{\text{indep. calc.}} + \Delta P(T,\mu), \qquad \underbrace{\frac{\Delta P(T,\mu)}{T^4} = \sum_{k=1} c_{2k}(T) \left(\frac{\mu}{T}\right)^{2k}}_{\text{indep. calc.}}$$

 $c_{2k} = \langle \text{Tr}(\text{ degree } 2k \text{ polynomial in } \not D^{-1}, \frac{\partial \not D}{\partial \mu}) \rangle_{\mu=0} \to \text{vanilla HMC}$

From {c_{2k}}, obtain all thermodynamic info: EOS and T_c(μ) and crit. pt. and ...
As μ//_T increases, need higher-order c_{2k}'s to control truncation error



Taylor expansion: nitty-gritty

hep-lat/0501030, Appendix A for generic observable \mathcal{O} :

$$\langle \mathcal{O}
angle \, = \, rac{1}{\mathcal{Z}} \int \mathcal{D} U \mathcal{O}(\det M)^{n_{\mathrm{f}}/4} e^{-S_{\mathrm{g}}} \quad ,$$

$$\frac{\partial \langle \mathcal{O} \rangle}{\partial \mu} = \left\langle \frac{\partial \mathcal{O}}{\partial \mu} \right\rangle + \frac{n_{\rm f}}{4} \left(\left\langle \mathcal{O} \; \frac{\partial (\ln \det M)}{\partial \mu} \right\rangle - \left\langle \mathcal{O} \right\rangle \left\langle \frac{\partial (\ln \det M)}{\partial \mu} \right\rangle \right)$$

$$\begin{split} \frac{\partial \ln \det M}{\partial \mu} &= \operatorname{tr} \left(M^{-1} \frac{\partial M}{\partial \mu} \right), \\ \frac{\partial^2 \ln \det M}{\partial \mu^2} &= \operatorname{tr} \left(M^{-1} \frac{\partial^2 M}{\partial \mu^2} \right) - \operatorname{tr} \left(M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial M}{\partial \mu} \right), \\ \frac{\partial^3 \ln \det M}{\partial \mu^3} &= \operatorname{tr} \left(M^{-1} \frac{\partial^3 M}{\partial \mu^3} \right) - \operatorname{3tr} \left(M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial^2 M}{\partial \mu^2} \right) \\ &+ 2 \operatorname{tr} \left(M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial M}{\partial \mu} M^{-1} \frac{\partial M}{\partial \mu} \right), \quad \text{etc...} \end{split}$$

Taylor expansion: nitty-gritty

$$\begin{split} &\frac{\partial^{6}\ln\det M}{\partial\mu^{6}} = \operatorname{tr}\left(M^{-1}\frac{\partial^{6}M}{\partial\mu^{6}}\right) - \operatorname{ftr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^{5}M}{\partial\mu^{5}}\right) \\ &-15\operatorname{tr}\left(M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}M^{-1}\frac{\partial^{4}M}{\partial\mu^{4}}\right) - \operatorname{10tr}\left(M^{-1}\frac{\partial^{3}M}{\partial\mu^{3}}M^{-1}\frac{\partial^{3}M}{\partial\mu^{3}}\right) \\ &+30\operatorname{tr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^{4}M}{\partial\mu^{4}}\right) + \operatorname{fotr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}M^{-1}\frac{\partial^{3}M}{\partial\mu^{3}}\right) \\ &+ \operatorname{fotr}\left(M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^{3}M}{\partial\mu^{3}}\right) + \operatorname{fotr}\left(M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}\right) \\ &- \operatorname{fotr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}\right) \\ &- \operatorname{fotr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}\right) \\ &- \operatorname{fotr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}\right) \\ &+ \operatorname{fotr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu^{2}}M^{-1}\frac{\partial^{2}M}{\partial\mu^{2}}\right) \\ &- \operatorname{fotr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu^{2}}M^{-1}\frac{\partial M}{\partial\mu^{2}}\right) \\ &- \operatorname{fotr}\left(M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu}M^{-1}\frac{\partial M}{\partial\mu^{2}}M^{-1}\frac{\partial M}{\partial\mu^{2}}\right) . \end{split}$$

Now estimate all Traces by sandwiching between noise vectors... GPUs

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Complexity of Taylor expansion approach?

Effects of increasing Taylor order k:

- $c_{2k} = \langle \text{Tr}(\text{ degree } 2k \text{ polynomial in } \not D^{-1}, \frac{\partial \not D}{\partial \mu}) \rangle_{\mu=0} \rightarrow \text{nb. terms} \sim 6^{2k}$
- Cancellations: c_{2k} finite as $V o \infty$, but sum of terms possibly $\sim V^{2k}$

ie. the sign problem fights back!

- c_{2k} obtained as average over less and less Gaussian dist. \rightarrow stat. error?
- $c_{2k} \sim 2k$ -point function \rightarrow need larger volumes

Current best: $N_t = 6$, 8th order Gavai & Gupta, 0806.2233

Need *much* higher order to estimate convergence radius \rightarrow critical point

Karsch, Schaefer et al, 1009.5211

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Imaginary μ : same, but simpler

- Simulate at several values of $\mu = i\mu_l$: no sign pb. ($|\mu_l| < \frac{\pi T}{3}$, Roberge-Weiss singularity)
- Fit $\langle \mathcal{O} \rangle(\mu_I) = \sum_k \frac{d_k}{k!} \mu_I^k \rightarrow d_k$ is estimator of $\frac{\partial^k \mathcal{O}}{\partial \mu_I^k}$ Analytic continuation trivial: $i\mu_I \rightarrow \mu$
- For pressure, take eg. $\mathcal{O}=n_B=\frac{\partial P}{\partial \mu_B}$ and integrate fitted polynomial
- Error analysis simple: data at different μ_I 's uncorrelated
- No free lunch: *k*th derivative damped by *k*!
- Data fitted by *truncated* Taylor series or Pade → systematic error? Conformal mapping to unit disk
 Morita et al., 1008.4549



Frequent problem (here for $T_c(\mu)$): the series in $(i\mu_I)^2$ is *alternating* D'Elia et al., 0905.1292

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New hope with imaginary μ : tricritical scaling

- Rich phase diagram as a function of $(\mu = i\mu_I, m_{u,d}, m_s)$:
 - Roberge-Weiss transition at $\frac{\mu_I}{T} = \frac{2\pi}{3}(2k+1)$
 - Two tricritical lines in Columbia plot $(m_{u,d},m_s)$ for $rac{\mu_l}{T}=rac{2\pi}{3}$



Crosschecks



State of the art I

• Curvature of $T_c(\mu)$ in continuum limit (5 deriv. of P) Fodor, Katz et al.



- $T_c(\mu)$ very flat \rightarrow critical point far from freeze-out curve
- continuum curvature \approx same as $N_t = 4 \rightarrow$ small discretization error ?
- No evidence of critical point for $\mu_q/T \lesssim \mathcal{O}(1)$

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State of the art II

 Curvature of critical surface on coarse lattices (N_t = 4) to O(μ/T)⁴ (8 deriv. of P)
 PdF & Philipsen

Region $(m_{u,d}, m_s)$ of first-order transition shrinks as μ is turned on



Results I and II use same numerical method (small imag. μ) 0711.0262

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Tame the sign problem at strong coupling

Avoid complex determinant by reversing order of integration: links, then fermions

No conservation law for sign pb.! Chandrasekharan, Wenger, PdF, ...

$$Z = \int \mathcal{D}A\mathcal{D}ar{\psi}\mathcal{D}\psi \exp\left[d^{3}xd au\left(-rac{1}{4}F_{\mu
u}F_{\mu
u}+\sum_{i=1}^{N_{f}}ar{\psi}_{i}(
ot\!\!D+m_{i}+\mu_{i}\gamma_{0})\psi_{i}
ight)
ight]$$

- Problem: $-\frac{1}{4}F_{\mu\nu}F_{\mu\nu} \rightarrow \frac{1}{g_0^2} \text{Tr} U_{\text{Plaquette}}$, ie. 4-link interaction
- Solution: set $g_0 = \infty$, strong coupling limit (\leftrightarrow continuum limit)
- Then integral over gauge links factorizes: $\sim \int \prod dU \exp(\bar{\psi}_x U_{x,\hat{\mu}} \psi_{x+\hat{\mu}})$
- analytic 1-link integral \rightarrow only color singlets survive
- perform Grassmann integration last \rightarrow hopping of color singlets

 \rightarrow hadron (baryon, meson) worldlines

(staggered quarks so far)

- sample gas of worldlines by Monte Carlo
- baryons make *self-avoiding* loops:

Point-like, hard-core baryons in pion bath

No πNN vertex: just hard-core repulsion?

Worldline configurations in (1+1)d



Constraint at every site: 3 blue symbols (• $\bar{\psi}\psi$, meson hop) or a baryon loop

Sign problem mild at all densities \rightarrow complete numerical solution

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The dense (crystalline) phase: 1 baryon per site; no space left $\rightarrow \langle \bar{\psi}\psi \rangle = 0$

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Sign problem? Monitor $-\frac{1}{V}\log\langle sign \rangle$



• $\langle \text{sign} \rangle = \frac{Z}{Z_{||}} \sim \exp(-\frac{V}{T} \Delta f(\mu^2))$ as expected; $\Delta f \sim \mu^2 + \mathcal{O}(\mu^4)$

• Determinant method $ightarrow \Delta f \sim \mathcal{O}(1)$. Why is worldline so much better??

- no conservation law for sign pb. (eg. use eigenbasis of H)

- negative sign caused by spatial baryon hopping: no baryon \rightarrow no sign pb no silver blaze pb.

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Results I – Crude nuclear matter: spectroscopy



- Can compare masses of differently shaped "isotopes"
- $am(A) \sim a\mu_B^{crit}A + (36\pi)^{1/3}\sigma a^2 A^{2/3}$, ie. (bulk + surface tension) Bethe-Weizsäcker parameter-free (μ_B^{crit} and σ measured separately)
- "Magic numbers" with increased stability: A = 4, 8, 12 (reduced area)

Results II – Nuclear interactions and Phase diagram

- Baryon: point-like core (self-avoiding loop) disturbs pion bath \Rightarrow macroscopic pion cloud $\Delta E_{\pi}(R) \propto \frac{\exp(-m_{\rho/\omega}R)}{R} \times (-1)^{x+y+z} \times (-1)^{x+y+z}$
- Nuclear interaction from nucleon's core disturbing other nucleon's pion cloud Linear response $\Rightarrow V_{NN}(R) \approx -2 \times \Delta E_{\pi}(R)$, ie. Yukawa!

• Phase diagram for $m_q = 0$: chiral transition line, with tricritical point



Going beyond strong coupling limit

• At $\beta = 0$: measure gauge observables (plaquette, Polyakov loop)

w/Fromm, Langelage, Miura,...

Polyakov loop vs T across chiral transition $m_q = 0, \ \mu = 0$



• Simulate $\mathcal{O}(\beta)$ action: in progress

• Beyond $\mathcal{O}(\beta)$: decouple the 4 links in each plaquette by *auxiliary fields*? Hubbard-Stratonovich: $\int d\phi^* d\phi \exp(-|\phi - \phi_0|^2) = \text{const. indep. of }\phi_0$ Variant: $\exp(\alpha AB) \propto \int d\phi^* d\phi \exp[-\alpha(|\phi|^2 - \phi^*A - B\phi)] \quad \forall \alpha \in R^+$ Take $A = U_1 U_2, B = U_3 U_4,$ ϕ along diagonal Further decoupling to "1-link" action \rightarrow link integration possible $\forall \beta$

Conclusions (from LAT09 Beijing plenary)

- Finite density QCD is important enough to keep trying
- Analytic understanding of severity of sign problem
- Crosschecks among LQCD methods and with effective models
- Slow but steady progress for small μ : $T_c(\mu)$ OK, crit. pt. ?? Try to control $a \rightarrow 0$ extrapolation
- Confucius: Real knowledge is to know the extent of one's ignorance
- Future: -Start with link integration still vague beyond $\beta = 0$ -Complex Langevin do miracles really happen?

• Not covered: - canonical ensemble - density of states method Backup: complex Langevin 80's revival Aarts, Seiler, Stamatescu, Berges,...

• Real action S: Langevin evolution in Monte-Carlo time τ Parisi-Wu $\frac{\partial \phi}{\partial \tau} = -\frac{\delta S[\phi]}{\delta \phi} + \eta$, ie. drift force + noise Can prove: $\langle W[\phi] \rangle_{\tau} = \frac{1}{2} \int \mathcal{D}\phi \exp(-S[\phi]) W[\phi]$

• Complex action S ? Parisi, Klauder, Karsch, Ambjorn,... Drift force complex \rightarrow complexify field $(\phi^R + i\phi^I)$ and simulate as before With luck: $\langle W \left[\phi^R + i\phi^I \right] \rangle_{\tau} = \frac{1}{Z} \int \mathcal{D}\phi \exp(-S\left[\phi\right]) W\left[\phi\right]$

- Only change since 1980's: adaptive stepsize \rightarrow runaway sols disappear
- Gaussian example:

$$Z(\lambda) = \int dx \exp(-x^2 + \mathbf{i}\lambda \mathbf{x})$$

Complexify: $\frac{d}{d\tau}(x + iy) = -2(x + iy) + i\lambda + \eta$

For any observable W, $\langle W(x + iy) \rangle_{\tau} = \langle W(x) \rangle_{Z}$

