The struggle against the sign problem

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Monte Carlo: no pain, no gain...

Monte Carlo highly efficient: *importance sampling* $\mathrm{Prob}(\mathrm{conf}) \propto \exp[-S(\mathrm{conf})]$

- But all low-hanging fruits have been picked by now
- Further progress requires tackling the "sign problem":

$$\boxed{\exists \text{ conf s.t. "Boltzmann weight" } \exp[-S(\mathrm{conf})] \notin \mathbb{R}_{\geq 0}}$$

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Real-time quantum evolution

dynamics of chemical reactions, protein folding, entanglement, ...

limited to small systems / short times, or classical approximation

weight in path integral $\propto \exp(-\frac{i}{\hbar}Ht) \longrightarrow$ phase cancellations

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High T_c superconductivity: still mysterious after $\sim$ 30 years

Hubbard model: repulsion $U n_\uparrow n_\downarrow \xrightarrow[\text{Hubbard-Stratonovich}]{} \det_\uparrow \det_\downarrow$

can be negative except at half-filling (particle-hole symmetry)

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QCD at non-zero density / chemical potential μ

integrate out the fermions $\det(\not{D} + \mu\gamma_0)^2$ $(N_f = 2)$

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Real > 0 "Boltzmann weight" is the exception rather than the rule

Interdisciplinary sign pb conferences, etc...

Computational complexity of the sign pb

- How to study: $Z_\rho \equiv \int dx\ \rho(x), \quad \rho(x) \in \mathbf{R}$, with $\rho(x)$ sometimes negative ?

  Reweighting: sample with $|\rho(x)|$ and "put the sign in the observable":

$$\langle W \rangle_f \equiv \frac{\int dx\ W(x)\rho(x)}{\int dx\ \rho(x)} = \frac{\int dx\ [W(x)\mathrm{sign}(\rho(x))]\ |\rho(x)|}{\int dx\ \mathrm{sign}(\rho(x))\ |\rho(x)|} = \boxed{\frac{\langle W \mathrm{sign}(\rho)\rangle_{|\rho|}}{\langle \mathrm{sign}(\rho)\rangle_{|\rho|}}}$$

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- $\langle \mathrm{sign}(\rho)\rangle_{|\rho|} = \frac{\int dx\ \mathrm{sign}(\rho(x))|\rho(x)|}{\int dx\ |\rho(x)|} = \boxed{\frac{Z_\rho}{Z_{|\rho|}}} = \exp(-\frac{V}{T}\underbrace{\Delta f(\mu^2, T)}_{\text{diff. free energy dens.}})$, exponentially small

  Each meas. of $\mathrm{sign}(\rho)$ gives value $\pm 1 \Longrightarrow$ statistical error $\approx \frac{1}{\sqrt{\#\ \text{meas.}}}$

  Constant relative accuracy $\Longrightarrow$ $\boxed{\text{need statistics} \propto \exp(+2\frac{V}{T}\Delta f)}$

  Large V, low T inaccessible: signal/noise ratio degrades exponentially

"Figure of merit" Δf: measures severity of sign pb.

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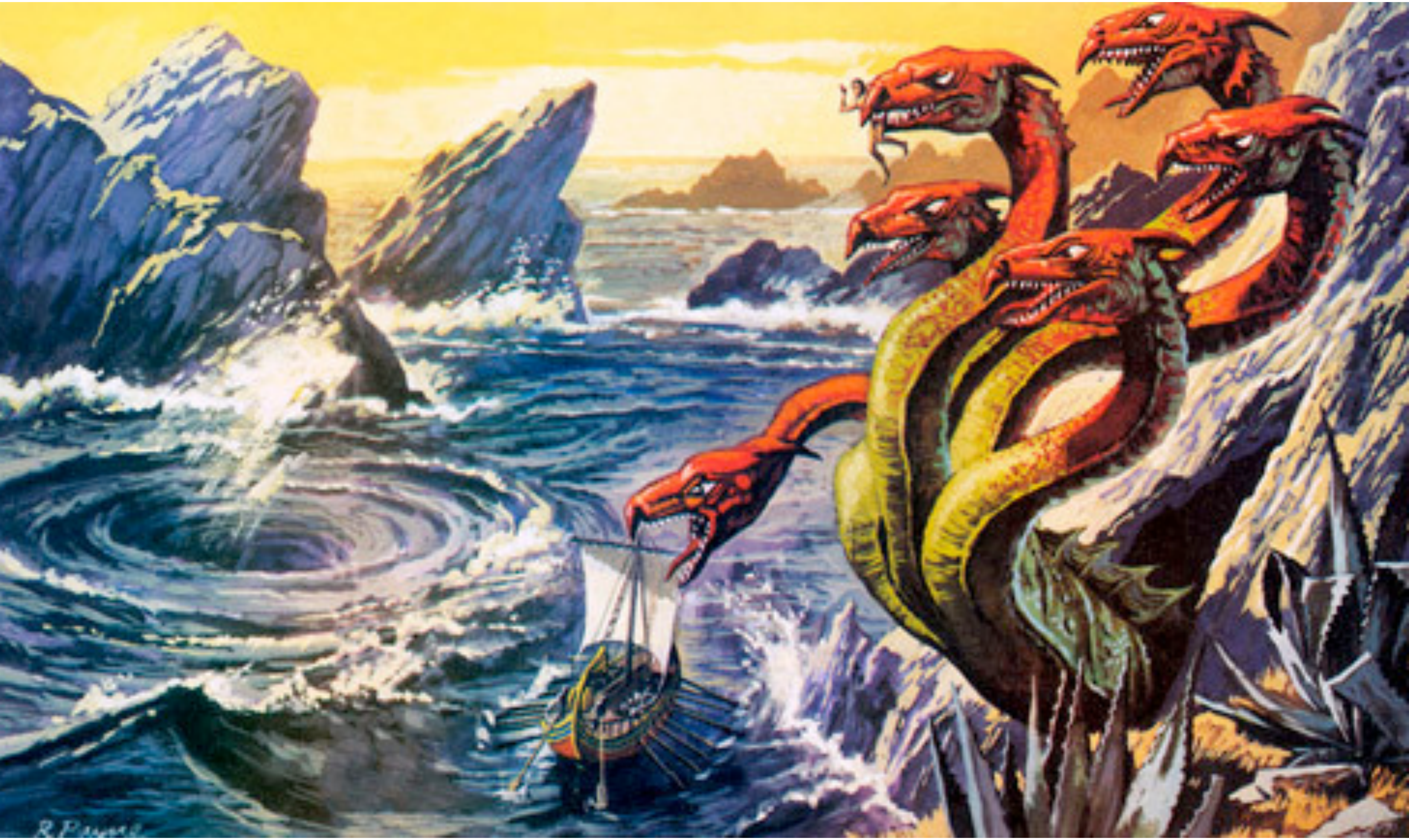
More general factorization: $\underbrace{\rho = \rho_{MC}}_{\text{non-negative, used for sampling}} \times \underbrace{\frac{\rho}{\rho_{MC}}}_{\text{reweighting factor}}$ but (1) Δf increases, AND (2) $\cdots$



Sign pb

Overlap pb

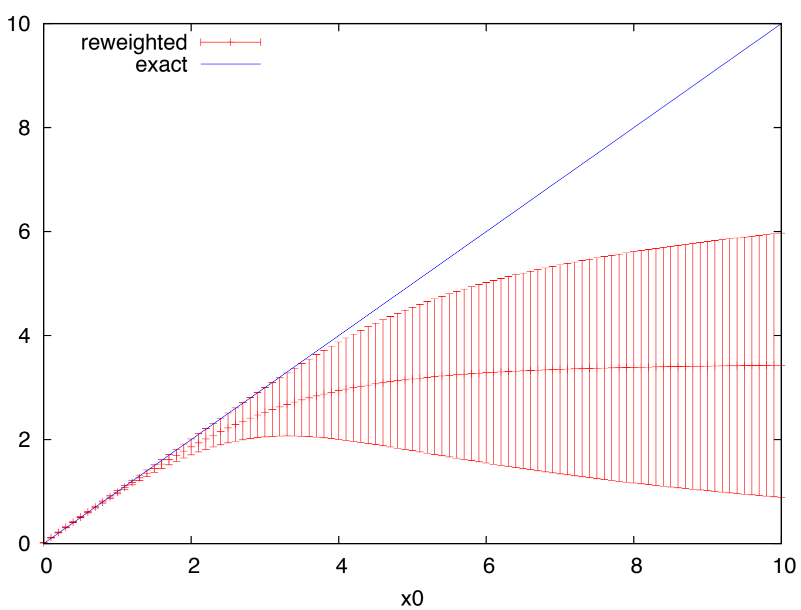
More difficulties: the overlap problem

- Further danger: insufficient overlap between sampled and reweighted ensembles

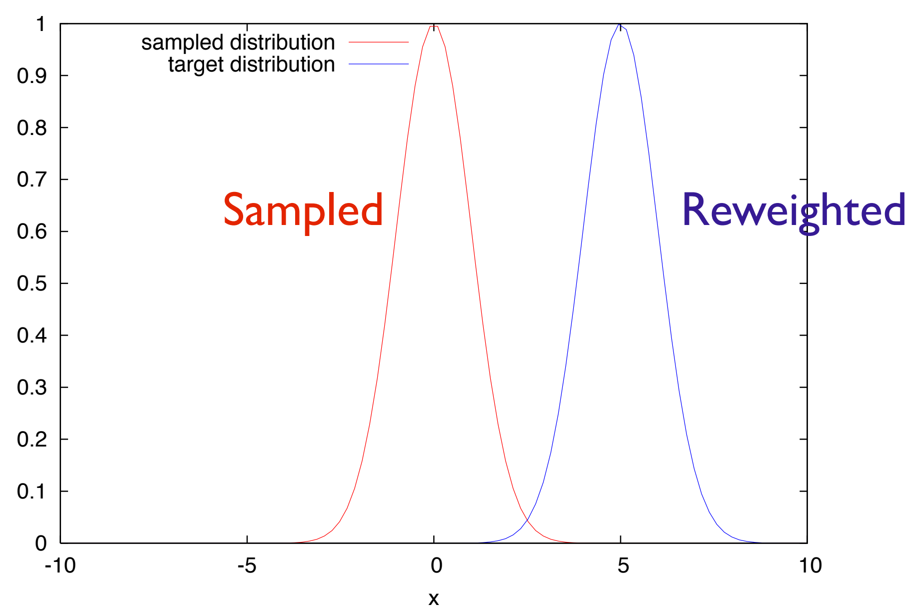
Very large weight carried by very rarely sampled states

$\rightarrow$ WRONG estimates in reweighted ensemble for finite statistics

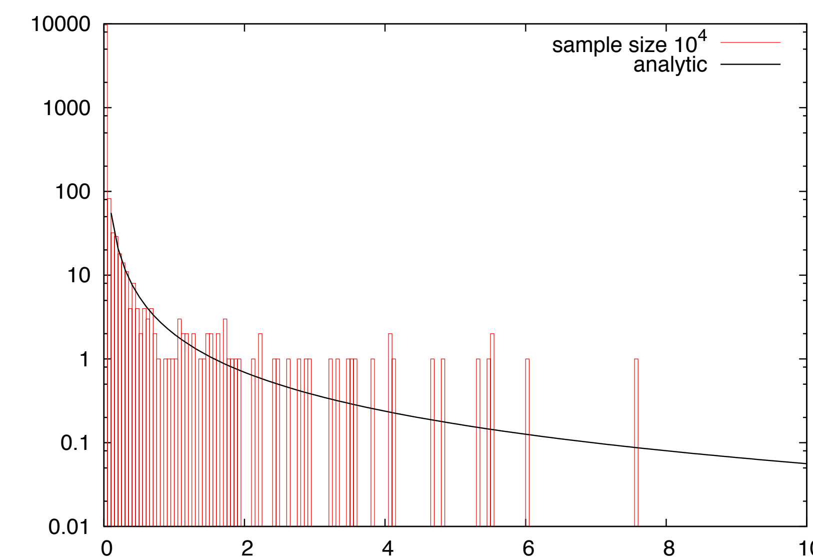
- Example: sample $\exp(-\frac{x^2}{2})$, reweight to $\exp(-\frac{(x-x_0)^2}{2}) \rightarrow \langle x \rangle = x_0$?



- Estimated $\langle x \rangle$ saturates at largest sampled x-value
- Error estimate too small



Insufficient overlap ($x_0 = 5$)



Very non-Gaussian distribution of reweighting factor

Log-normal Kaplan et al.

Solution: Need stats $\propto \exp(\Delta S)$

Semantics: what does "solving the sign pb" mean?

- Idealist: "eliminate" the sign pb (ie. sign-pb-free representation of Z)

  eg. flux ("dual") variables for complex bosonic field ϕ with chem. pot.
  integrate out the phase of ϕ (plays no explicit role in physical states)

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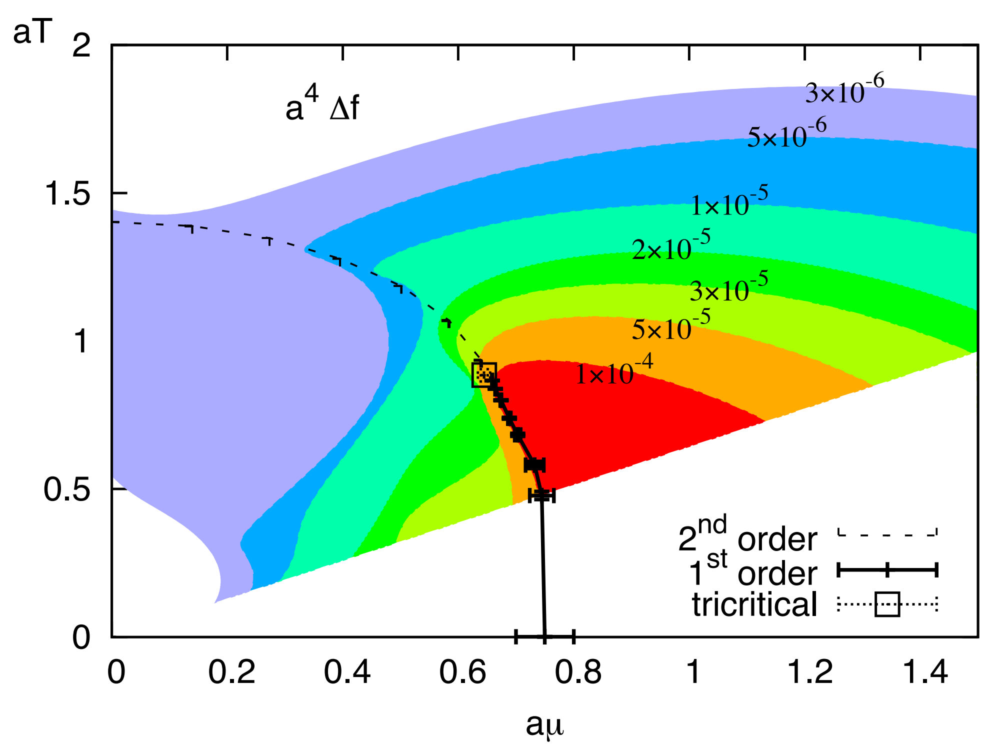
- Pragmatist: "mollify" the sign pb

$\langle \text{sign} \rangle = \exp(-\frac{V}{T}\Delta f) \rightarrow$ reduce Δf $\rightarrow$ simulate "large enough" volumes

eg. lattice QCD with chemical potential in strong-coupling limit
integrate out colored gauge links (plays no role in physical states,
except at short distance)



Compare with $\sim \rho_N(m_N - \frac{3}{2}m_\pi)$

$\rightarrow \Delta F$ reduced by $\sim 10^4$

General guiding principle ?

Steve Weinberg's
Third Law of Progress in Theoretical Physics

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in "Asymptotic realms of physics", 1983

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- Second Law: do not trust arguments based on lowest-order perturbation theory

- First Law: you will get nowhere by just churning equations

How to make the sign problem milder?

- Severity of sign pb. is representation dependent:

$$\text{generically, } Z = \mathrm{Tr} e^{-\beta H} = \mathrm{Tr}\left[e^{-\frac{\beta}{N}H}\left(\sum |\psi\rangle\langle\psi|\right)e^{-\frac{\beta}{N}H}\left(\sum |\psi\rangle\langle\psi|\right)\cdots\right]$$

Any complete set $\{|\psi\rangle\}$ will do

If $\{|\psi\rangle\}$ form an eigenbasis of H, then $\langle\psi_k|e^{-\frac{\beta}{N}H}|\psi_l\rangle = e^{-\frac{\beta}{N}E_k}\delta_{kl} \geq 0 \rightarrow$ no sign pb

- Strategy: $\boxed{\text{choose } \{|\psi\rangle\} \text{ ``close'' to physical eigenstates of } H}$

without full-fledged diagonalization of H

Strategy is general – “deep” optimization? tensor networks?

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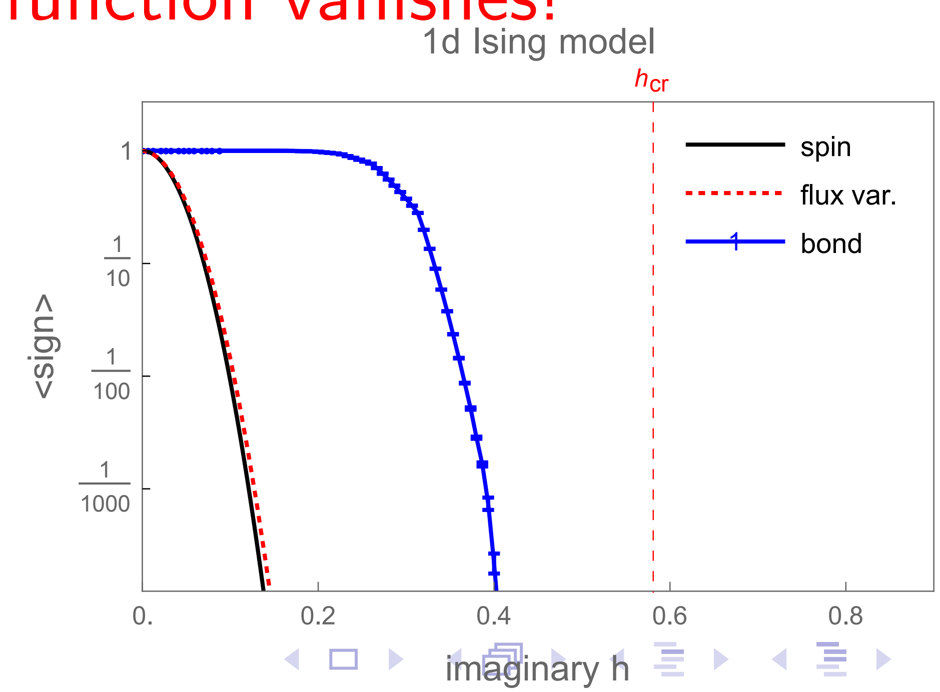
- Worse: are there irreducible sign problems?

YES: when the partition function vanishes!

Example: spin system in complex magnetic field (Lee-Yang zeros of Z)

Rindlisbacher & PdF



Catalogue of approaches to bypass the QCD sign pb

- Analytic continuation from imaginary μ (no sign pb there): data is cheap
  How to control systematic error?? (fitting ansatz)

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- Density of states:
  $S = S_R + iS_I$; select one observable eg. $S_I \rightarrow Z_x = \int \mathcal{D}U e^{-S_R} \delta(S_I - x)$
  $Z = \int dx\ Z_x\ e^{ix}$, i.e. Fourier transform
  old: Gocksch (1988), Fodor Katz & Schmidt, 2007, ..
  significant progress: Langfeld, Lucini & Rago, 2012
  Solves overlap pb
  consensus(?): data alone not accurate enough to beat sign pb:
  need "smoothing" or "fitting" ansatz LLR; Gattringer
  $\rightarrow$ bias PdF & Rindlisbacher, XQCD 2016

Catalogue of approaches to bypass the QCD sign pb: going complex

e.g. gauge field: $A_\mu \to A^R_\mu + iA^I_\mu$ $\quad$ S extended by analytic continuation

- QCD problem I:
  S is not analytic: $\log\det(\not{D})$ has poles and is multi-valued

- QCD problem II:
  gauge group $SU(3) \to SL(3,\mathcal{C})$, departure from $SU(3) \sim A^I_\mu$
  $SL(3,\mathcal{C})$ gauge transformations $\Rightarrow$ flat directions $A_\mu \to i\infty$
  $\Rightarrow$ runaway solutions; large, diverging force; roundoff error; etc..
  - gauge cooling — Seiler, Sexty & Stamatescu
  - irrelevant (?) $SU(3)$-restoring force — Attanasio & Jäger

Hope: find probability $P(A^R_\mu, A^I_\mu) \in \mathcal{R}^+$ in complexified space, which yields correct vevs for all observables

Catalogue of approaches to bypass the QCD sign pb: going complex

- Intelligent design: construct "representation" $P(A_\mu^R, A_\mu^I) \in \mathcal{R}^+$ such that

  $\langle W(A_\mu^R)\rangle_{\exp(-S_R - iS_I)} = \langle W(A_\mu^R + iA_\mu^I)\rangle_P \quad \forall W$ Salcedo, Wosiek

  Example: $S = (x-i)^2 \;\rightarrow\; P(x,y) = \delta(y-1)\exp(-x^2)$

Finding suitable "representation" more difficult than solving the sign problem?

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- Complex Langevin: *conjecture* by Parisi and by Klauder, 1983
  S complex $\rightarrow$ complex drift force ∇S, $+$ complex noise
  Outcomes: runaway, convergence to correct or to wrong answers
  When does complex Langevin give correct results?
  - infinite set of conditions (Seiler et al) – not practical
  - no boundary in parameter space separating correct and wrong results
    $\rightarrow$ always wrong? Kogut & Sinclair?
  - real noise only
  - may give wrong answers in the absence of sign pb ($3d$ XY model, Aarts & James, 2010)

Catalogue of approaches to bypass the QCD sign pb: going complex

- Lefschetz thimble:

Idea: deform integration contour in the complex plane,
such that $S_I = \text{constant} \to \approx$ constant phase

- do NOT explore full complexified space ($\leftrightarrow$ complex Langevin)
- to find the thimble: start at saddle point $\partial_z S(z) = 0$
  keep S_I fixed
  move to increase S_R (steepest ascent)
- IF one thimble, then constant phase e^{iS_I} cancels in vevs
  residual, mild sign pb from Jacobian along [not straight] thimble
  technical difficulty of sampling along thimble can be overcome

Di Renzo et al, Tanizaki et al, Fujii et al, Bedaque et al

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Problem: number of thimbles $\sim \exp(\text{Volume})$?

- Keep dominant thimble only (OK as $V \to \infty$?) but, eg. phase transitions??
- Keep all thimbles: - relative phase $\to$ sign pb reappears
  - ergodic sampling?

Catalogue of approaches to bypass the QCD sign pb: going complex

- Holomorphic gradient flow: Alexandru, Bedaque et al, 1512.08764,..

Idea: tuning knob (flow time) to $\boxed{\text{interpolate between real manifold and thimble}}$

- $t = 0 \rightarrow$ original field ϕ
- $t > 0 \rightarrow \frac{d\phi}{dt} = \overline{\frac{\partial S}{\partial \phi}}$

Along flow, S_I remains constant, and S_R keeps increasing
ie. $\exp(-S_R)$ keeps decreasing, except for critical points $\partial S/\partial\phi = 0$
$\Longrightarrow$ approach Lefschetz thimbles as $t \rightarrow \infty$

Flow time:	0	$\longrightarrow$	∞
Difficulty:	sign pb		ergodicity pb
		sweet spot	

Note: sign pb requires $\exp(V)$ resources, ergodicity pb ALSO
$\rightarrow$ don't expect "sweet spot" to beat $\exp(V)$ complexity – only Δf smaller

- Reason for optimism: real-time quantum dynamics 1605.08040

Catalogue of approaches to bypass the QCD sign pb:

a sobering story (Ph.D. thesis, Slavo Kratochvila, ETH, 2005)

- Toy problem: estimate $\langle W(\lambda)\rangle = \frac{\int_{-\infty}^{+\infty} dx \;\; e^{-x^2+i\lambda x}}{\int dx \;\; e^{-x^2}}$

Exact answer: $\langle W(\lambda)\rangle = \langle e^{i\lambda x}\rangle_{\lambda=0} = e^{-\lambda^2/4} \rightarrow$ exponentially large cancellations

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- Observation: optimum is to go through $\boxed{x = i\lambda/4,}$ ie. neither saddle point!

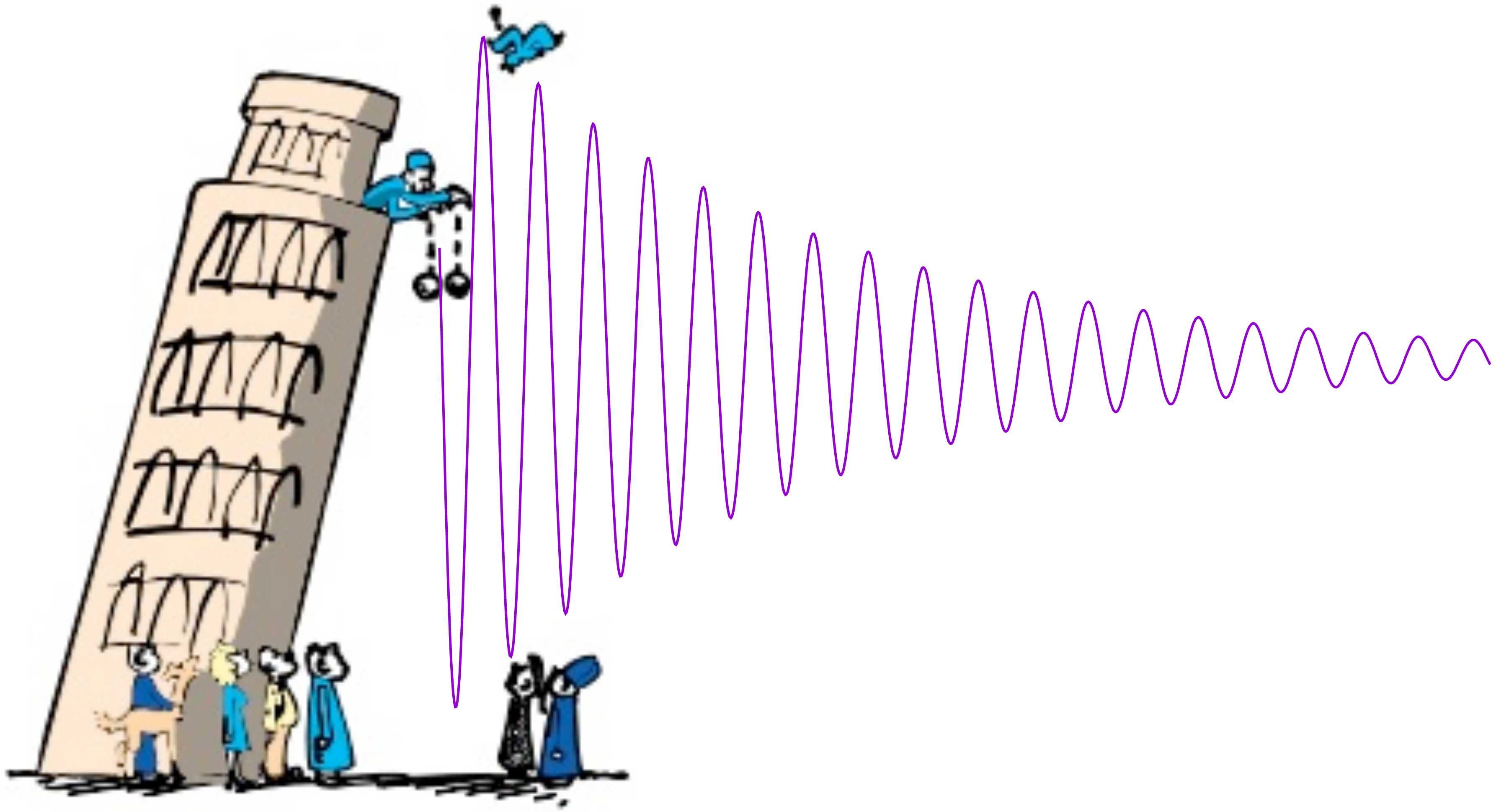
  Why? Moving the contour away from real axis renders denominator oscillatory

Sign problem is shifted between numerator and denominator!
Optimum contour is a compromise (half-way between the two saddle points)
which depends on observable W

Lesson for realistic problems:

an innocent observable may become oscillatory when analytically continued
$\rightarrow$ danger of simply reshuffling the sign pb from Z to W

cf. optimization of contour via cost-function Ohnishi et al, 1705.05605



The struggle continues...

Backup

Sampling for QCD at finite μ

- QCD: sample with $|\mathrm{Re}(\det(\mu)^{N_f})|$ optimal, but not equiv. to Gaussian integral

  Can choose instead: $|\det(\mu)|^{N_f}$, i.e. "phase quenched"

  $|\det(\mu)|^{N_f} = \det(+\mu)^{\frac{N_f}{2}} \det(-\mu)^{\frac{N_f}{2}}$, ie. isospin chemical potential $\mu_u = -\mu_d$

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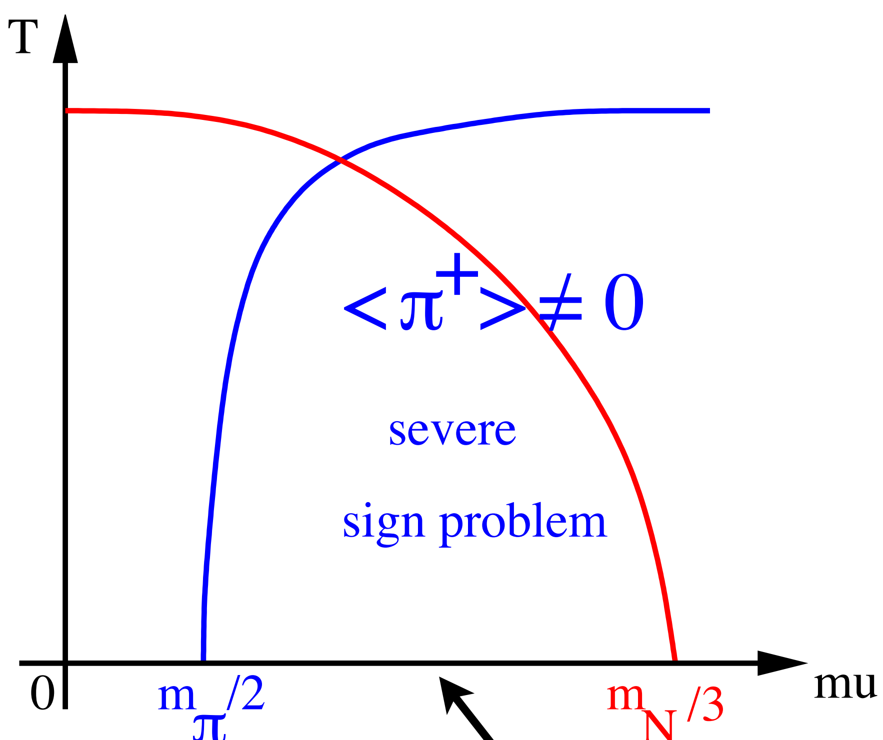

$\Delta f(\mu^2, T)$ large in the Bose phase
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"Silverblaze pb": phase of det changes groundstate

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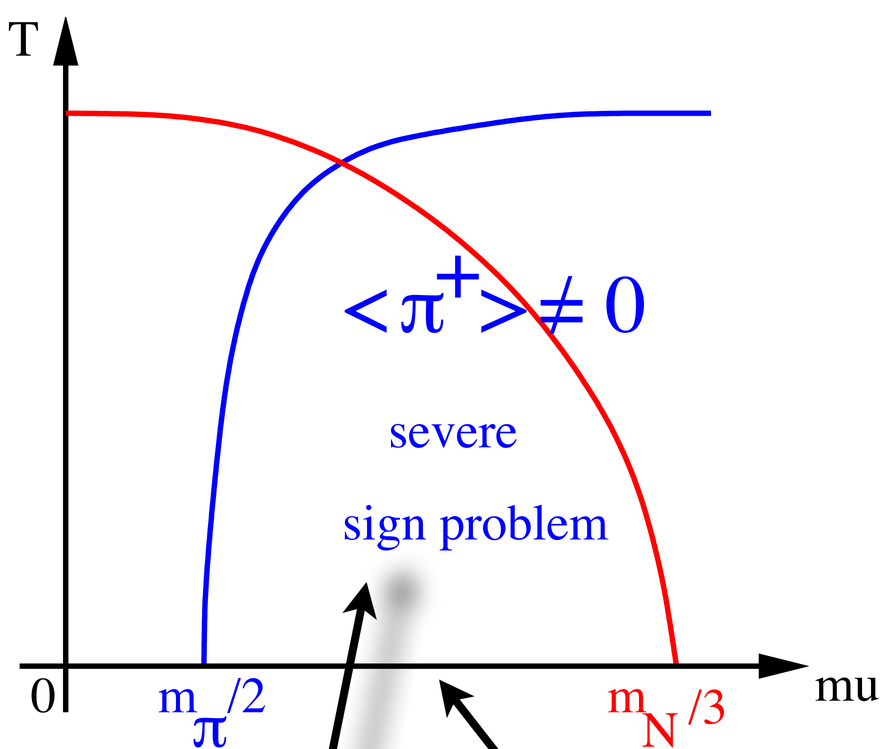

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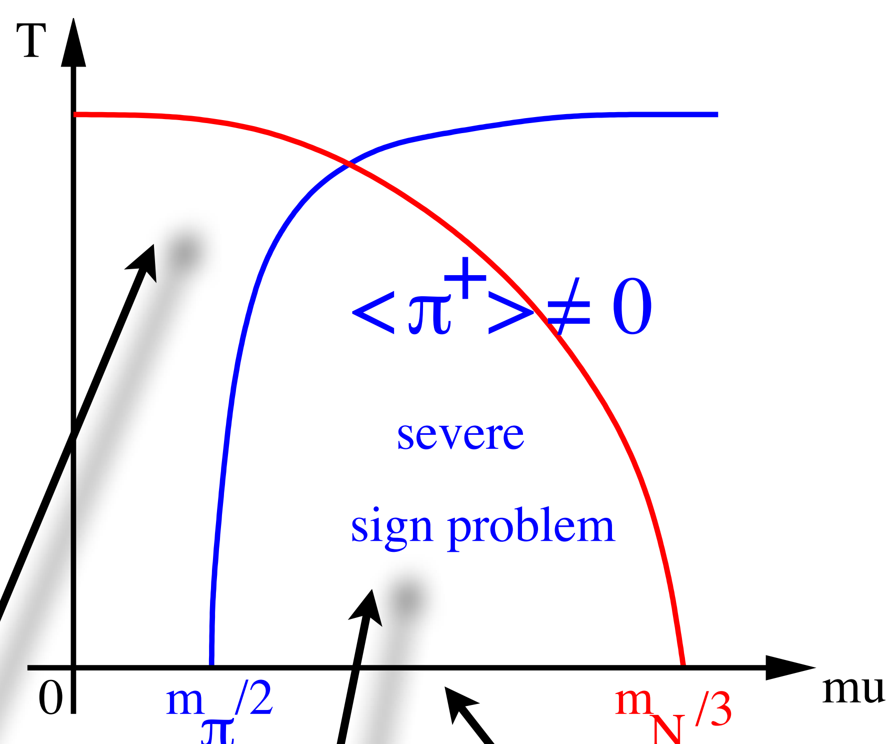

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Extremely hard

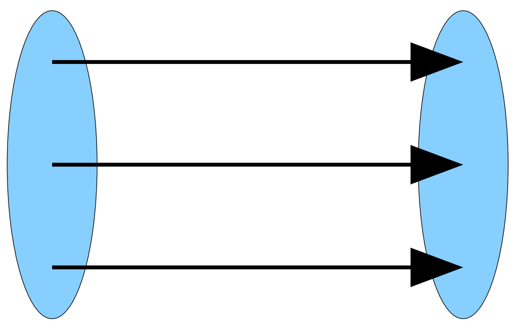
Not as hard

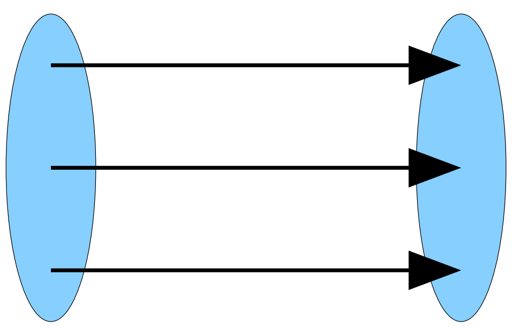
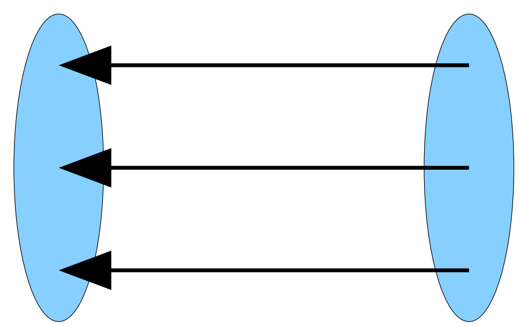
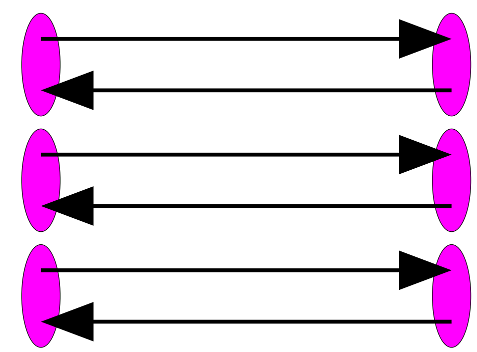
$\frac{\mu}{T} \lesssim 1$

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

Signal-to-noise ratio of N-baryon correlator $\propto \exp(-N(m_B - \frac{3}{2} m_\pi)t)$

Lepage 1989

$C_B(t) \quad =$  $\sim \mathbf{e^{-m_B t}}$

$|C_B(t)|^2 =$  x  $\sim$  $\sim \mathbf{e^{-3m_\pi t}}$

- 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$\rightarrow$72 *pions or kaons* Detmold et al., eg. 0803.2728

  (cf. isospin-μ: no sign pb.)