Going with the flow

a solution to your sign problems

Gökçe Başar

University of Illinois, Chicago

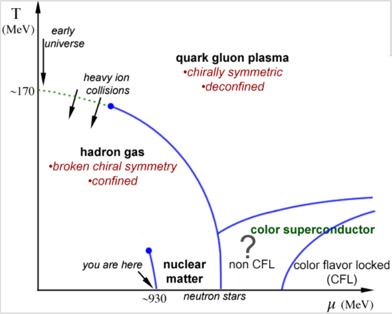
September 20, 2017
Keio QFT Workshop

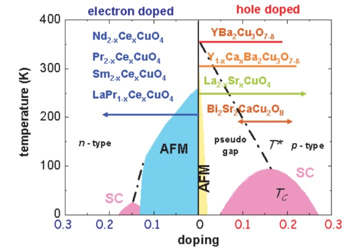
with A. Alexandru, P. Bedaque, G. Ridgway, N. Warrington

refs: 1510.03258, 1512.08764, 1604.00956, 1605.08040, 1606.02742, 1703.02414 , 1704.06404

Motivations:

- many body systems with finite density:
  QCD, strongly correlated electrons, Hubbard model, . . .





[Hartinger, DFG FG 538]

- real time physics: transport coefficients, out of equilibrium physics, thermalization, quantum chaos, . . .

Monte-Carlo method and the sign problem

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int D\phi \; e^{-S[\phi]} \mathcal{O}[\phi] \quad \Rightarrow \quad \langle \mathcal{O} \rangle = \frac{1}{\mathcal{N}} \sum_a \mathcal{O}[\phi^{(a)}]$$

$\phi^{(a)}$ sampled according to the distribution $P[\phi] = e^{-S[\phi]}/Z$

what if S is complex ? as in...

- many body systems with non-zero density: QCD, nuclear matter, Hubbard model, graphene, ...
- real time dynamics: transport coefficients, out-of-equilibrium physics, thermalization, ...
- QCD with non-zero θ

Monte-Carlo method and the sign problem

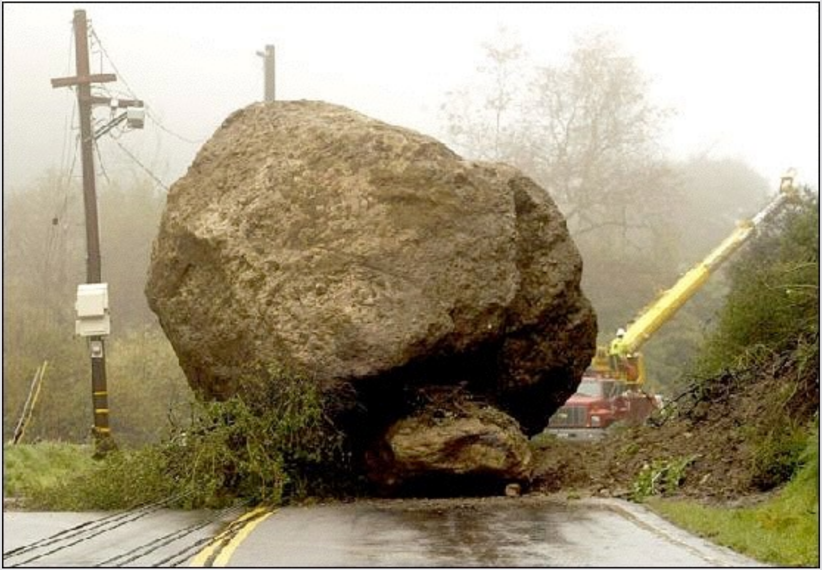
"reweighting"

$$\langle \mathcal{O} \rangle = \frac{\int D\phi\; e^{-S_R[\phi]} e^{-iS_I[\phi]} \mathcal{O}[\phi]}{\int D\phi\; e^{-S_R[\phi]} e^{-iS_I[\phi]}}$$

$$= \frac{\int D\phi\; e^{-S_R} e^{-iS_I} \mathcal{O}}{\int D\phi\; e^{-S_R}} \frac{\int D\phi\; e^{-S_R}}{\int D\phi\; e^{-S_R} e^{-iS_I}}$$

$$= \frac{\langle \mathcal{O}\, e^{-iS_I} \rangle_{S_R}}{\langle e^{-iS_I} \rangle_{S_R}}$$

- S_I grows with the volume $(\beta L^3) \rightarrow$ large fluctuations
- needs exponentially large resources $\Rightarrow$ ~~reweighting~~



Main idea of this talk:

complexify the fields

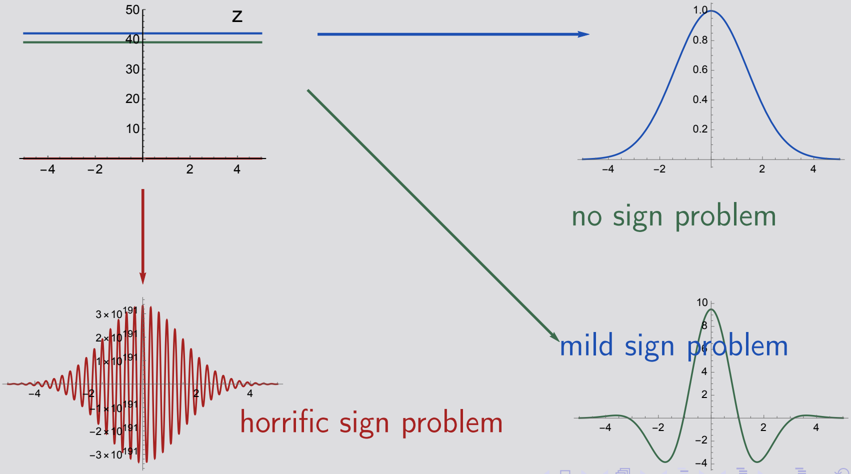
deform the integration domain such that $\mathbb{Im}(S[\phi])$ varies mildly on the new domain $\Rightarrow$ reweighing $\checkmark$

[Alexandru, GB, Bedaque, Ridgway, Warrington]

- based on Picard-Lefschetz theory (complex Morse theory)
- new domain: generalization of the *Lefschetz thimble* [“multi-dimensional stationary phase contour“ $\mathbb{Im}(S[\phi])=$ constant]
  [Cristoforetti et. al.; Aarts et. al.; Fujii, et. al. ; Tanizaki et. al., Fukushima, Alexandru, GB, Bedaque, Ridgway, Warrington; Makri, Miller, Chang (chemical physics)]
- similar ideas [Complex Langevin: Aarts, Berges, Sexty, Stamatescu; Nishimura, Ito, Nagata, Shimasaki, ...] [de Forcrand; Lombardo,Splittorff,Verbaarschot,...]

Solving the sign problem: an example

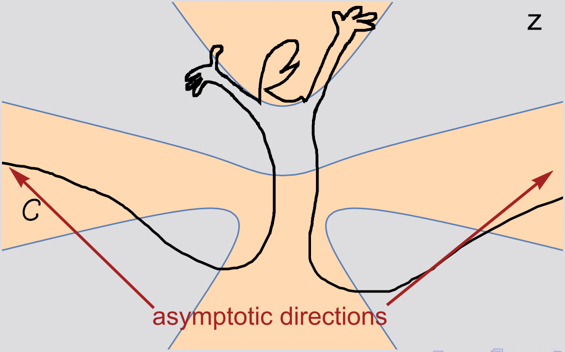
$$\int_{-\infty}^{\infty} e^{-\frac{1}{4}(z+42i)^2}\, dz = 2\sqrt{\pi}$$



Solving the sign problem: another example

$$\mathcal{Z} = \int_{\mathbb{R}} e^{-\left(\frac{1}{2}z^2+\frac{1}{4}\lambda z^4+3iz\right)}\, dz = \int_{\mathcal{C}} e^{-\left(\frac{1}{2}z^2+\frac{1}{4}\lambda z^4+3iz\right)}\, dz$$

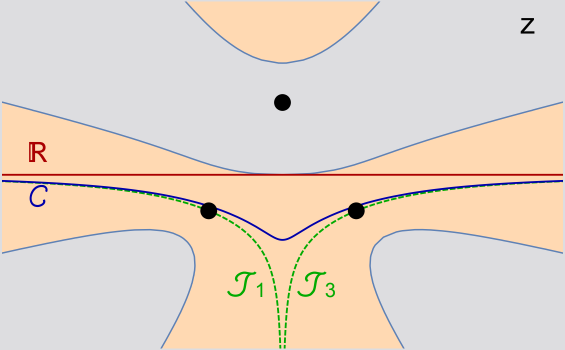
- freedom in choosing the integration contour: integral only depends on asymptotic directions
- family of equivalent contours ⇒ a notion of topology



Solving the sign problem: another example

$$\mathcal{Z} = \int_{\mathbb{R}} e^{-\left(\frac{1}{2}z^2+\frac{1}{4}\lambda z^4+3iz\right)}\,dz = \int_{\mathcal{C}} e^{-\left(\frac{1}{2}z^2+\frac{1}{4}\lambda z^4+3iz\right)}\,dz$$

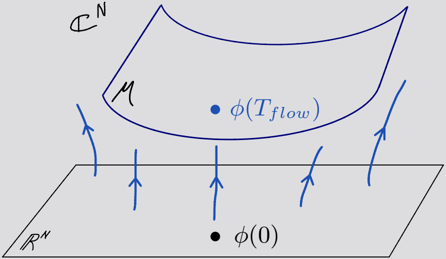
$$= 1\times\int_{\mathcal{J}_1} dz\, e^{-i\left(\alpha z^2+\frac{1}{4}z^4\right)} + 1\times\int_{\mathcal{J}_3} dz\, e^{-i\left(\alpha z^2+\frac{1}{4}z^4\right)}$$



Higher dimensions: QFT

holomorphic gradient flow

$$\frac{d\phi_a}{d\tau} = \overline{\frac{\partial S}{\partial \phi_a}}, \quad \phi_a \equiv x_a + i y_a \begin{cases} \frac{dx_a}{d\tau} = \frac{\partial S_R}{\partial x_a} = \frac{\partial S_I}{\partial y_a} \\ \frac{dy_a}{d\tau} = \frac{\partial S_R}{\partial y_a} = -\frac{\partial S_I}{\partial x_a} \end{cases}$$

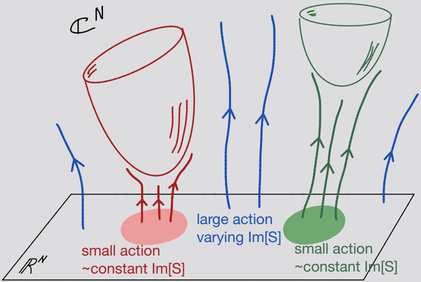


- *gradient flow:* increases S_R
  $\Rightarrow$ integral is well defined
- *Hamiltonian flow:* preserves S_I

- defines a class of alternative manifolds $\mathcal{M}$ parameterized by the "flow time" T_{flow} with identical path integrals

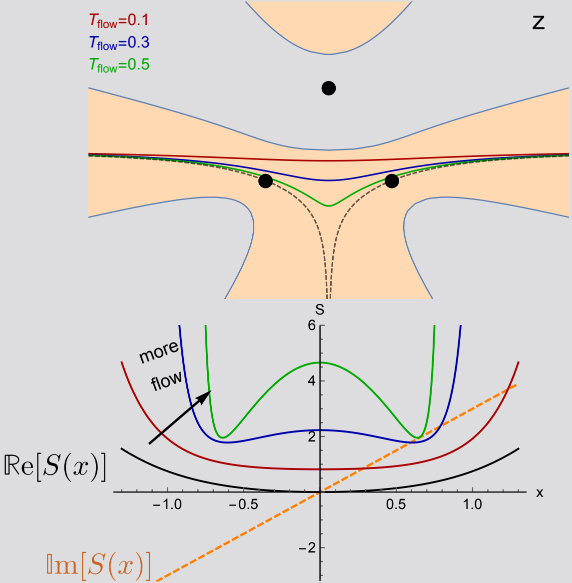
Higher dimensions: QFT

holomorphic gradient flow: $\frac{d\phi_a}{d\tau} = \overline{\frac{\partial S}{\partial \phi_a}}$



- flow $\rightarrow$ only small regions where S_I varies little contribute significantly to the integral: milder sign problem ☺
- too much flow $\rightarrow$ isolated pockets, harder to sample ☹
- adjust T_{flow} to find the best manifold $\mathcal{M}$

Back to the simple example

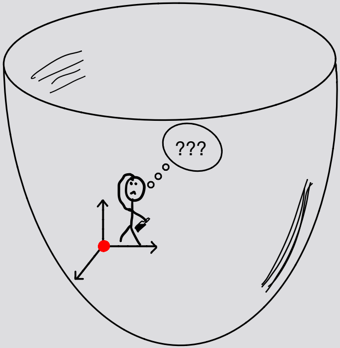


Monte-Carlo on $\mathcal{M}$?

- Metropolis: $\phi_{pr.} \in \mathcal{M}$, $P(\phi_{old} \to \phi_{pr.}) = P(\phi_{pr.} \to \phi_{old})$

$$P_{accept} = \min(1, e^{-S[\phi_p]+S[\phi_{old}]})$$

- random walk on $\mathcal{M}$ is tricky (no local characterization)

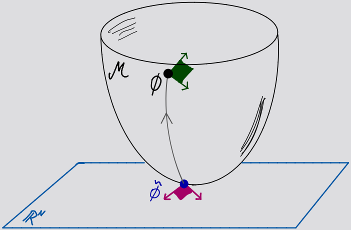


Monte-Carlo on $\mathcal{M}$ ✓

Metropolis algorithm on $\mathcal{M}$: [Alexandru, GB, Bedaque, Ridgway, Warrington]

- parameterize $\mathcal{M}$ with the points on $\mathbb{R}^N$
- accept / reject w.r.t. $S_{eff} = \mathbb{R}\mathrm{e}[S[\phi(\tilde{\phi})] - \log\det J]$
- reweight the remaining phase: $\mathbb{I}\mathrm{m}[S[\phi(\tilde{\phi})] - \log\det J]$

$$\langle\mathcal{O}\rangle = \frac{\int d\phi_i\, \mathcal{O} e^{-S(\phi)}}{\int d\phi_i\, e^{-S(\phi)}} = \frac{\int d\tilde{\phi}_i\, \mathcal{O}\ \overbrace{det\left(\frac{\partial\phi_i}{\partial\tilde{\phi}_i}\right)}^{J=\text{volume elm.}} e^{-S[\phi(\tilde{\phi})]}}{\int d\tilde{\phi}_i\, det\left(\frac{\partial\phi_i}{\partial\tilde{\phi}_i}\right)\ e^{-S[\phi(\tilde{\phi})]}}$$



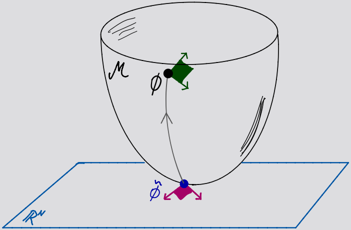
$$\frac{dJ_{ij}}{d\tau} = \overline{\frac{\partial^2 S}{\partial z_i \partial z_k} J_{kj}}$$

Monte-Carlo on $\mathcal{M}$✓

Metropolis algorithm on $\mathcal{M}$: [Alexandru, GB, Bedaque, Ridgway, Warrington]

- parameterize $\mathcal{M}$ with the points on $\mathbb{R}^N$
- accept / reject w.r.t. $S_{eff} = \mathbb{R}\mathrm{e}[S[\phi(\tilde{\phi})] - \log\det J]$
- reweight the remaining phase: $\mathbb{I}\mathrm{m}[S[\phi(\tilde{\phi})] - \log\det J]$

$$\langle \mathcal{O} \rangle = \frac{\left\langle \mathcal{O}\, e^{-i\,\mathbb{I}\mathrm{m}(S - \log\det J)} \right\rangle_{S_{eff}}}{\left\langle e^{-i\,\mathbb{I}\mathrm{m}(S - \log\det J)} \right\rangle_{S_{eff}}}$$



$$\frac{dJ_{ij}}{d\tau} = \overline{\frac{\partial^2 S}{\partial z_i \partial z_k} J_{kj}}$$

Results

real time physics

- 0+1d anharmonic oscillator
- 1+1d ϕ^4 theory

finite density QFT

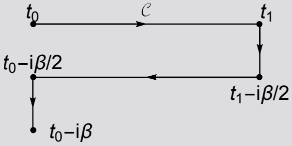
- 2d Thirring model
- 4d interacting Bose gas

Real time physics

Motivation: compute out-of-equilibrium correlators, transport coefficients non-perturbatively from first principles

main object:
$$\begin{aligned}\langle \mathcal{O}_1(t)\mathcal{O}_2(0)\rangle &= Tr[\mathcal{O}_1(t)\mathcal{O}_2(0)\, e^{-\beta H}] \\ &= Tr[e^{-iHt}\mathcal{O}_1(0)e^{iHt}\mathcal{O}_2(0)e^{-\beta H}]\end{aligned}$$

path integral representation: closed time contour [Schwinger, Keldsyh]



$t_0 \sim t_0 - i\beta$

$$S_{SK}[\phi] = \int_{\mathcal{C}} dt\, L[\phi]$$

$$\langle \mathcal{O}_1(t)\mathcal{O}_2(t')\rangle = \frac{1}{Z}\int \mathcal{D}\phi\, e^{iS_{SK}[\phi]}\mathcal{O}_1(t)\mathcal{O}_2(t')$$

$\langle e^{i\mathbb{R}\mathrm{e}[S_{SK}]}\rangle = 0$ for $x \in \mathbb{R}^N$: reweighting is not possible even with infinite statistics $\Rightarrow$ the ultimate sign problem!

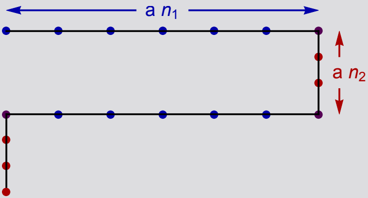
Real time physics

(1605.08040, Phys. Rev. Lett. 117, 081602)

$$L = \frac{1}{2}\dot{x}^2 + \frac{1}{2}x^2 + \frac{\lambda}{4!}x^4$$

discretization:

- lattice spacing: a,
  \# of points: $N = 2(n1 + n_2)$
- real time extent: $2n_1 a$
  imaginary time extent: $2n_2 a$
  (will take $n_1 = 10, n_2 = 2$)

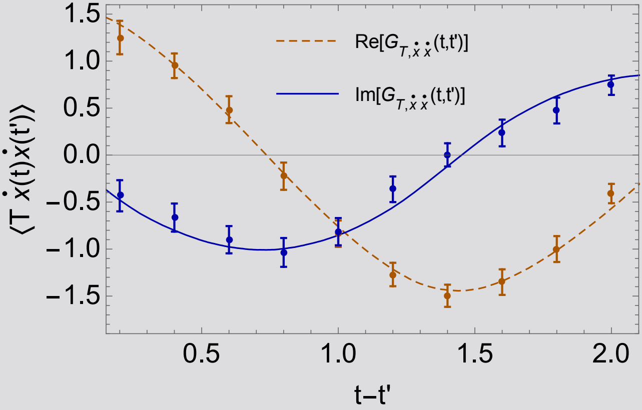


$$S = -i\sum_{i=0}^{N}\Delta t_i\left[\frac{1}{2}\left(\frac{x_{i+1}-x_i}{\Delta t_i}\right)^2 - V(x_i)\right]$$

$$\langle\mathcal{O}\rangle = \frac{\int dx_i\, e^{-S[x]}\,\mathcal{O}[x]}{\int dx_i\, e^{-S[x]}}$$

Real time physics

- consider $G(t,t') = \langle \mathrm{T}\,\dot{x}(t)\dot{x}(t')\rangle$
- response to an external force, analogue of conductivity



Real time physics

some remarks

- this problem was studied via complex Langevin [Berges, Stamatescu,'05; Berges, Borsanyi, Sexty, Stamatescu, '06] which converges to the wrong result for $T_{max} > \beta$.

  Our approach does not have such a problem.

- slow convergence (large autocorrelation time, improvements needed)
- computation of J is costly

Real time physics: 1+1d QFT

(1704.06404, Phys. Rev. D95 114501)

$$\mathcal{L}[\phi] = \frac{1}{2}(\partial\phi)^2 + \frac{1}{2}m^2\phi^2 + \frac{\lambda}{4!}\phi^4$$

two algorithmic improvements:

- avoiding the explicit calculation of $\det J$ ($\mathcal{O}(N^3)$)
- better proposals $\rightarrow$ faster convergence

main idea:

Grady algorithm: the effect of the jacobian is embedded in a bias of the proposals that are isotropic in the flowed manifold. instead of $\det J$, one needs to compute $J\eta$

further simplification: Use free field J for proposals and re-weight the difference at measurements: ("J_0 method")

Real time physics: 1+1d QFT

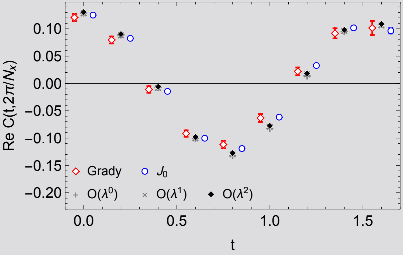
(1704.06404, Phys. Rev. D95 114501)

$$C(t,p) = \left\langle \phi(t,p)\phi(0,p)^\dagger \right\rangle_\beta \quad \text{with} \quad \phi(t,p) \equiv \frac{1}{N_x} \sum_{n=0}^{N_x-1} e^{ipn} \phi_{t,n} \,.$$

$$n_1 = 8, n_2 = 2, n_x = 8$$

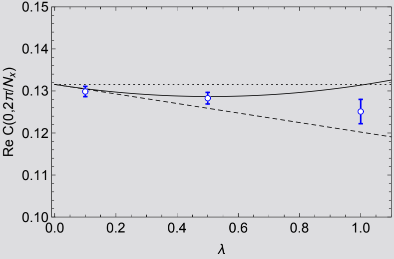
results:

comparison of Grady and J_0 methods:



(data points are offset for clarity)

J_0 method vs perturbation theory:



Finite density QFT: 2d Thirring model

(1609.01730, Phys. Rev. D. 95, 014502)

a theory of interacting fermions

$$S = \int d^2x\bar{\psi}^a\left(\gamma^\mu\partial_\mu + m + \mu\gamma^0\right)\psi^a + \frac{g^2}{2N_f}(\bar{\psi}^a\gamma^\mu\psi^a)(\bar{\psi}^b\gamma_\mu\psi^b)$$

$$\rightarrow \frac{N_F}{2g^2}\int d^2x\, A_\mu A_\mu + \ln\det(\not{\partial} + \not{A} + \mu\gamma_0 + m)$$

discretization:

$$S_{lat.} = N_F\left(\frac{1}{g^2}\sum_{x,\nu}(1-\cos A_\nu(x)) - \gamma\log\det D(A)\right)$$

Wilson, $\gamma = 1$:

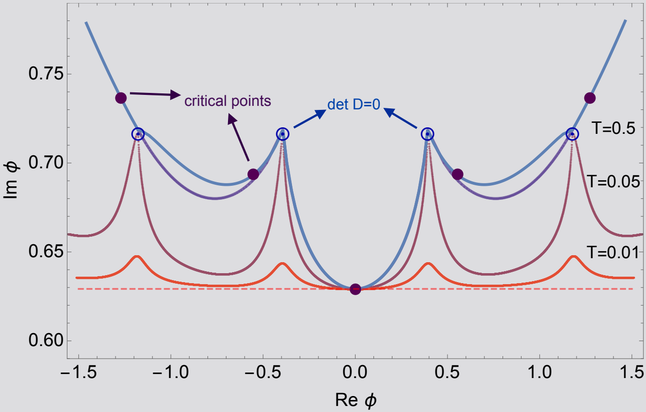
$$D^W_{xy} = \delta_{xy} - \kappa\sum_{\nu=0,1}\left[(1-\gamma_\nu)e^{iA_\nu(x)+\mu\delta_{\nu 0}}\delta_{x+\nu,y} + (1+\gamma_\nu)e^{-iA_\nu(x)-\mu\delta_{\nu 0}}\delta_{x,y+\nu}\right]$$

staggered (Kogut-Susskind), $\gamma = 1/2$:

$$D^{KS}_{xy} = m + \frac{1}{2}\sum_{\nu=0,1}\left[\eta_\nu e^{iA_\nu(x)+\mu\delta_{\nu 0}}\delta_{x+\nu,y} - \eta^\dagger_\nu e^{-iA_\nu(x)-\mu\delta_{\nu 0}}\delta_{x,y+\nu}\right]$$

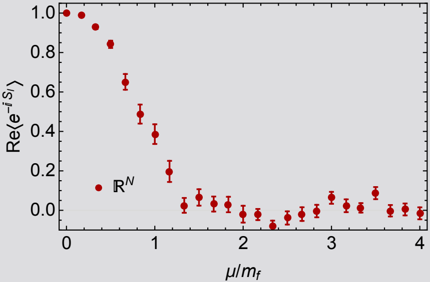
2d Thirring model

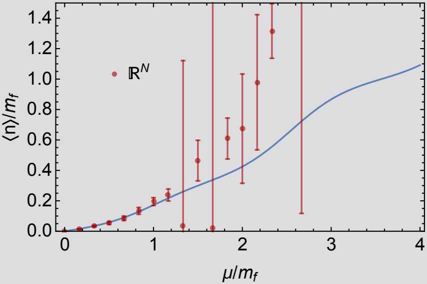
integration manifolds:



projection: $$\phi = \frac{1}{L^2} \sum_x A_0(x)$$

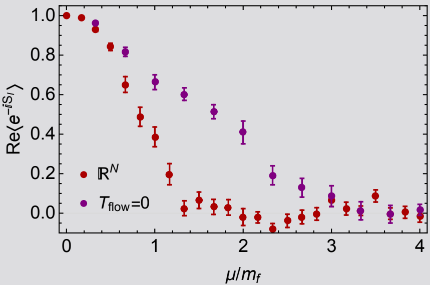
2d Thirring model

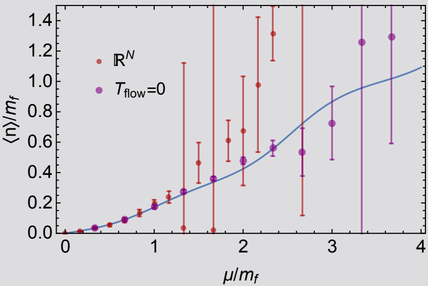




Wilson fermions, $N_f = 2$, $N_t \times N_x = 10 \times 10$

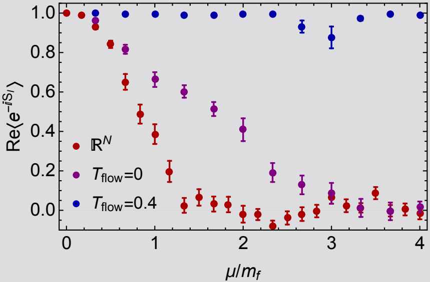
2d Thirring model

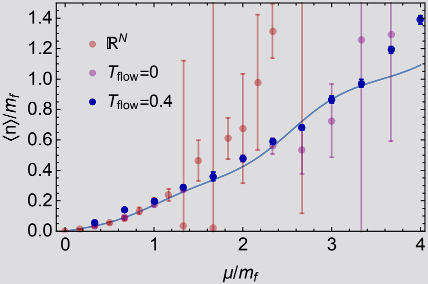




Wilson fermions, $N_f = 2$, $N_t \times N_x = 10 \times 10$

2d Thirring model

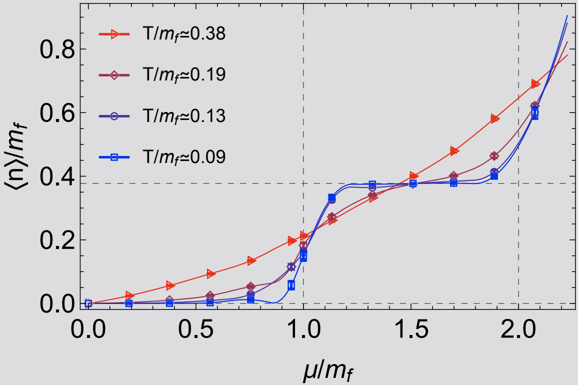




Wilson fermions, $N_f = 2$, $N_t \times N_x = 10 \times 10$

2d Thirring model

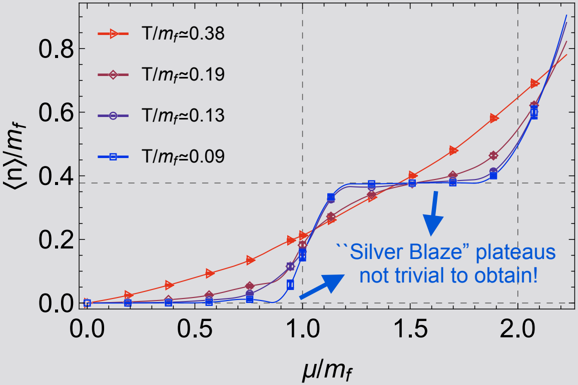
low temperature limit



staggered fermions, $N_f = 2$

2d Thirring model

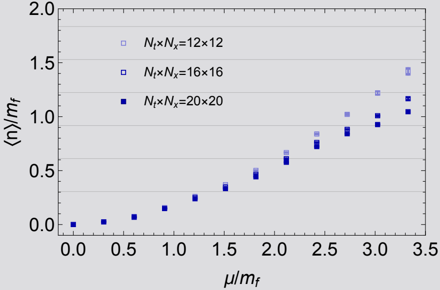
low temperature limit



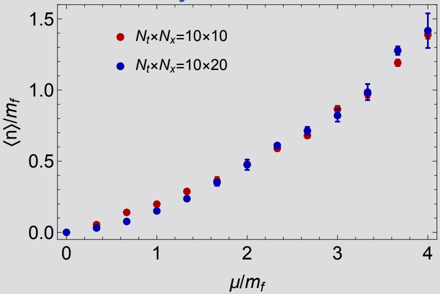
staggered fermions, $N_f = 2$

2d Thirring model

continuum limit



thermodynamic limit



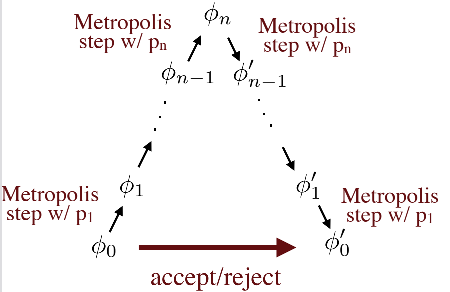
staggered fermions, $N_f = 2$

Tempered transitions

(1703.02414, Phys.Rev. D96 034513) [also: Fukuma, Umeda, 2017]

problem: larger flows lead to multi-modal distributions that cause trapping in local minima during MC sampling

a solution: *tempered transitions* [R. Neal, Statistics and Computing, 6:353 (1996)]
make proposals via a successive accept/reject steps with gradually varying flow time

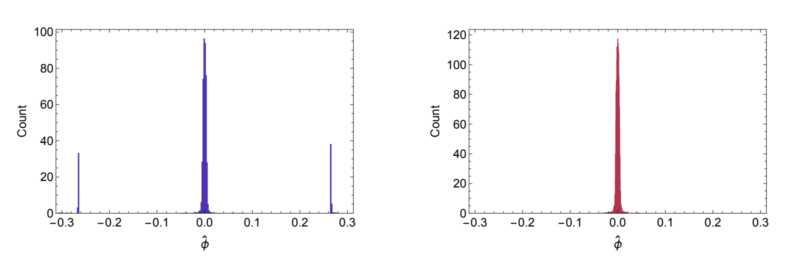


Tempered transitions

(1703.02414, Phys.Rev. D96 034513) [also: Fukuma, Umeda, 2017]

results: (1d Thirring model, low T limit)

tempered transitions correctly sample the sub-dominant “thimbles” that are beyond the reach of regular Metropolis steps



blue:tempered, red:non-tempered, trapped in local minimum

4d QFT: interacting Bose gas

(1606.02742, Phys.Rev. D93 (2016) no.1, 014504)

complex scalar field: $\phi = \phi^1 + i\phi^2$

$$\mathcal{L} = |\partial_\mu \phi|^2 + (m^2 - \mu^2)|\phi|^2 + \mu\left(\phi^* \partial_0 \phi - \phi \partial_0 \phi^*\right) + \lambda|\phi|^4 + h(\phi^1 + \phi^2)$$

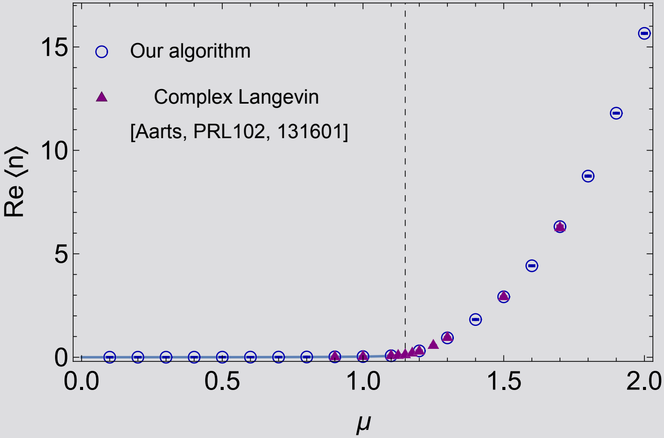
sign problem here!

discretization:

$$S_{lat.} = \sum_x \left[\left(4 + \frac{m^2}{2}\right) \phi_x^a \phi_x^a + \frac{\lambda}{4} (\phi_x^a \phi_x^a)^2 - h(\phi_x^1 + \phi_x^2) - \sum_{\nu=1}^{3} \phi_x^a \phi_{x+\hat{\nu}}^a - \cosh\mu\ \phi_x^a \phi_{x+\hat{0}}^a - i \sinh\mu\ \epsilon_{ab} \phi_x^a \phi_{x+\hat{0}}^b \right]$$

sign problem here!

4d QFT: interacting Bose gas



parameters: $m = 1.0, \lambda = 1.0, h = 0.001(1 + 0.1i), V = 4^4$

Conclusions

- if you have a sign problem, complexifying of the fields is good for you
- holomorphic gradient flow: knob to control the sign problem
- QFT (fermionic, bosonic), real time ✓

Outlook

- the manifolds can be bumpy: smarter proposals
- det J is costly: estimators, pseudo-fermions
- gauge theories, transport coefficients ...

Some Remarks I

computing $\log\det J$ at every MC step is costly: $\mathcal{O}(N^3)$

- instead of computing J, compute a cheaper substitute for $\log\det J$: *"wrongian"* ($\sim$ estimator)

  (1604.00956, Phys.Rev.D93, 9, 094514)

$$\log W_1 = \int_0^{T_{flow}} dt \sum_a \rho^a \mathrm{Tr}[\bar{H}(t)]\bar{\rho}^a \quad , \quad \log W_2 = \int_0^{T_{flow}} dt \; \mathrm{Tr}[\bar{H}(t)]$$

where $H(z) = \partial^2 S(z)/\partial z_i \partial z_j$, $\overline{H\rho^a} = \lambda^a \rho^a$, ρ^a: basis for $\mathcal{T}$

- correct the error by reweighing with $\det J/W$
- wrongians cost $\mathcal{O}(N)$: substantial gain in computing time
- a good estimator for the real time problem?

Some Remarks II

the landscape of the field space is not homogeneous

- has steep and flat directions w.r.t. $S_{eff}(\tilde{\phi})$

  e.g. *gaussian* $S(z) = \vec{z} \cdot H \cdot \vec{z} = \sum_a \lambda^a \, c_a^2$ (diagonalized)

  flow: $\tilde{z} = z(0) = \sum_a \tilde{c}_a \rho^a \mapsto z(t) = \sum_a \tilde{c}_a \, e^{\lambda_a t} \rho^a$

  $$\Rightarrow S_{eff}(\tilde{z}) = \sum_a \lambda^a \, e^{2\lambda_a t} \tilde{c}_a^2$$

- for a reasonable thermalization and decorrelation time make educated proposals

  $$\tilde{c}_a \to \tilde{c}_a + \frac{e^{-\lambda_a t}}{\sqrt{\lambda_a}} \, \delta$$

- similar construction for flowing from (=proposals on) $\mathbb{R}^N$?