Going with the flow:
a solution to your sign problems

Gökçe Başar

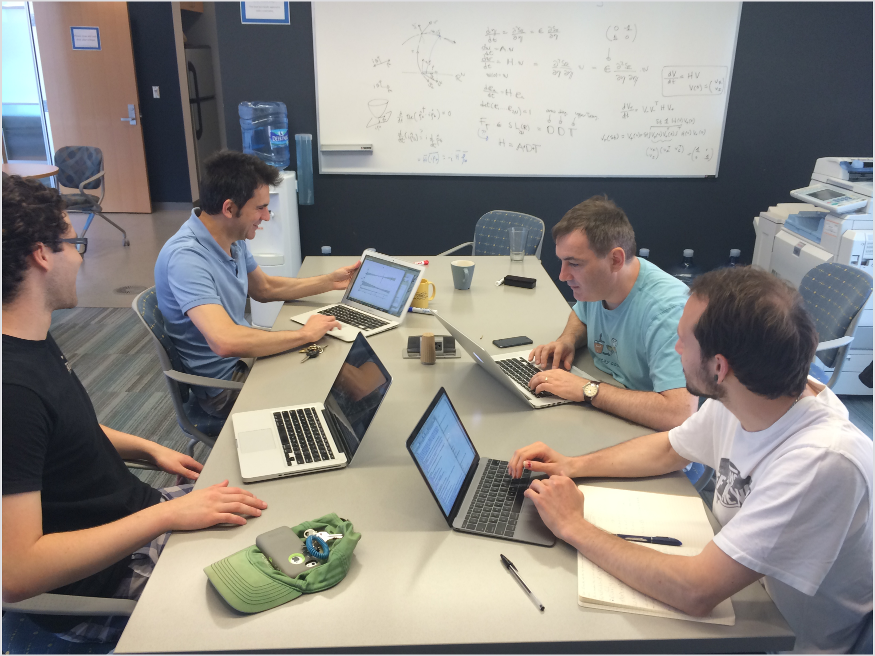
University of Maryland

January 10, 2017

WWND 2017

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

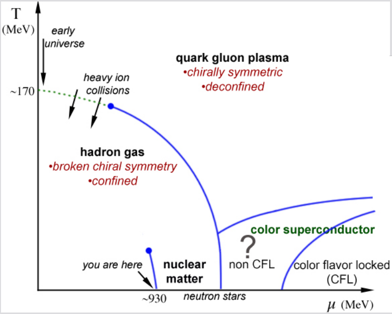
based on: 1510.03258, 1512.08764, 1604.00956, 1605.08040, 1606.02742

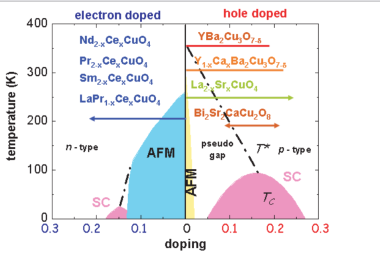


Motivations:

- 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

a robust method to study strongly coupled QFTs

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

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

Monte-Carlo method and the sign problem

a robust method to study strongly coupled QFTs

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

$\phi^{(a)}$ 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
- ...

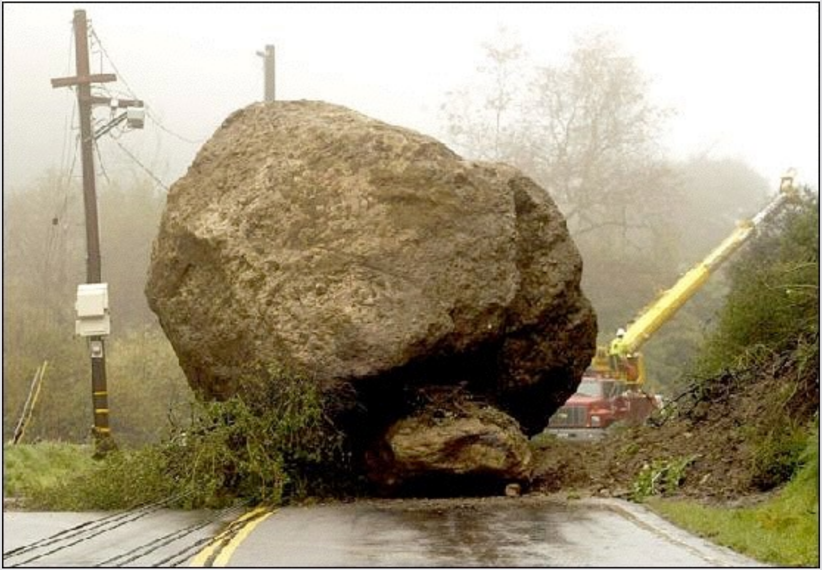
Monte-Carlo method and the sign problem

reweighting:

$$\begin{aligned}\langle \mathcal{O} \rangle &= \frac{\int D\phi\ e^{-S_R[\phi]} e^{-iS_I[\phi]} \mathcal{O}[\phi]}{\int D\phi\ e^{-S_R[\phi]} e^{-iS_I[\phi]}} \\ &= \frac{\int D\phi\ e^{-S_R} e^{-iS_I} \mathcal{O}}{\int D\phi\ e^{-S_R}} \frac{\int D\phi\ e^{-S_R}}{\int D\phi\ e^{-S_R} e^{-iS_I}} \\ &= \frac{\langle \mathcal{O}\ e^{-iS_I} \rangle_{S_R}}{\langle e^{-iS_I} \rangle_{S_R}}\end{aligned}$$

S_I grows with the volume (βL^3) $\rightarrow$ large fluctuations

$\Rightarrow$ ~~reweighting~~



Main idea in this talk: complexify the fields

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

$\Rightarrow$ reweighing ✓

[Alexandru, GB, Bedaque, Ridgway, Warrington]

- generalization of the multi-dimensional stationary phase contour where $\mathbb{Im}(S[\phi])$ stays constant *"Lefschetz thimble "*

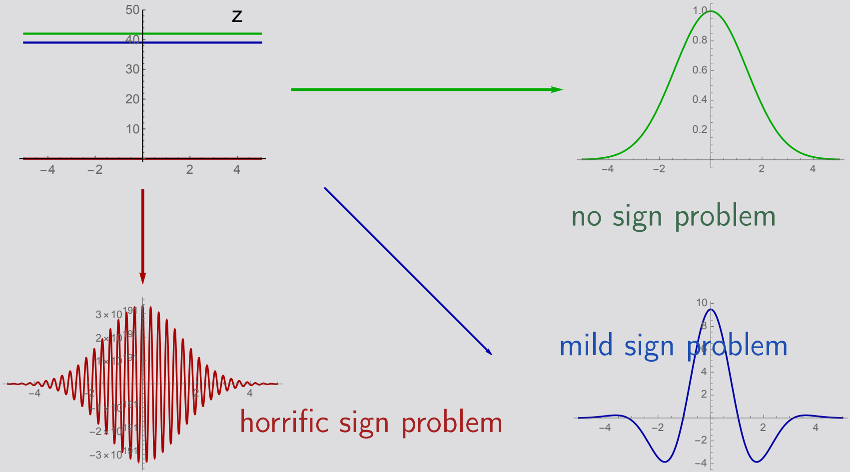
  [Cristoforetti et. al.; Aarts et. al.; Fujii, Honda, Kato, Kikukawa, Komatsu, Sano; Tanizaki et. al. Alexandru, GB, Bedaque, Ridgway, Warrington; Makri, Miller, Chang (chemical physics)]

  [resurgence: Pham; Witten; Argyres, GB, Cherman, Dorigoni, Dunne, Sulejmanpasic,Ünsal . . .]

- similar ideas: [Complex Langevin: Aarts, Berges, Sexty, Stamatescu; Nishimura, Ito, Nagata, Shimasaki, ...] [de Forcrand; Lombardo,Splittorff,Verbaarschot,...]

an example

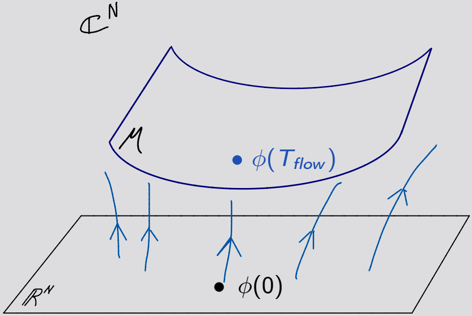
$$\int_{-\infty}^{\infty} e^{-\frac{1}{4}(z+42i)^2}\, dz = 2\sqrt{\pi}$$



Higher dimensions

holomorphic gradient flow:

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



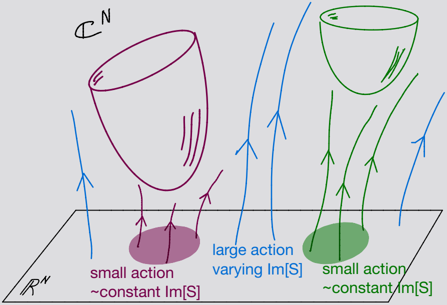
- *gradient flow:* increases S_R
  $\Rightarrow$ integral is well defined
- *Hamiltonian flow:* preserves S_I

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

Higher dimensions

holomorphic gradient flow:

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



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

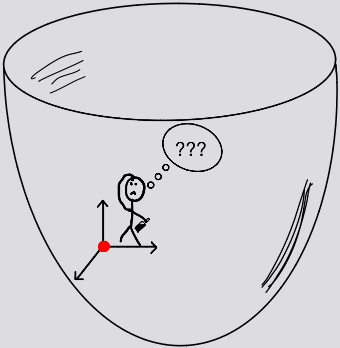
- defines a class of alternative manifolds $\mathcal{M}$ parameterized by the "flow time" T_{flow} with identical path integrals

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)

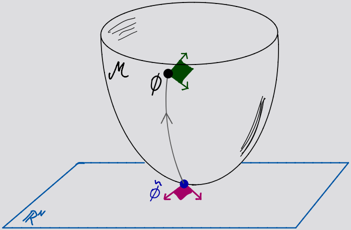


Monte-Carlo on $\mathcal{M}$ ✓

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

- parameterize $\mathcal{M}$ with the points on $\mathbb{R}^N$
- make proposals 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: $\mathbb{I}\mathrm{m}[S[\phi(\tilde{\phi})] - \log\det J]$

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



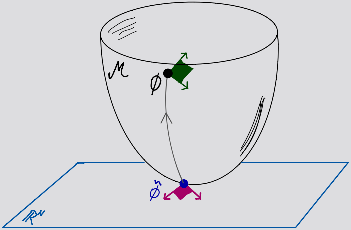
$$\frac{dJ_{ij}}{d\tau} = \overline{\frac{\partial^2 S}{\partial z_i \partial z_k} J_{kj}}$$

Monte-Carlo on $\mathcal{M}$ ✓

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

- parameterize $\mathcal{M}$ with the points on $\mathbb{R}^N$
- make proposals 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: $\mathbb{I}\mathrm{m}[S[\phi(\tilde{\phi})] - \log\det J]$

$$\langle \mathcal{O} \rangle = \frac{\int d\tilde{\phi}_i\, \mathcal{O} e^{-i\,\mathbb{I}\mathrm{m}(S-\log\det J)}\, e^{\overbrace{-\mathbb{R}\mathrm{e}\,(S_R - \log\det J)}^{S_{eff}}}}{\int d\tilde{\phi}_i\, e^{-i\,\mathbb{I}\mathrm{m}(S-\log\det J)}\, e^{-S_{eff}}}$$



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

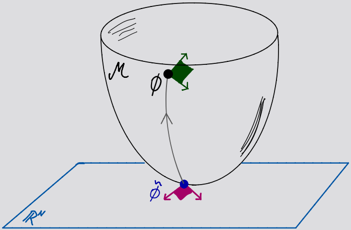
Monte-Carlo on $\mathcal{M}$ ✓

Metorpolis algorithm on $\mathcal{M}$:

[Alexandru, GB, Bedaque, Ridgway, Warrington]

- parameterize $\mathcal{M}$ with the points on $\mathbb{R}^N$
- make proposals 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: $\mathbb{I}\mathrm{m}[S[\phi(\tilde{\phi})] - \log\det J]$

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



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

Results

finite density

- 2d Thirring model
- 4d interacting Bose gas

real time physics

- 0+1d anharmonic oscillator

2d Thirring model

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

$$
\begin{aligned}
S &= \int d^2x \bar{\psi}^a \left(\gamma^\mu \partial_\mu + m + \mu\gamma^0\right) \psi^a + \frac{g^2}{2N_f} (\bar{\psi}^a \gamma^\mu \psi^a)(\bar{\psi}^b \gamma_\mu \psi^b) \\
&\to \frac{N_F}{2g^2} \int d^2x \, A_\mu A_\mu + \ln \det(\not{\partial} + \not{A} + \mu\gamma_0 + m)
\end{aligned}
$$

2d Thirring model

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

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

$$\rightarrow \frac{N_F}{2g^2} \int d^2x\, A_\mu A_\mu + \ln\det(\partial\!\!\!/ + A\!\!\!/ + \mu\gamma_0 + m)$$

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, $\gamma = 1$:

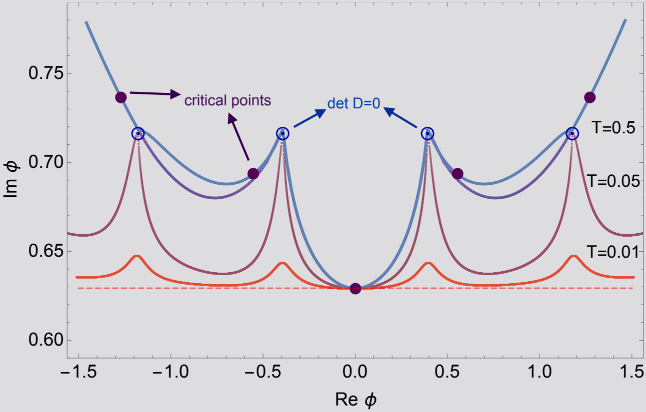
$$D^W_{xy} = \delta_{xy} - \kappa \sum_{\nu=0,1} \left[(1-\gamma_\nu) e^{iA_\nu(x) + \mu\delta_{\nu 0}} \delta_{x+\nu,y} + (1+\gamma_\nu) e^{-iA_\nu(x) - \mu\delta_{\nu 0}} \delta_{x,y+\nu} \right]$$

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

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

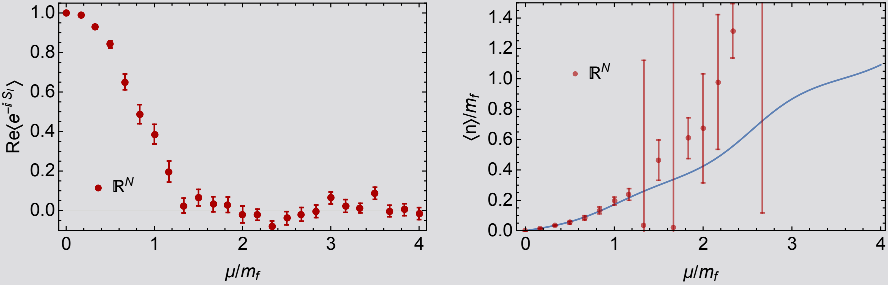
2d Thirring model

integration manifolds:



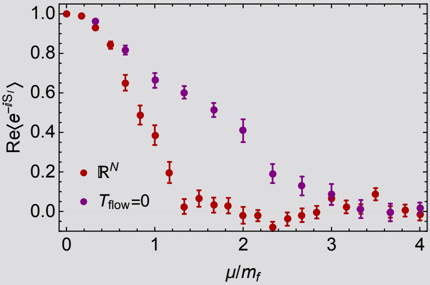
projection: $$\phi = \frac{1}{L^2} \sum_x A_0(x)$$

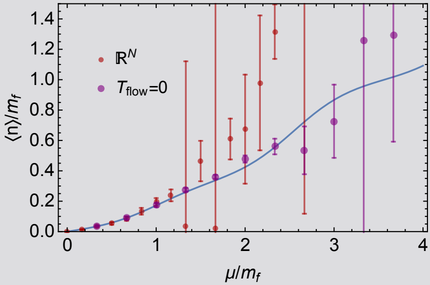
2d Thirring model



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

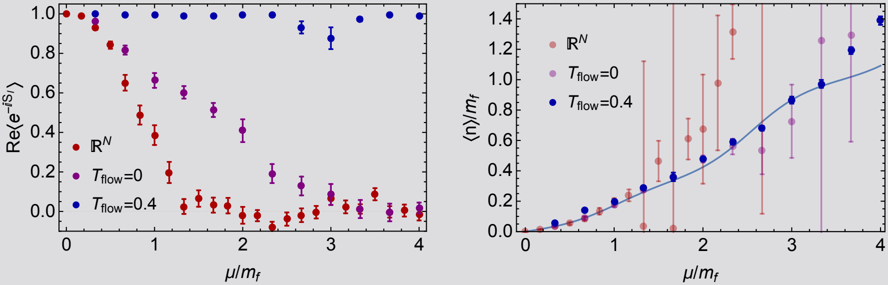
2d Thirring model





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

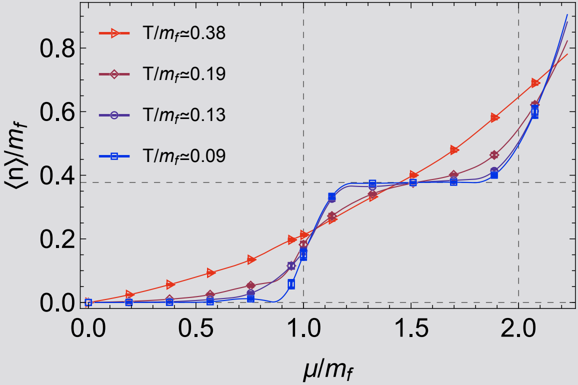
2d Thirring model



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

2d Thirring model

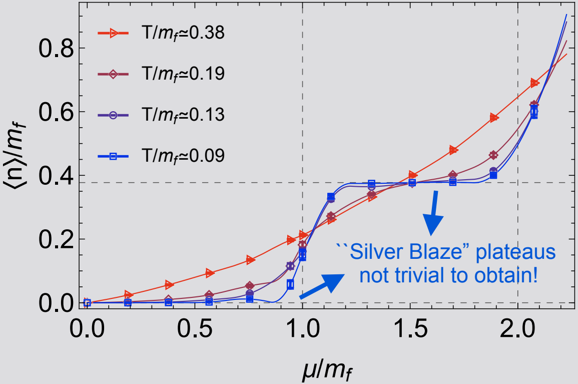
low temperature limit



staggered fermions, $N_f = 2$

2d Thirring model

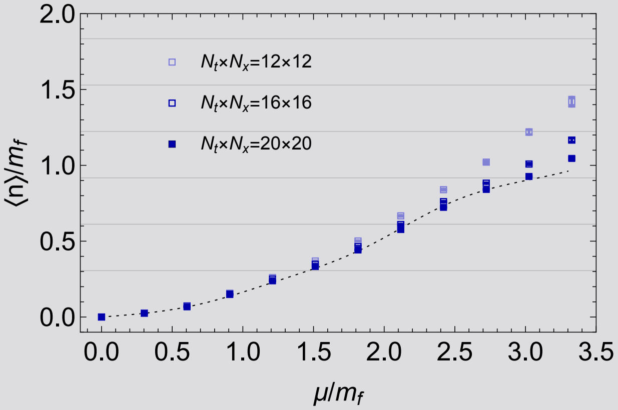
low temperature limit



staggered fermions, $N_f = 2$

2d Thirring model

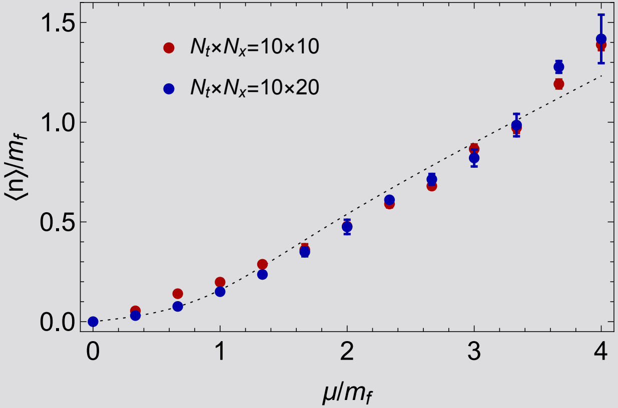
continuum limit



staggered fermions, $N_f = 2$

2d Thirring model

thermodynamic limit



staggered fermions, $N_f = 2$

Real time physics

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

main object:

$$\langle \mathcal{O}_1(t)\mathcal{O}_2(t')\rangle \;=\; Tr[\mathcal{O}_1(t)\mathcal{O}_2(t')\,\hat{\rho}], \quad \hat{\rho} = e^{-\beta H}$$

e.g. transport coefficients:

$$\eta = \frac{1}{20}\lim_{\omega\to 0}\frac{2T}{\omega}\mathbb{Im}\int d^4x e^{i\omega t}\langle T^{ij}(t,x)T_{ij}(0,0)\rangle_R \quad \text{shear viscosity}$$

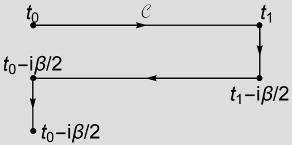
$$\sigma = \frac{1}{6}\lim_{\omega\to 0}\frac{2T}{\omega}\mathbb{Im}\int d^4x e^{i\omega t}\langle J^{i}(t,x)J_{i}(0,0)\rangle_R \quad \text{conductivity}$$

Real time physics

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]



$t_0 \sim t_0 - i\beta$

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

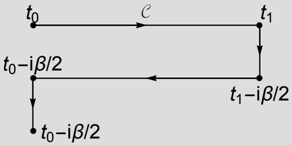
$$\langle \mathcal{O}_1(t)\mathcal{O}_2(t')\rangle = \frac{1}{Z}\int \mathcal{D}\phi\, e^{iS_{SK}[\phi]}\mathcal{O}_1(t)\mathcal{O}_2(t')$$

Real time physics

main object:

$$\langle \mathcal{O}_1(t)\mathcal{O}_2(0)\rangle = Tr[\mathcal{O}_1(t)\mathcal{O}_2(0)\, e^{-\beta H}]$$
$$= Tr[e^{-iHt}\mathcal{O}_1(0)e^{iHt}\mathcal{O}_2(0)e^{-\beta H}]$$

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



$t_0 \sim t_0 - i\beta$

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

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

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

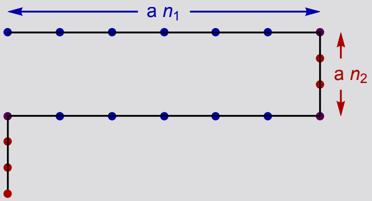
Real time physics

(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 $n_1 = 10, n_2 = 2$)

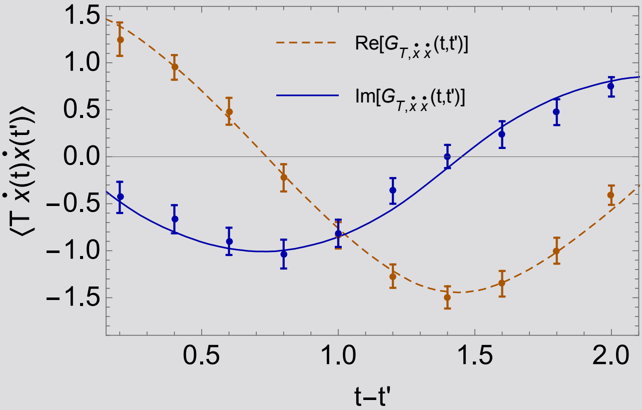


$$S = -i\sum_{i=0}^{N} \Delta t_i \left[\frac{1}{2}\left(\frac{x_{i+1} - x_i}{\Delta t_i}\right)^2 - V(x_i)\right]$$

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

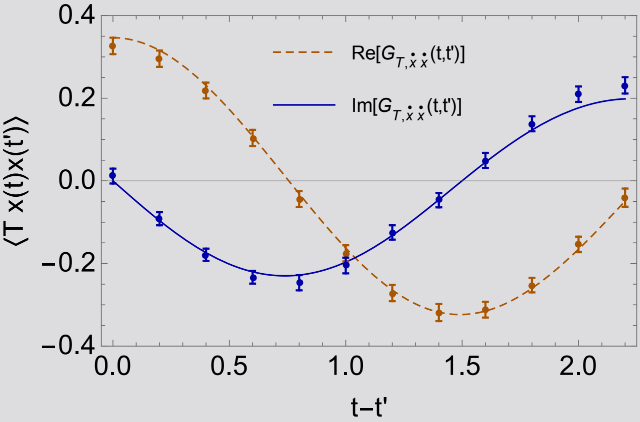
Real time physics: anharmonic oscillator

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



Real time physics: anharmonic oscillator

$$\langle x(t)x(t')\rangle$$



Real time physics: anharmonic oscillator

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, improvements needed

Conclusions

- *holomorphic gradient flow*: knob to control the sign problem
- Lefschetz thimble decomposition is a limiting case, problematic if multiple thimbles contribute
- QFT (ferminoic, bosonic), real time ✓
- chiral symmetry breaking (on the way)

Outlook

- the manifolds can be bumpy: smarter proposals
- det J is costly: estimators, pseudo-fermions
- multimodal distributions: tempered transitions?

  [R. Neal, Statistics and Computing, 6:353 (1996)]
- gauge theories, transport coefficients ...

a bunch of other stuff

4d interacting Bose gas

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

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

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

discretization:

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

4d 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!

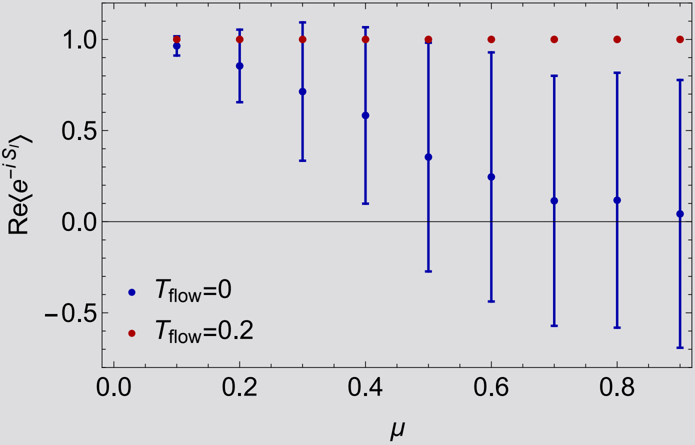
discretization:

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

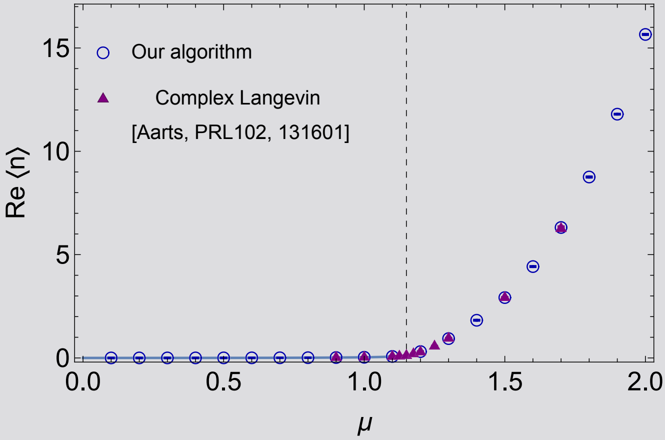
sign problem here!

4d interacting Bose gas

sign problem ?



4d interacting Bose gas



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

General 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?

General Remarks II

the landscape of the space of proposals ($\mathcal{T}$ or $\mathbb{R}^N$) 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) $\mathbb{R}^N$?