

PATH INTEGRALS, THIMBLES AND MCMC

Paul Saffin

University of Nottingham



Science & Technology
Facilities Council

in collaboration with
Zong-Gang Mou, Anders Tranberg, Simon Woodward
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OVERVIEW OF TALK

- motivation



- The problem

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}\Phi \mathcal{O} e^{iS/\hbar}}{\int \mathcal{D}\Phi e^{iS/\hbar}}$$

- A solution



- what next?

?

REAL-TIME EVOLUTION IN QUANTUM FIELD THEORY

- Preheating

- Berges, Felder, Garcia-Bellido, Garcia-Perez, Gelfand, Gonzalez-Arroyo, Khlebnikov, Kofman, Linde, Micha, Mou, Prokopec, Pruschke, Roos, Tkachev

- Baryogenesis

- Bodecker, Grigoriev, Hu, Kusenko, Moore, Mou, Muller, Rummukainen, PMS, Shaposhnikov,, Smit, Tranberg

- FRW evolution

- Baacke, Covi, Heitmann, Kevlishvili, Patzold, Tranberg

- Soliton dynamics

- Berges, Borsanyi, Hertzberg, Hindmarsh, Mou, PMS, Roth, Tognarelli, Tranberg

- Thermalization

- Aarts, Attems, Berges, Bonini, Gelfand, Kurkela, Philipsen, Pruschke, Schlichting, Sexty, Shafer, Wagenbach, Wetterich, Zafeiropoulos

- Phase transitions

- Blaizot, Hatta, Rajantie, Sexty, Smit, Tranberg, Tsutsui

- Langevin

- Aarts, Scherzer, Seiler, Sexty, Stamatescu

THE PATH INTEGRAL

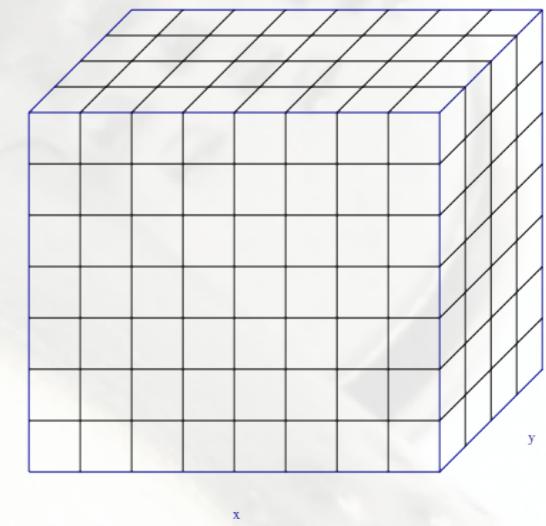
$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}\Phi \ \mathcal{O} e^{iS/\hbar}}{\int \mathcal{D}\Phi \ e^{iS/\hbar}}$$

THE PATH INTEGRAL

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}\Phi \ \mathcal{O} e^{iS/\hbar}}{\int \mathcal{D}\Phi \ e^{iS/\hbar}}$$

- It's big

$$\int \mathcal{D}\Phi = \int d\Phi(x_1^\mu) d\Phi(x_2^\mu) d\Phi(x_3^\mu) \dots$$

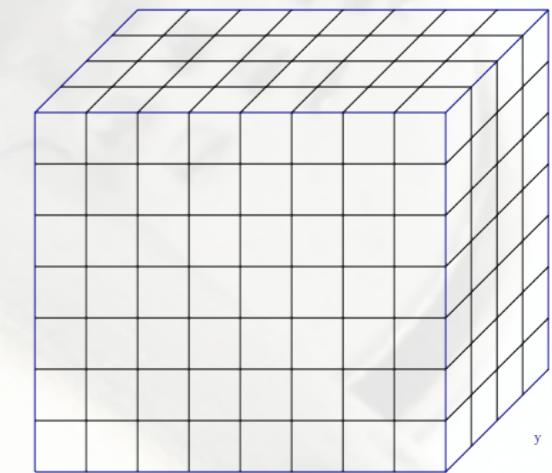


THE PATH INTEGRAL

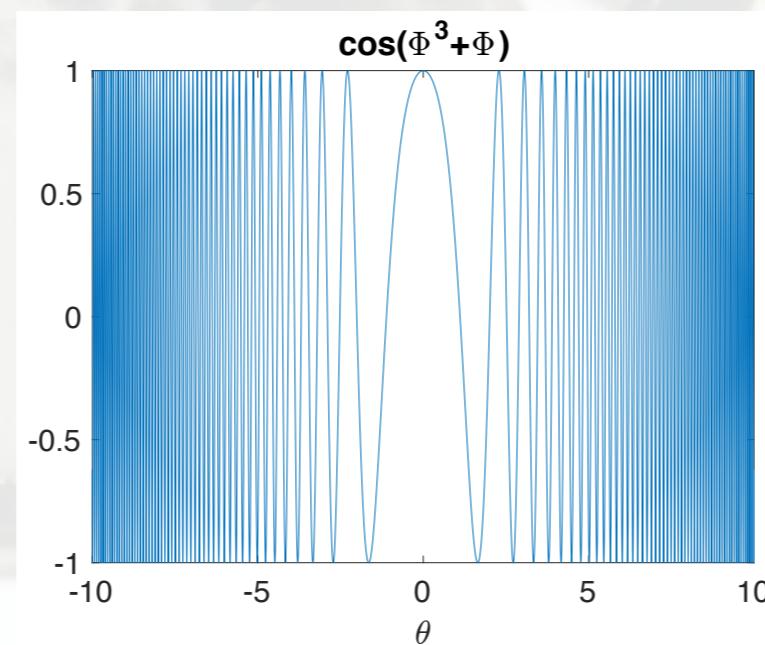
$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}\Phi \mathcal{O} e^{iS/\hbar}}{\int \mathcal{D}\Phi e^{iS/\hbar}}$$

- It's big

$$\int \mathcal{D}\Phi = \int d\Phi(x_1^\mu) d\Phi(x_2^\mu) d\Phi(x_3^\mu) \dots$$



- It's a phase



THE PATH INTEGRAL

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}\Phi \ \mathcal{O} e^{iS/\hbar}}{\int \mathcal{D}\Phi \ e^{iS/\hbar}}$$

- It's big:
 - use Monte Carlo sampling to evaluate the integrals

THE PATH INTEGRAL

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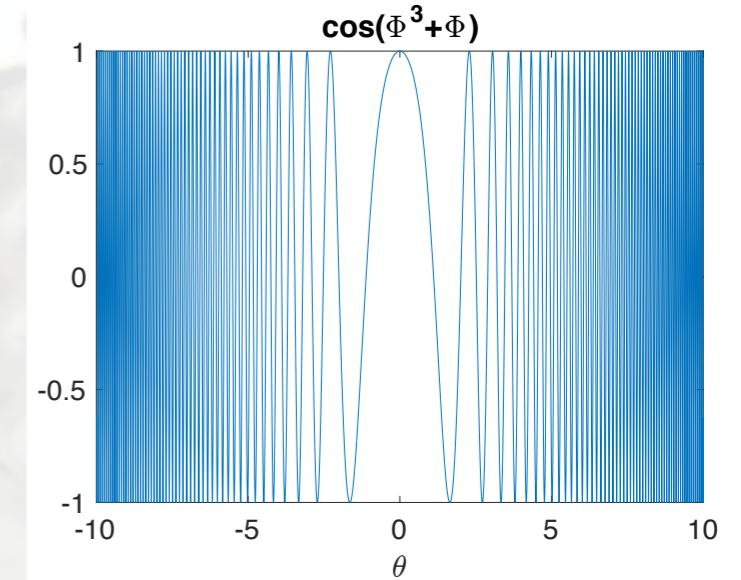
- It's big:
 - use Monte Carlo sampling to evaluate the integrals
- It's a phase:
 - use Picard-Lefschetz (Cauchy's theorem) to improve convergence
- Aarts, Alexandru, Basar, Bedaque, Christoforetti, , Feldbrugge, Fujii, Honda, Kato, Kikuwa, Komatsu, Lehners, Di Renzo, Ridgeway, Sano, Scorzato, Seiler, Sexty, Turok, Warrington, Witten, ...

IMPROVING CONVERGENCE:

$$\int \mathcal{D}\Phi \exp\left(\frac{i}{\hbar}S(\Phi)\right)$$

IMPROVING CONVERGENCE:

$$Ai(x) = \int_{-\infty}^{\infty} \frac{d\phi}{2\pi} \exp \left(i \left[\frac{1}{3}\phi^3 + x\phi \right] \right)$$
$$\int \mathcal{D}\Phi \exp \left(\frac{i}{\hbar} S(\Phi) \right)$$

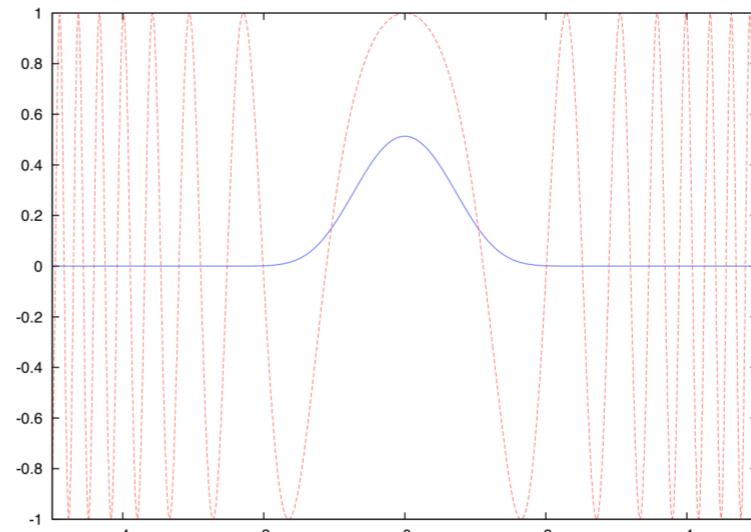
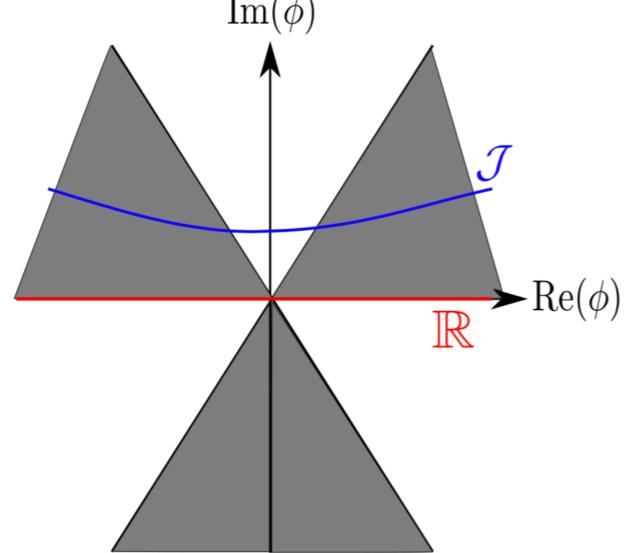
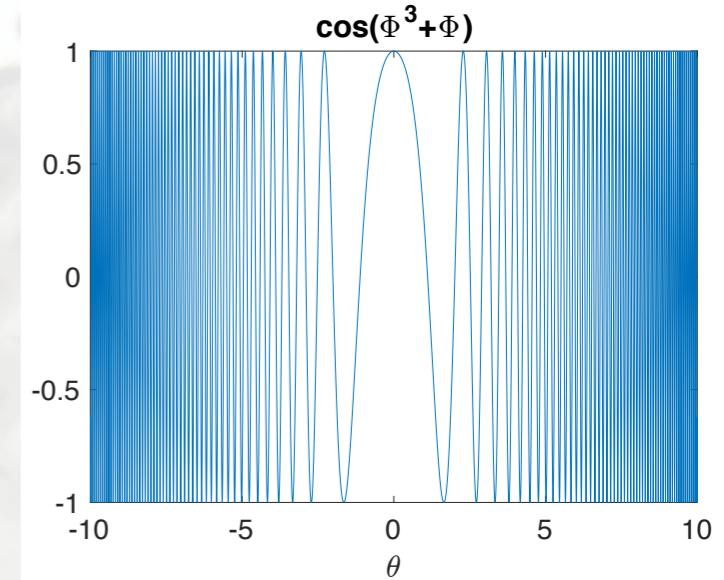


IMPROVING CONVERGENCE:

$$Ai(x) = \int_{-\infty}^{\infty} \frac{d\phi}{2\pi} \exp \left(i \left[\frac{1}{3}\phi^3 + x\phi \right] \right)$$

$$\int \mathcal{D}\Phi \exp \left(\frac{i}{\hbar} S(\Phi) \right)$$

$$\phi \in \mathbb{R} \rightarrow \phi \in \mathbb{C}$$

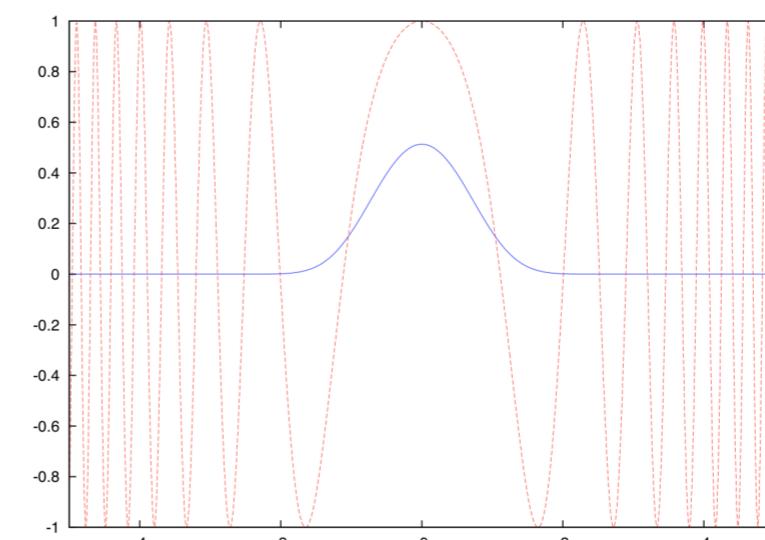
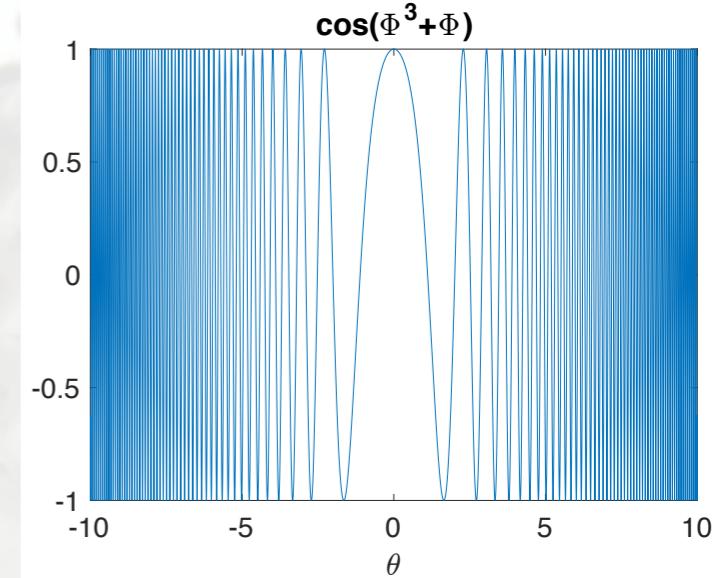
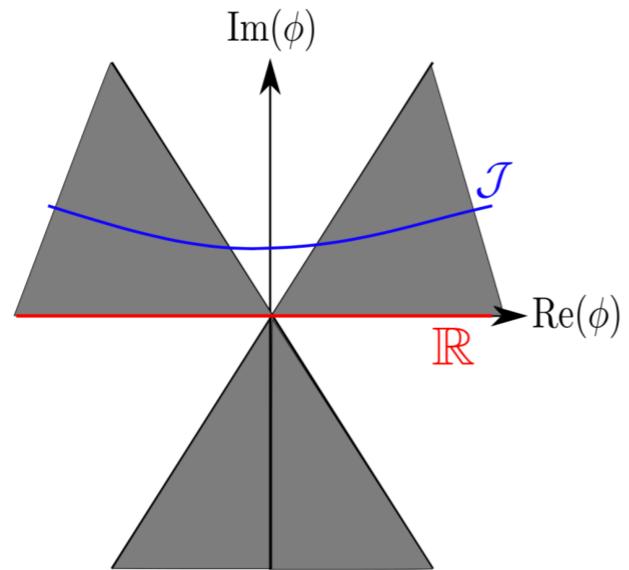


IMPROVING CONVERGENCE:

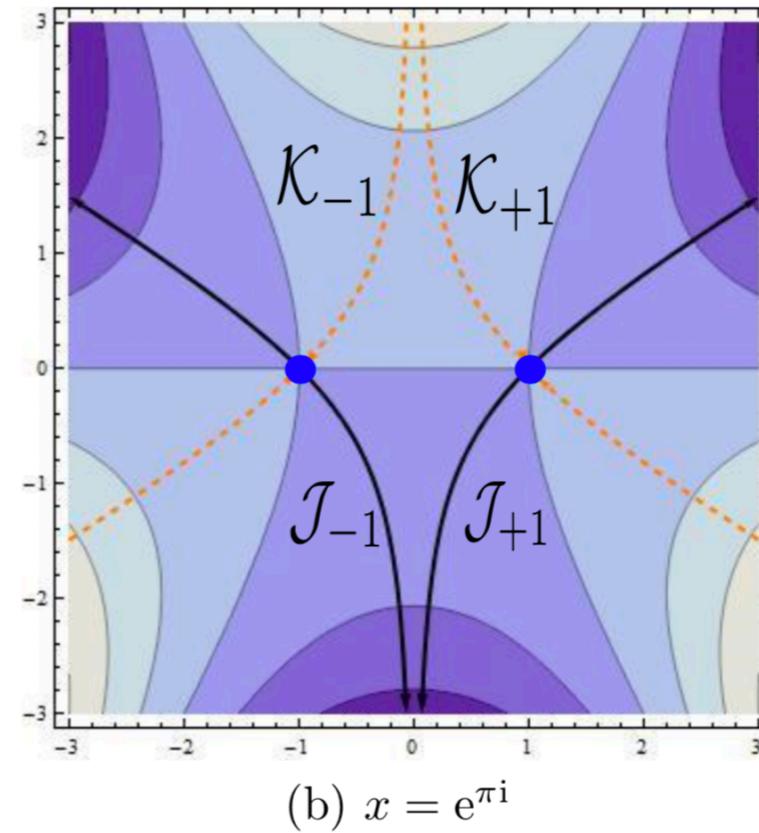
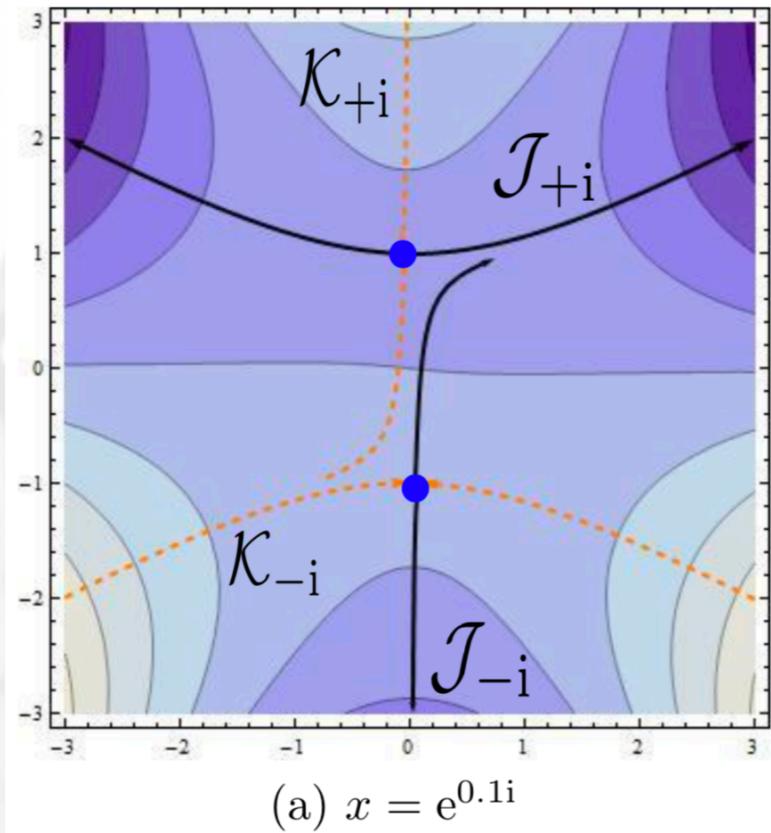
$$Ai(x) = \int_{-\infty}^{\infty} \frac{d\phi}{2\pi} \exp \left(i \left[\frac{1}{3}\phi^3 + x\phi \right] \right)$$

The "best" curve
is "the" thimble

$$\phi \in \mathbb{R} \rightarrow \phi \in \mathbb{C}$$

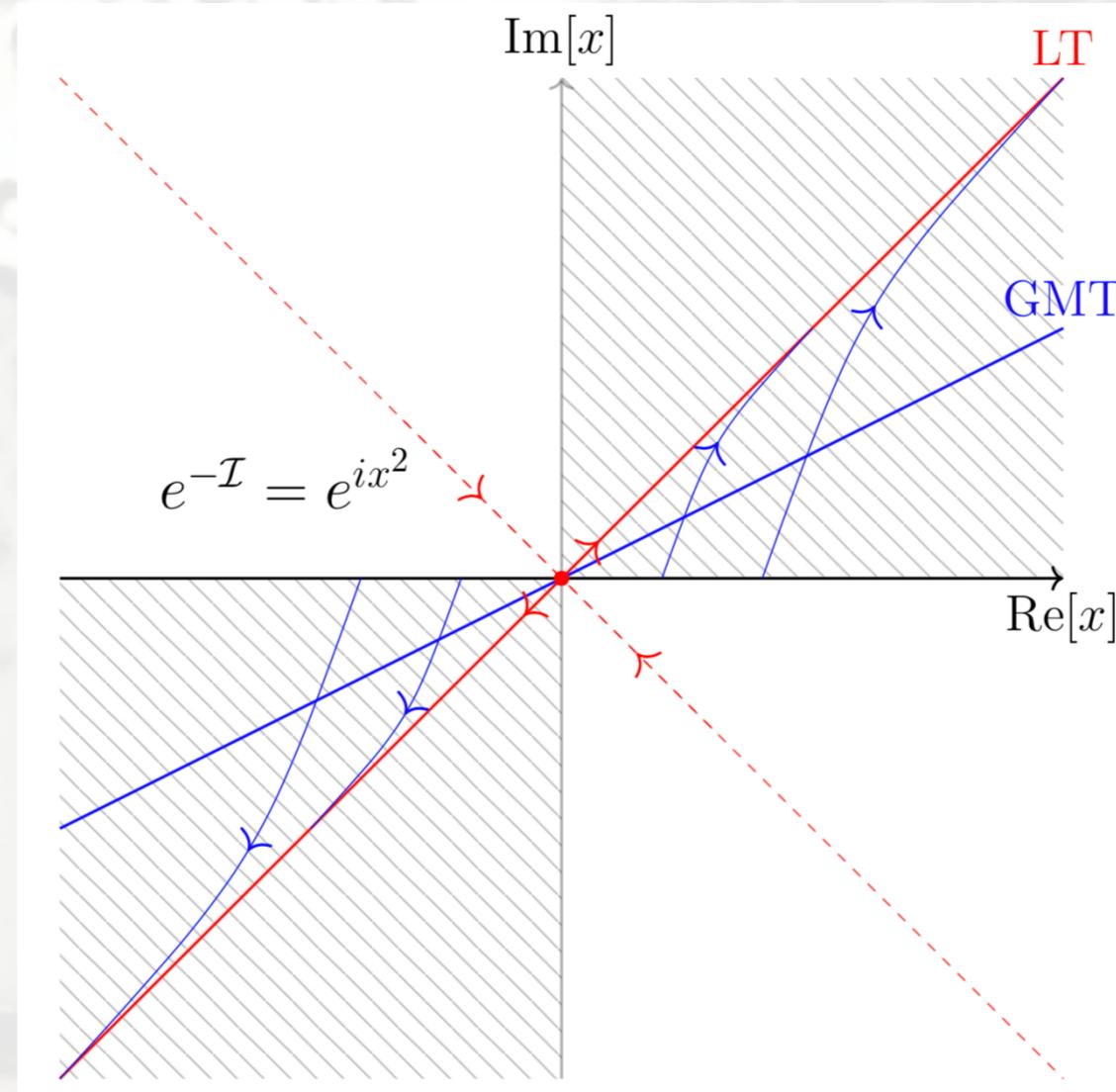


FINDING “THE” THIMBLE



GENERALIZED THIMBLE

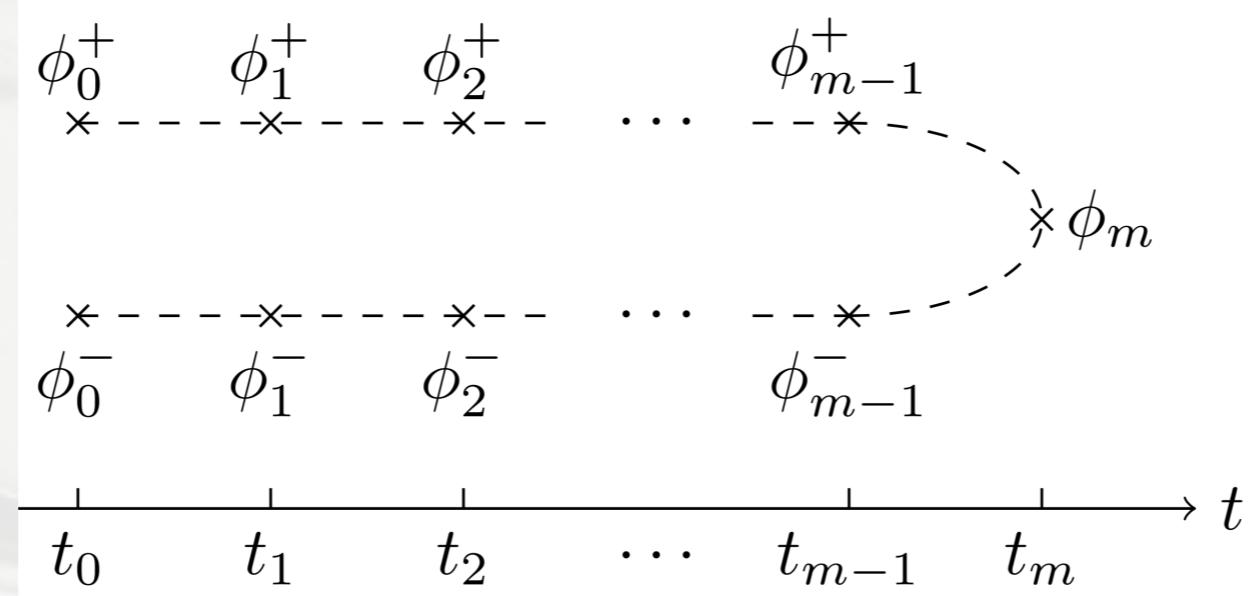
$$\int dx e^{-\mathcal{I}} \rightarrow \frac{dx}{d\tau} = \overline{\left(\frac{\partial \mathcal{I}}{\partial x} \right)} \rightarrow \frac{d\mathcal{I}}{d\tau} = \left| \frac{\partial \mathcal{I}}{\partial x} \right|^2 \geq 0$$



- Alexandru, Basar, Bedaque, Lamm, Lawrence.

WHAT WE WANT TO CALCULATE:

$$\begin{aligned}\langle \hat{\mathcal{O}}(t) \rangle &= \text{Tr} \left(\hat{\mathcal{O}}(t) \hat{\rho}(t_0) \right) = \int \mathcal{D}\phi \langle \phi_0^-; t_0 | \hat{\mathcal{O}}(t) \hat{\rho}(t_0) | \phi_0^-; t_0 \rangle \\ &= \frac{\int \mathcal{D}\phi \exp \left(\frac{i}{\hbar} \int_C dt L \right) \mathcal{O}(t) \langle \phi_0^+; t_0 | \hat{\rho}_0 | \phi_0^-; t_0 \rangle}{\int \mathcal{D}\phi \exp \left(\frac{i}{\hbar} \int_C dt L \right) \langle \phi_0^+; t_0 | \hat{\rho}_0 | \phi_0^-; t_0 \rangle}\end{aligned}$$



REAL-TIME EVOLUTION

$$\langle A \rangle = \frac{\int dx \; A(x) e^{-\mathcal{I}}}{\int dx \; e^{-\mathcal{I}}}$$

REAL-TIME EVOLUTION

$$\langle A \rangle = \frac{\int dx \ A(x) e^{-\mathcal{I}}}{\int dx \ e^{-\mathcal{I}}} \xrightarrow{\text{Picard-Lefschetz}} \frac{\int_{\Gamma} dz \ A(z) e^{-\mathcal{I}(z(x))}}{\int_{\Gamma} dz \ e^{-\mathcal{I}(z(x))}}$$

Picard-Lefschetz

Cauchy

REAL-TIME EVOLUTION

$$\langle A \rangle = \frac{\int dx A(x) e^{-\mathcal{I}}}{\int dx e^{-\mathcal{I}}}$$

Cauchy

Co-ordinate transformation

$$= \frac{\int_{\Gamma} dz A(z) e^{-\mathcal{I}(z(x))}}{\int_{\Gamma} dz e^{-\mathcal{I}(z(x))}}$$
$$= \frac{\int dx \frac{\partial z}{\partial x} A(z(x)) e^{-\mathcal{I}(z(x))}}{\int dx \frac{\partial z}{\partial x} e^{-\mathcal{I}(z(x))}}$$

REAL-TIME EVOLUTION

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$$= \frac{\int dx \frac{\partial z}{\partial x} A(z(x)) e^{-\mathcal{I}(z(x))}}{\int dx \frac{\partial z}{\partial x} e^{-\mathcal{I}(z(x))}}$$
$$= \frac{\langle A e^{i[\arg(\det(J)) - I_{im}]} \rangle_P}{\langle e^{i[\arg(\det(J)) - I_{im}]} \rangle_P}$$

$$P = e^{-\mathcal{I}_{re} + \ln(|\det(J)|)}$$

REAL-TIME EVOLUTION

$$\langle \phi_0^+; t_0 | \hat{\rho} | \phi_0^-; t_0 \rangle$$

REAL-TIME EVOLUTION

$$\langle \phi_0^+; t_0 | \hat{\rho} | \phi_0^-; t_0 \rangle$$

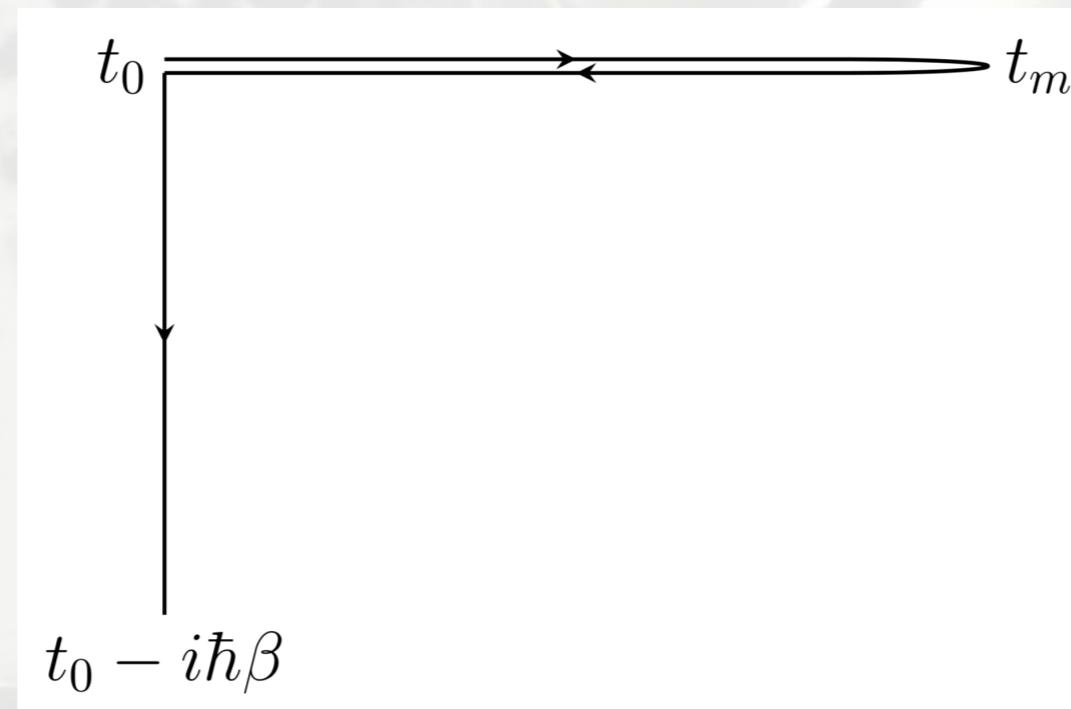
$$\hat{\rho} = e^{-\beta \hat{H}}$$

REAL-TIME EVOLUTION

$$\langle \phi_0^+; t_0 | \hat{\rho} | \phi_0^-; t_0 \rangle$$

$$\hat{\rho} = e^{-\beta \hat{H}}$$

$$\langle \phi_0^+; t_0 | \hat{\rho} | \phi_0^-; t_0 \rangle = \int_{\phi_0^-}^{\phi_0^+} \mathcal{D}e^{i \int_{t_0}^{t_0 - i\hbar\beta} S}$$



REAL-TIME EVOLUTION

$$\langle \phi_0^+;t_0 | \hat{\rho} | \phi_0^-;t_0 \rangle$$

$$\phi^{cl} = \frac{1}{2}(\phi^+ + \phi^-), \qquad \phi^q = \phi^+ - \phi^-$$

REAL-TIME EVOLUTION

$$\langle \phi_0^+;t_0|\hat{\rho}|\phi_0^-;t_0\rangle$$

$$\phi^{cl}=\frac{1}{2}(\phi^++\phi^-),\qquad \phi^q=\phi^+-\phi^-$$

$$Z = \int \mathcal{D}\phi \exp\left\{-\frac{1}{\hbar}\int \frac{\mathrm{d}^dp}{(2\pi)^d}\omega_p\left[\frac{(\phi_0^{cl})^2}{2n_p+1}+\frac{(\phi_0^q)^2}{4}(2n_p+1)\right]+\frac{i}{\hbar}\int_{\mathcal{C}}\mathrm{d}t\;L\right\}$$

$$n_p=\frac{1}{e^{\hbar\omega_p\beta}-1}$$

REAL-TIME EVOLUTION

$$\langle \phi_0^+;t_0|\hat{\rho}|\phi_0^-;t_0\rangle$$

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$$n_p=\frac{1}{e^{\hbar\omega_p\beta}-1}$$

$$Z = \int \mathcal{D}\phi \exp\left\{-\frac{1}{\hbar}\int \frac{\mathrm{d}^dp}{(2\pi)^d}\left[\omega_p\frac{(\phi_0^{cl})^2}{2n_p+1}+\frac{(\dot{\phi}_0^{cl})^2}{\omega_p(2n_p+1)}\right]+\frac{i}{\hbar}\int_{\mathcal{C}}\mathrm{d}t\;L\right\}$$

REAL-TIME EVOLUTION

$$\langle \phi_0^{cl}(p) \phi_0^{cl\dagger}(p') \rangle = \frac{\hbar}{\omega_p} \left(n_p + \frac{1}{2} \right) (2\pi)^d \delta(p - p')$$

$$\langle \dot{\phi}_0^{cl}(p) \dot{\phi}_0^{cl\dagger}(p') \rangle = \hbar \omega_p \left(n_p + \frac{1}{2} \right) (2\pi)^d \delta(p - p')$$

REAL-TIME EVOLUTION

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For a given $(\phi_0^{cl}, \phi_1^{cl})$ there is a unique critical point $\frac{\delta \mathcal{I}}{\delta \phi} = 0$

$$(\tilde{\phi}^{cl}, \phi^q = 0) \quad \left. \frac{\delta \mathcal{I}}{\delta \phi} \right|_{\tilde{\phi}^{cl}} = 0$$

One critical point

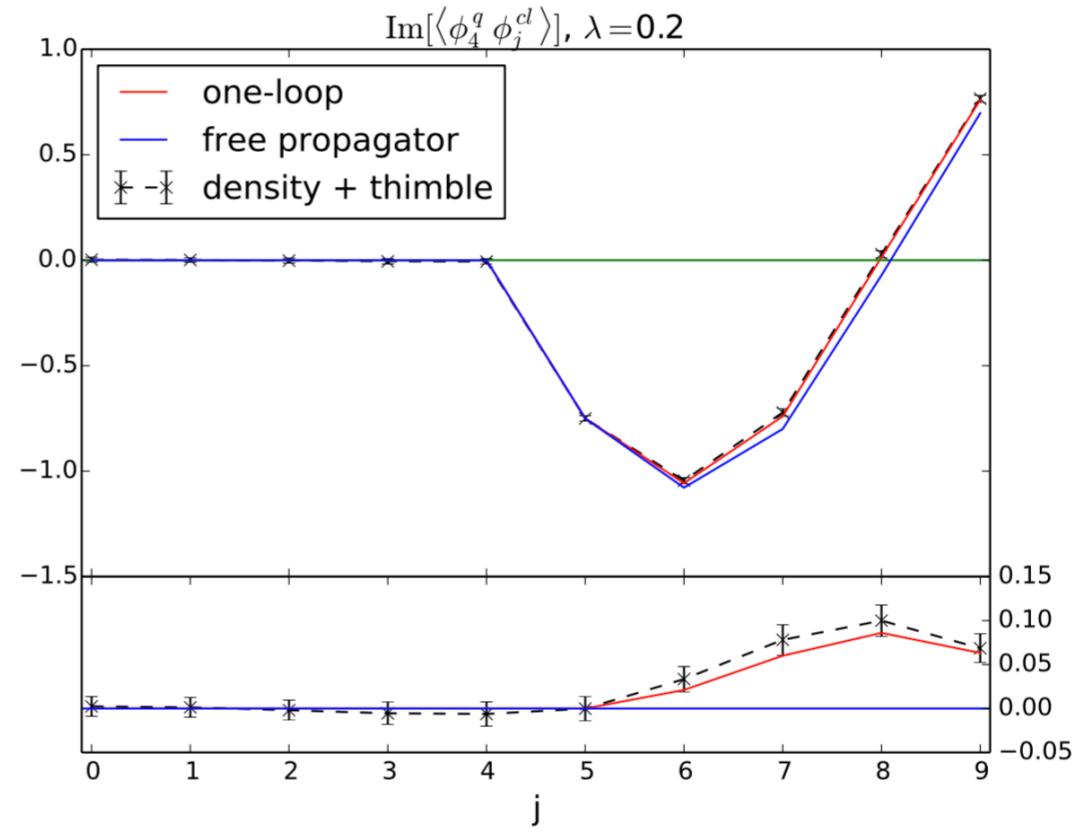
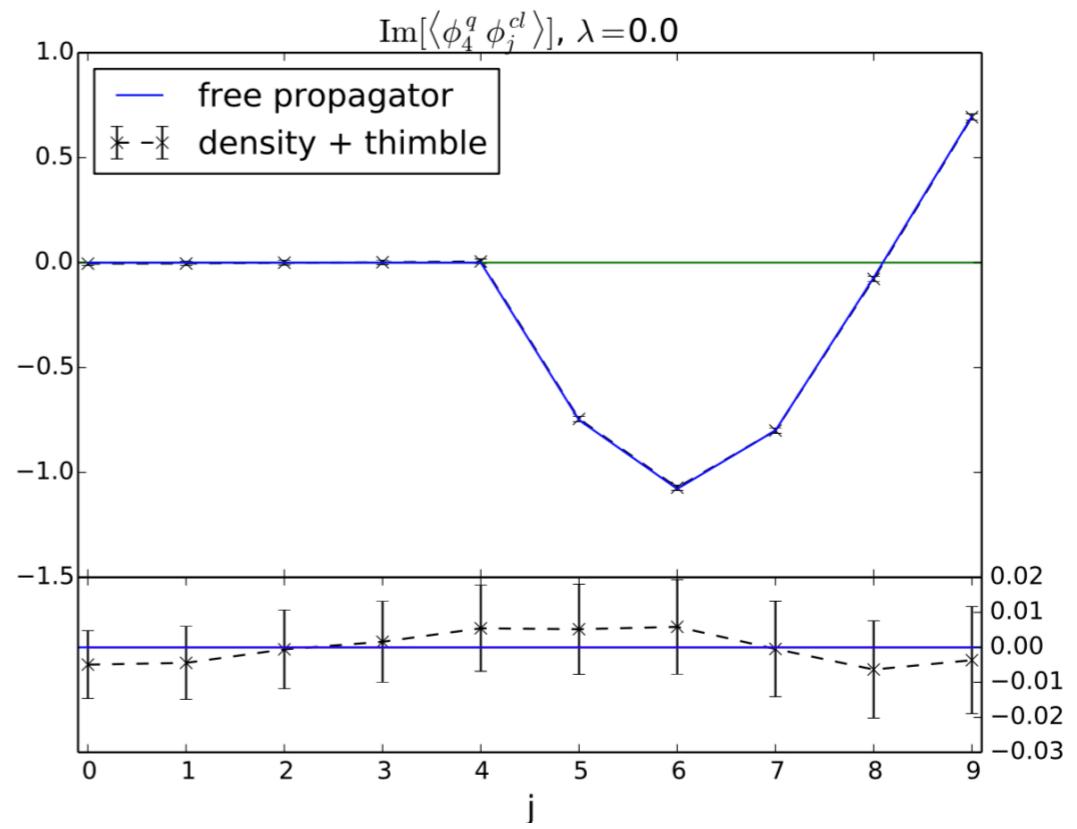
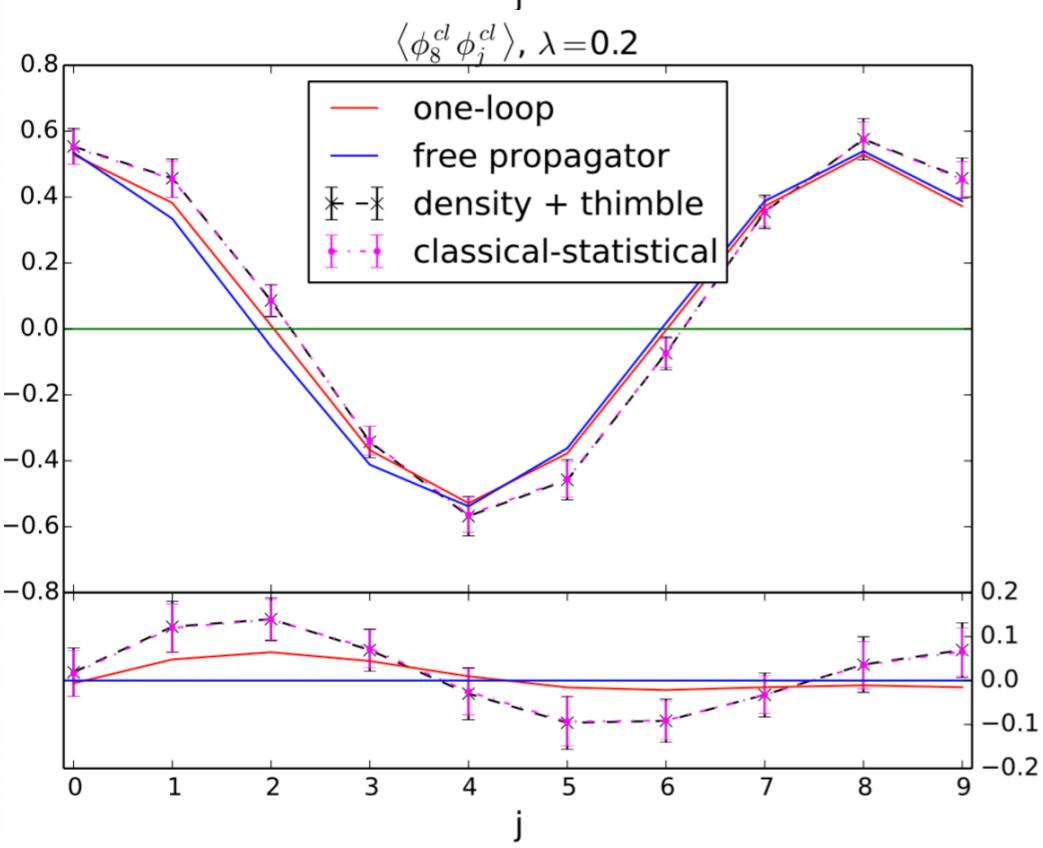
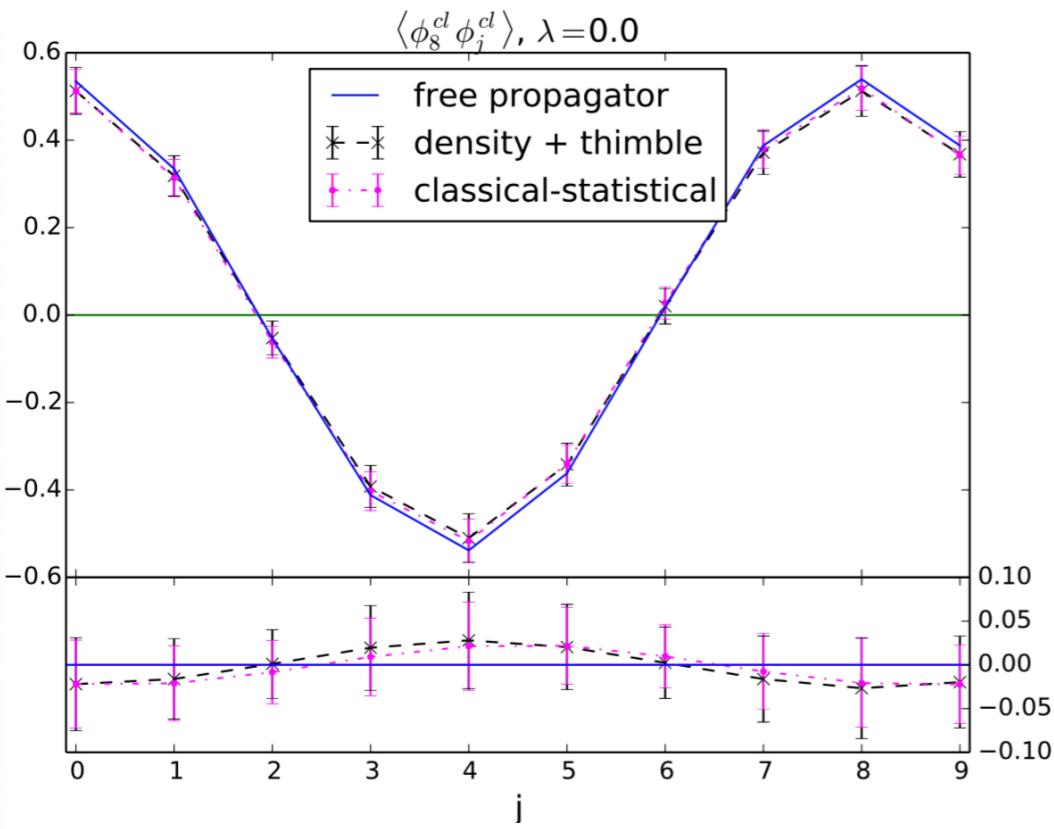


One thimble

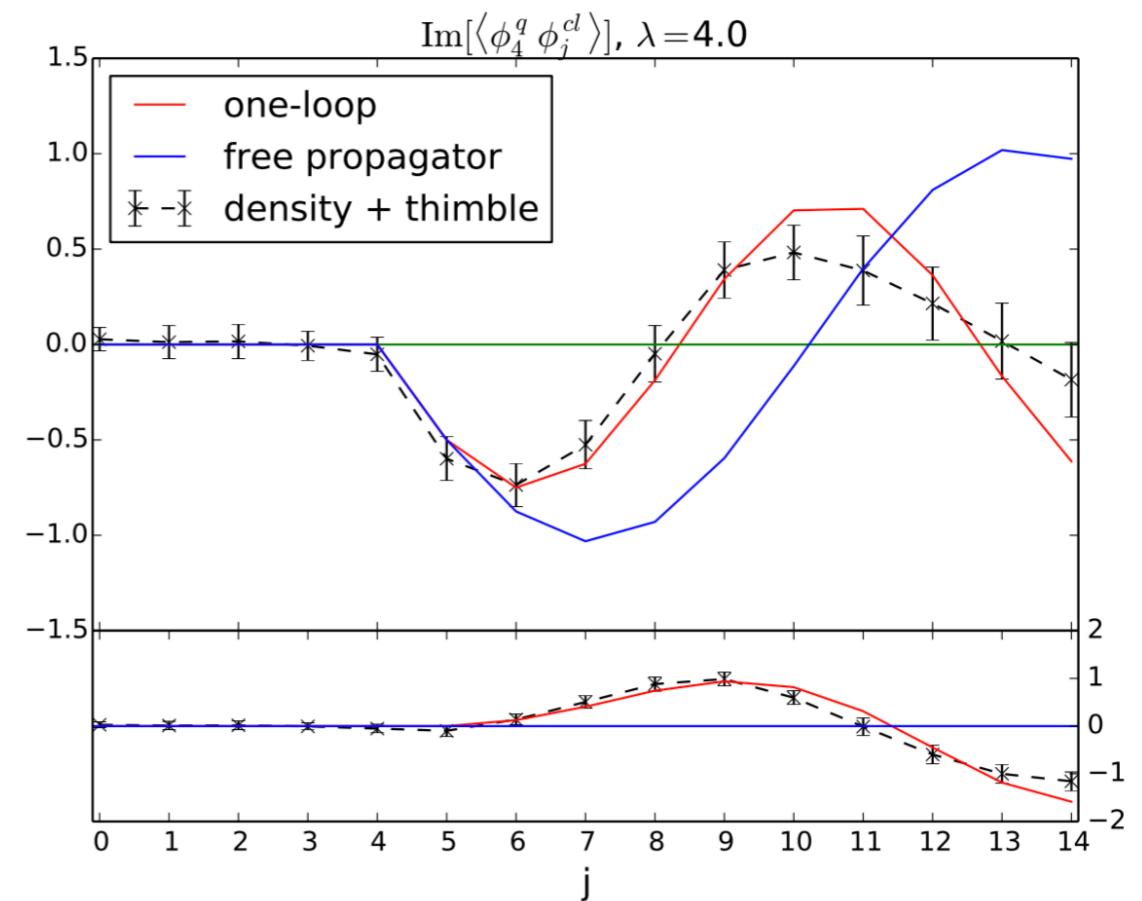
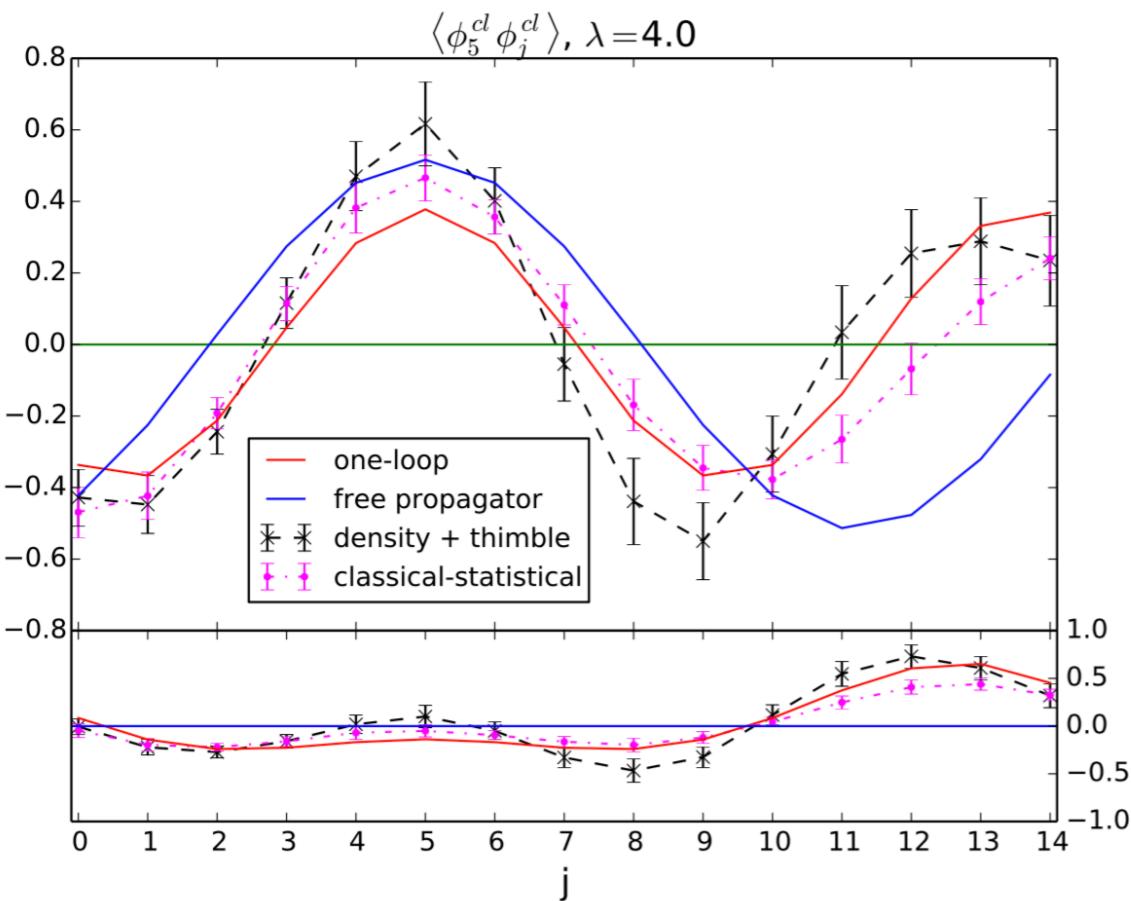


Well-behaved Monte Carlo

REAL-TIME EVOLUTION



REAL-TIME EVOLUTION



CONCLUSIONS + OUTLOOK

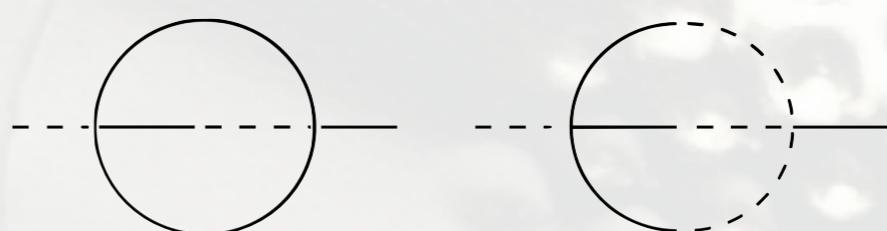
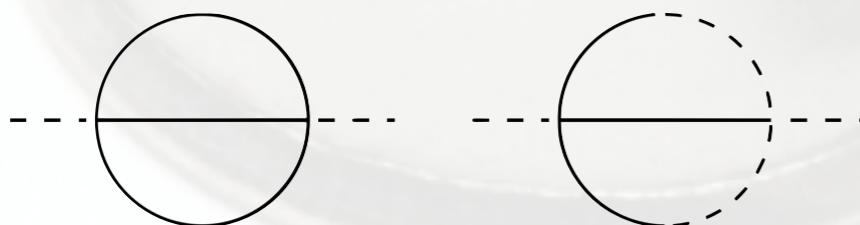
- Can solve the Lorentzian path integral using Picard-Lefschetz and Monte Carlo (scalar field)
 - Solves the sign problem
- Can we do fermions, gauge fields?
- How does this scale with dimension?
 - Is it practical for out of equilibrium studies?

CLASSICAL-STATISTICAL

$$\text{———} \quad \hbar \left(n_p + \frac{1}{2} \right) \frac{\cos(\omega_p[t_1 - t_2])}{\omega_p}$$

$$\text{-----} \quad -i\hbar\theta(t_2 - t_1) \frac{\sin(\omega_p[t_2 - t_1])}{\omega_p}$$

$$\text{—————} \quad -i\hbar\theta(t_1 - t_2) \frac{\sin(\omega_p[t_1 - t_2])}{\omega_p}$$



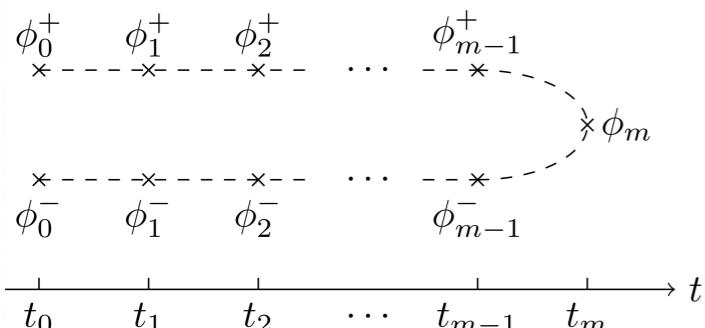
CRITICAL POINT

$$\hat{H} = \int d^d x \left(\frac{1}{2} \pi^2 + C(\Phi) \right)$$

$$E_i = \int d^d x \left[C \left(\phi_i^{cl}(x) + \frac{1}{2} \phi_i^q(x) \right) - C \left(\phi_i^{cl}(x) - \frac{1}{2} \phi_i^q(x) \right) \right]$$

E contains only odd powers of ϕ^q

$$\begin{aligned} \frac{\partial \mathcal{I}}{\partial \phi_i^q(x)} &= - \frac{i dt d^d x}{\hbar} \left[\frac{2\phi_i^{cl}(x) - \phi_{i-1}^{cl}(x) - \phi_{i+1}^{cl}(x)}{dt^2} - \frac{\partial E_i}{\partial \phi_i^q(x)} \right] & i \neq m \\ \frac{\partial \mathcal{I}}{\partial \phi_i^{cl}(x)} &= - \frac{i dt d^d x}{\hbar} \left[\frac{2\phi_i^q(x) - \phi_{i-1}^q(x) - \phi_{i+1}^q(x)}{dt^2} - \frac{\partial E_i}{\partial \phi_i^{cl}(x)} \right] & i \neq m \\ \frac{\partial \mathcal{I}}{\partial \phi_m(x)} &= \frac{i d^d x}{\hbar dt} \phi_{m-1}^q(x) \end{aligned}$$



REAL-TIME EVOLUTION



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