複素ランジュバン法のフェルミ原子気体への応用

筒井翔一朗
（理化学研究所仁科センター）

共同研究者:
土居孝寛 (阪大RCNP)
田島裕之 (高知大→東大)

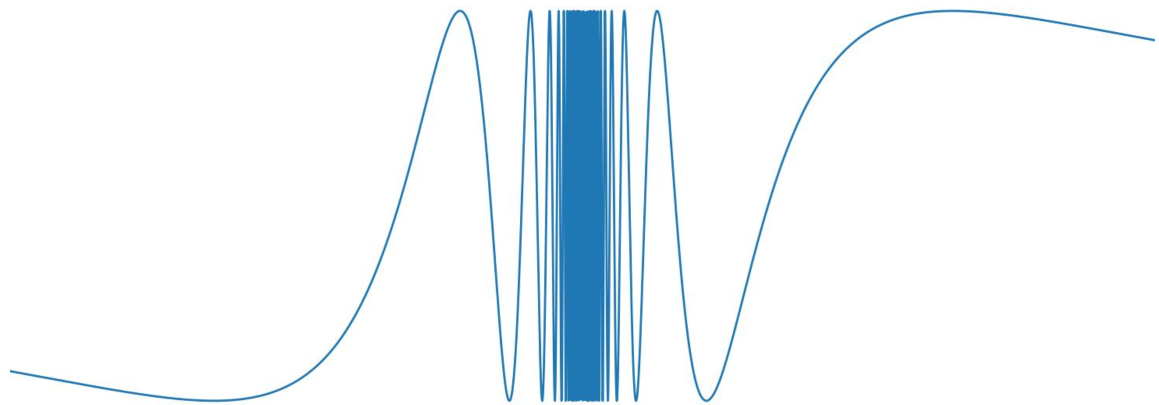
KEK 素核宇･物性 連携研究会 (online) 2021/3/29

Outline

- ◆ What is the sign problem ?
- ◆ Sign problem in cold Fermi gas
- ◆ Complex Langevin (theory and application)

Sign problem: an intuitive picture

$$\int dx \Bigg(\quad\Bigg)$$



Numerical evaluation of highly oscillatory integrals is difficult

Monte Carlo integration

Positive semi-definite

Random number

$$\int dx O(x) P(x) \sim \frac{1}{N} \sum_{i=1}^{N} O(x_i)$$

$P(x) \propto e^{-S(x)}$ is viewed as a probability density function if $S(x) \in \mathbb{R}$

Monte Carlo integration for complex P(x)

Non positive semi-definite

$$\frac{\int dx O(x) P(x)}{\int dx P(x)}$$

$P(x) \propto e^{-S(x)}$ is not viewed as a probability density function if $S(x) \in \mathbb{C}$

Monte Carlo integration for complex P(x)

$$\frac{\int dx O(x) P(x) / \int dx |P(x)|}{\int dx P(x) / \int dx |P(x)|}$$

Monte Carlo integration for complex P(x)

$$\frac{\int dx O(x) e^{i\theta(x)} |P(x)| / \int dx |P(x)|}{\int dx e^{i\theta(x)} |P(x)| / \int dx |P(x)|}$$

This procedure is known as reweighting.

Monte Carlo integration for complex P(x)

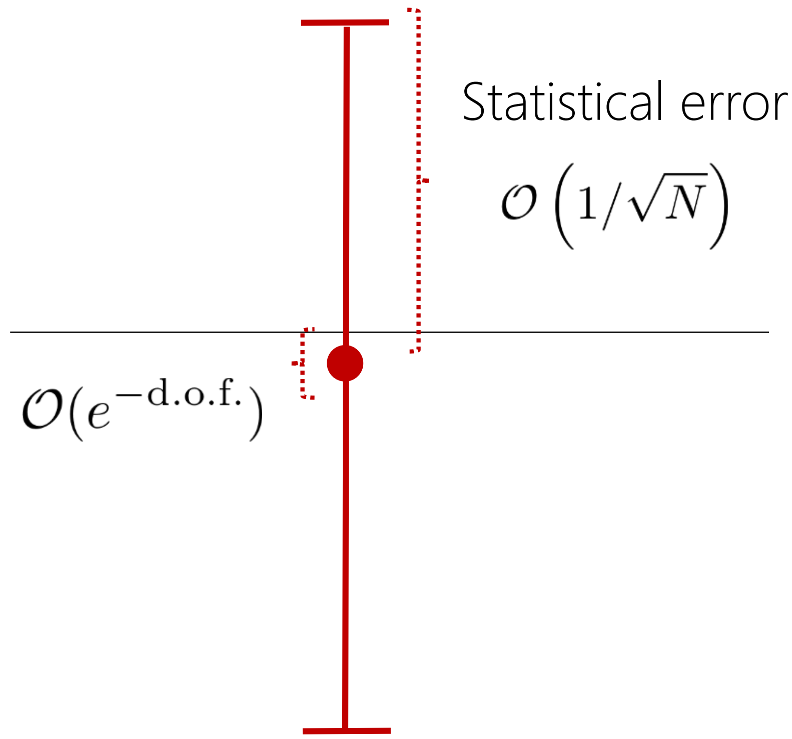
Positive semi-definite

$$\frac{\int dx O(x) e^{i\theta(x)} |P(x)| / \int dx |P(x)|}{\int dx e^{i\theta(x)} |P(x)| / \int dx |P(x)|}$$

Evaluate the numerator and denominator separately

Sign problem: more precise statement

$$\frac{\int dx e^{i\theta(x)}|P(x)|}{\int dx|P(x)|} \sim$$



Signal-to-noise ratio is **exponentially small**

Outline

- ◆ What is the sign problem ?
- ◆ Sign problem in cold Fermi gas
- ◆ Complex Langevin (theory and application)

Sign problem in cold Fermi gas

Grand partition function of the BCS model:

$$Z = \int \left(\prod_\sigma \mathcal{D}\bar{\psi}_\sigma \mathcal{D}\psi_\sigma \right) e^{-\int d\tau d^d x \left(\sum_\sigma \bar{\psi}_\sigma G_\sigma^{-1} \psi_\sigma - g \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow \right)}$$

$$= \int \mathcal{D}\phi \left(\prod_\sigma \mathcal{D}\bar{\psi}_\sigma \mathcal{D}\psi_\sigma \right) e^{-\int d\tau d^d x \left(\sum_\sigma \bar{\psi}_\sigma \left(G_\sigma^{-1} - \sqrt{g}\phi \right) \psi_\sigma + \frac{\phi^2}{2} \right)}$$

$$= \int \mathcal{D}\phi \det \left(G_\uparrow^{-1} - \sqrt{g}\phi \right) \det \left(G_\downarrow^{-1} - \sqrt{g}\phi \right) e^{-\int d\tau d^d x \frac{\phi^2}{2}}$$

Can be negative

When does the sign problem occur?

I assume that the partition function has a following form:

$$Z = \int \mathcal{D}\phi \det M(\phi) e^{-S(\phi)}$$

The fermion det. can be negative when

- there are even species of fermions with imbalance (↑≠↓)
- there are odd species of fermions
- repulsive interaction

↑ I will discuss this case later

Outline

- What is the sign problem ?
- Sign problem in cold Fermi gas
- Complex Langevin (theory and application)

Complex Langevin

$$\frac{d\phi}{dt} = -\frac{\partial S_{\mathrm{eff}}(\phi)}{\partial \phi} + \eta$$

Drift term White noise

Reach equilibrium

$$P_{\mathrm{eq}}(\phi_{\mathrm{R}}, \phi_{\mathrm{I}})$$

Parisi, Phys. Lett. 131B (1983) 393, Klauder PRA 29 (1984) 2036

Justification of complex Langevin

If P_{eq} or $\frac{\partial S_{\mathrm{eff}}}{\partial \phi}$ has "good" properties,

$$\int \mathcal{D}\phi_{\mathrm{R}} \mathcal{D}\phi_{\mathrm{I}} O(\phi_{\mathrm{R}} + i\phi_{\mathrm{I}}) P_{\mathrm{eq}}(\phi_{\mathrm{R}}, \phi_{\mathrm{I}}) = \frac{1}{Z} \int \mathcal{D}\phi O(\phi) e^{-S_{\mathrm{eff}}(\phi)}$$

Obtained by complex Langevin — Original path integral

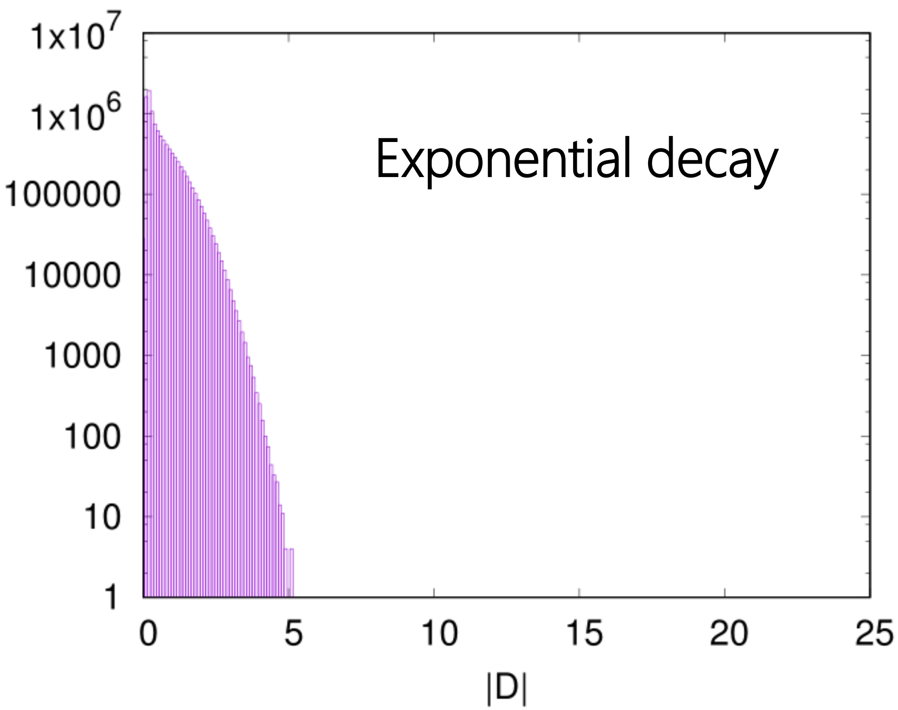
Aarts, Seiler, Stamatescu, PRD 81 (2010) 054608

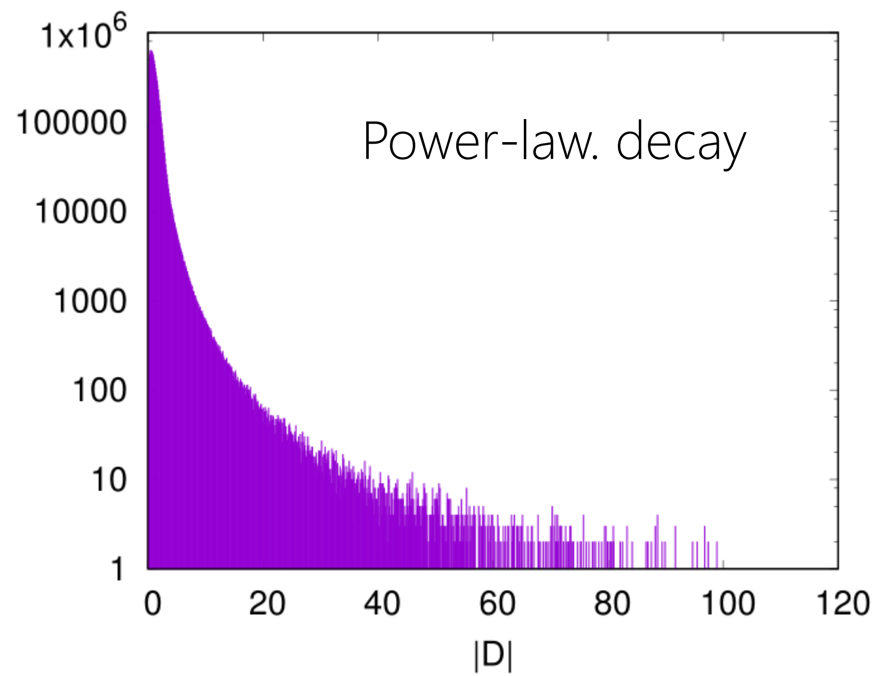
Aarts, James, Seiler, Stamatescu, EPJ C71 (2011) 1756

Nagata, Nishimura, Shimasaki, PRD 92 (2015) 011501, PTEP 2016 013B01

Practically useful criterion

Distribution of the drift term should decay **exponentially**.





Nagata, Nishimura, Shimasaki, PRD 92 (2015) 011501, PTEP 2016 013B01

Application

Our setup:

- Two-component Fermion ($\sigma = \uparrow, \downarrow$)
- Attractive contact interaction ($g > 0$)
- 1D

$$S = \int_0^\beta d\tau \int dx \left[\sum_{\sigma=\uparrow,\downarrow} \bar{\psi}_\sigma \left(\frac{\partial}{\partial \tau} - \frac{1}{2m_\sigma} \frac{\partial^2}{\partial x^2} - \mu_\sigma \right) \psi_\sigma - g \bar{\psi}_\uparrow \bar{\psi}_\downarrow \psi_\downarrow \psi_\uparrow \right]$$

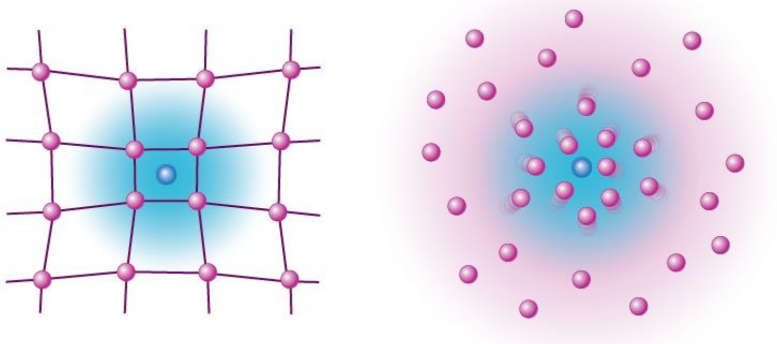
Dimensionless parameters:

$$\beta\mu = \beta(\mu_\uparrow + \mu_\downarrow)/2 \qquad \lambda = \sqrt{g^2 \beta}$$

$$\beta h = \beta(\mu_\uparrow - \mu_\downarrow)/2 \qquad r = a_\tau / a_s^2 \qquad m_\uparrow = m_\downarrow = 1$$

Corresponding Hamiltonian: $\hat{H} = -\sum_{\sigma=\uparrow,\downarrow} \sum_i \frac{1}{2m_\sigma} \frac{d^2}{dx_i^2} - \sum_{i<j} g\delta(x_i - x_j)$

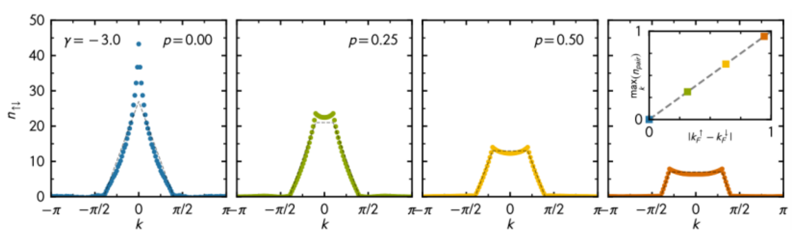
What is expected ?



Poralon (minority dressed by majority)

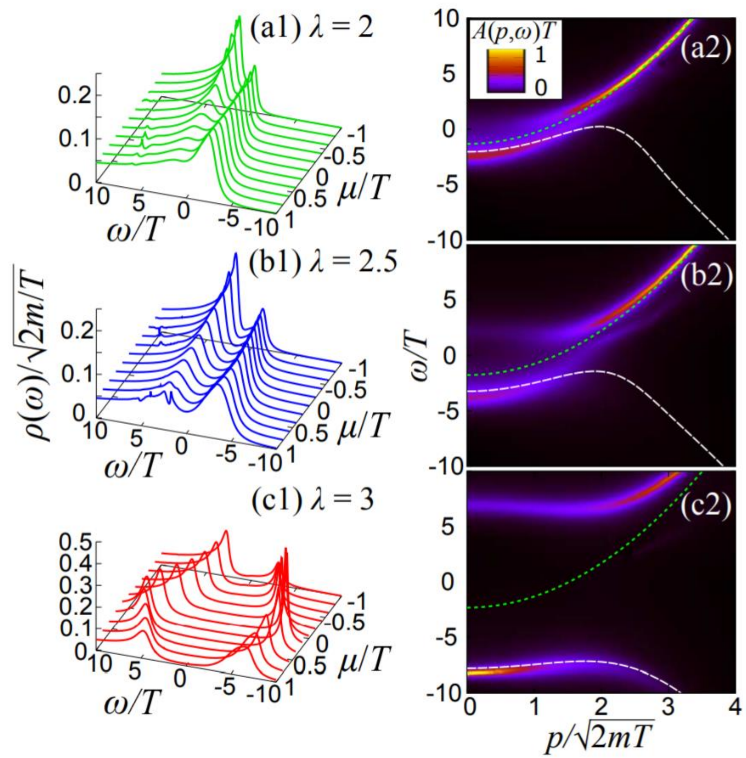
https://physics.aps.org/articles/v9/86

FFLO-like pairing



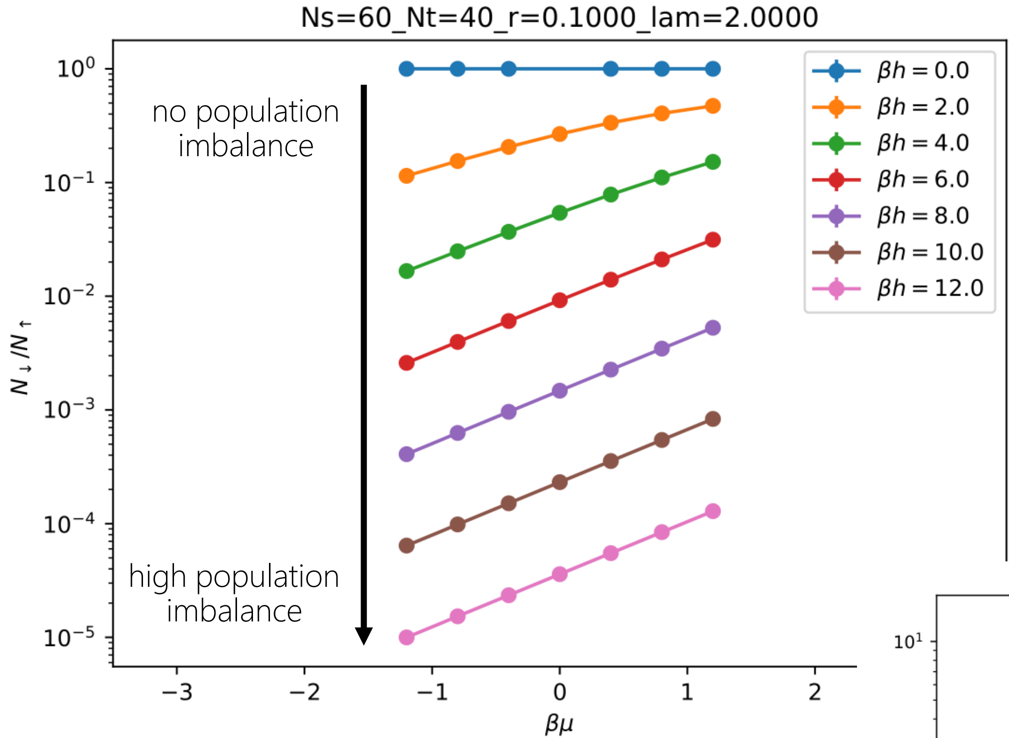
Rammelmüller, Drut, Braun
SciPost Phys. 9, 014 (2020)

Pseudogap



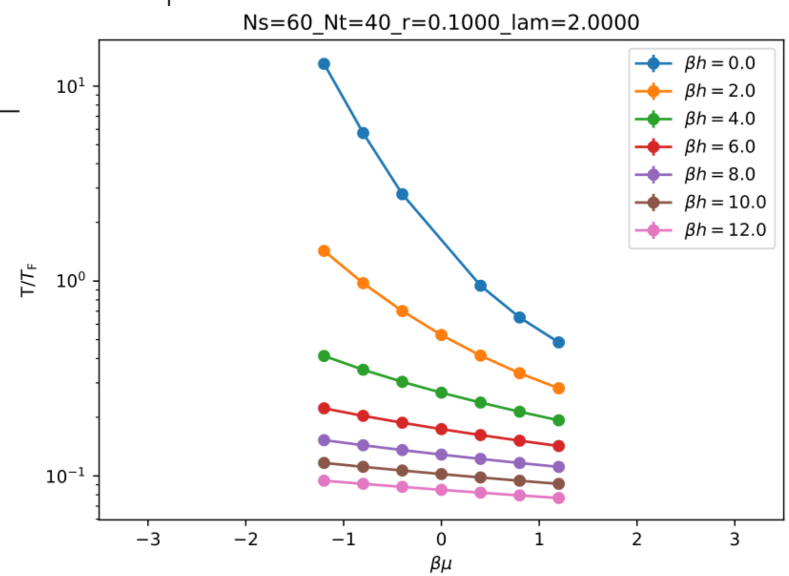
Tajima, ST, Doi, Phys. Rev. Research 2, 033441 (2020)

Complex Lanegvin simulation



Complex Langevin works for highly imbalanced cases

Cf) reliability of complex Langevin at βh=2.0 is reported by Alexandru, Badaque Warrington, Phys. Rev. D 98, 054514 (2018)



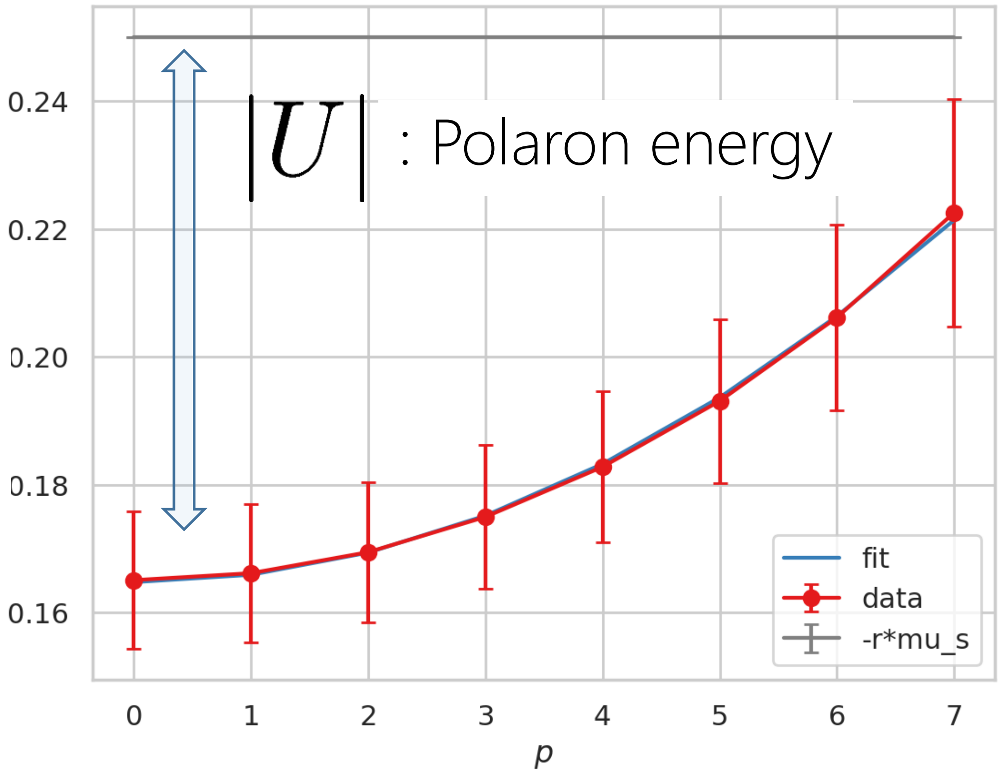
high population imbalance =

low temperature ($T/T_F < 1$)

Dispersion relation of polaron

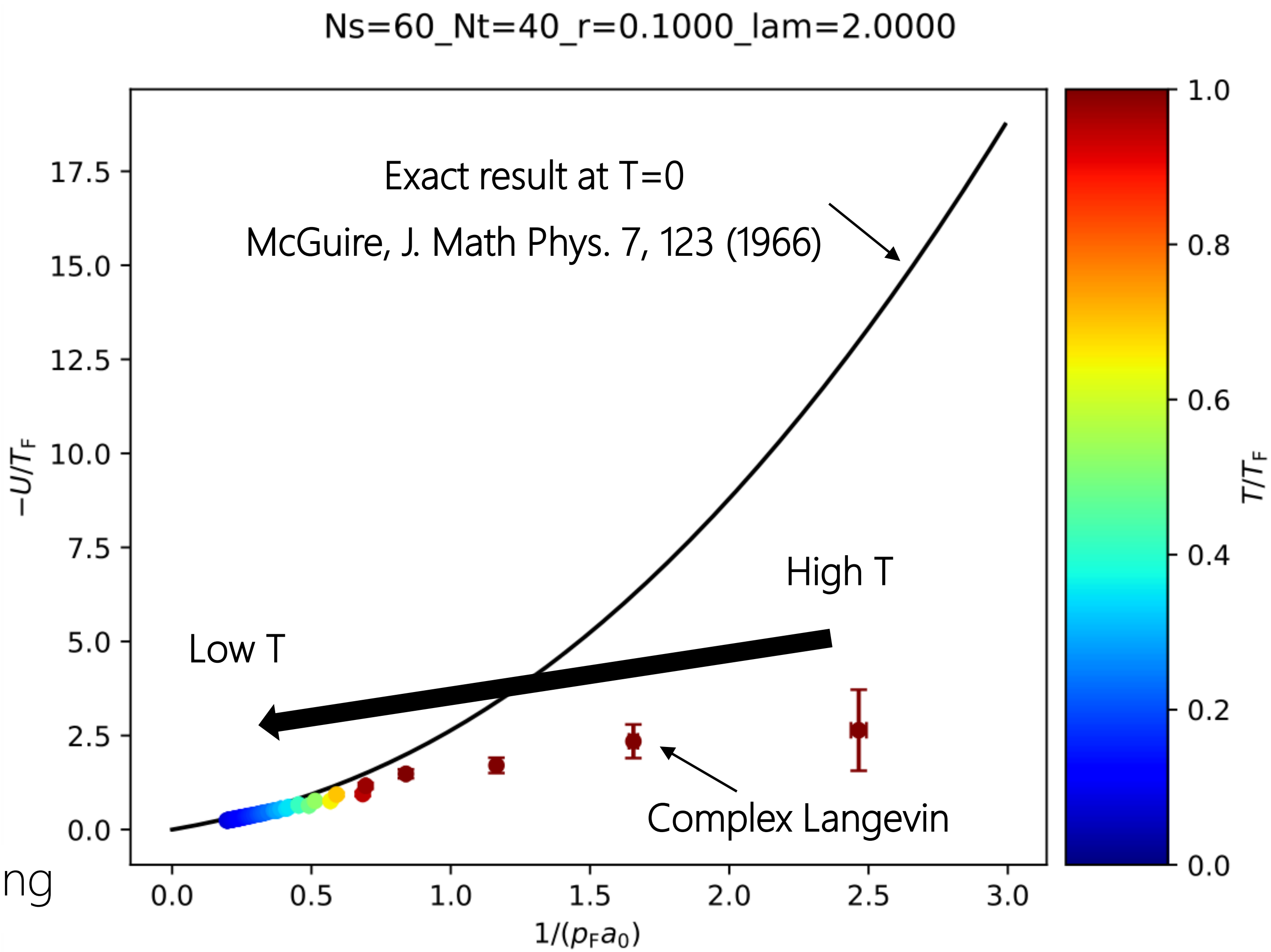
$$G(\tau) = \frac{1}{Z}\mathrm{Tr}\left[e^{-\beta(H-\sum_\sigma \mu_\sigma N_\sigma)}\psi_\downarrow^\dagger(\tau)\psi_\downarrow(0)\right] \sim A_0 e^{-\tau E}$$

$E(p)$



Fitting function: $$E(p) = \frac{p^2}{2} + U - r\mu_\downarrow$$

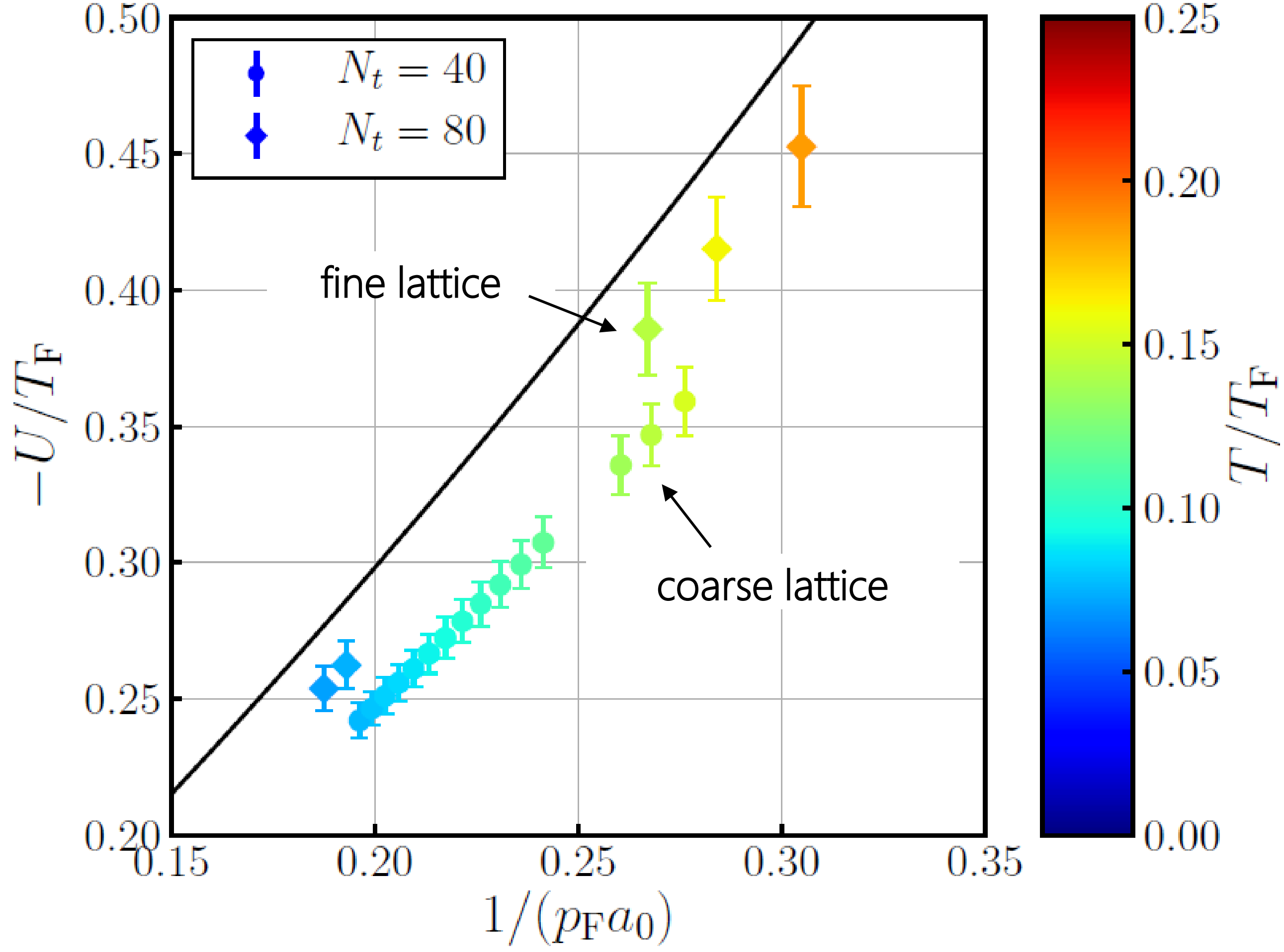
Temperature dependence of U



a_0 : scattering length

Complex Langevin results approach to the exact result as T→0

Taking continuum limit ($N_t \to \infty$)



Complex Langevin results approach to the exact result as $N_t \to \infty$

Summary

◆ What is the sign problem ?

- Exponentially small signal-to-noise ratio in Monte Carlo simulations

◆ Sign problem in cold Fermi gas

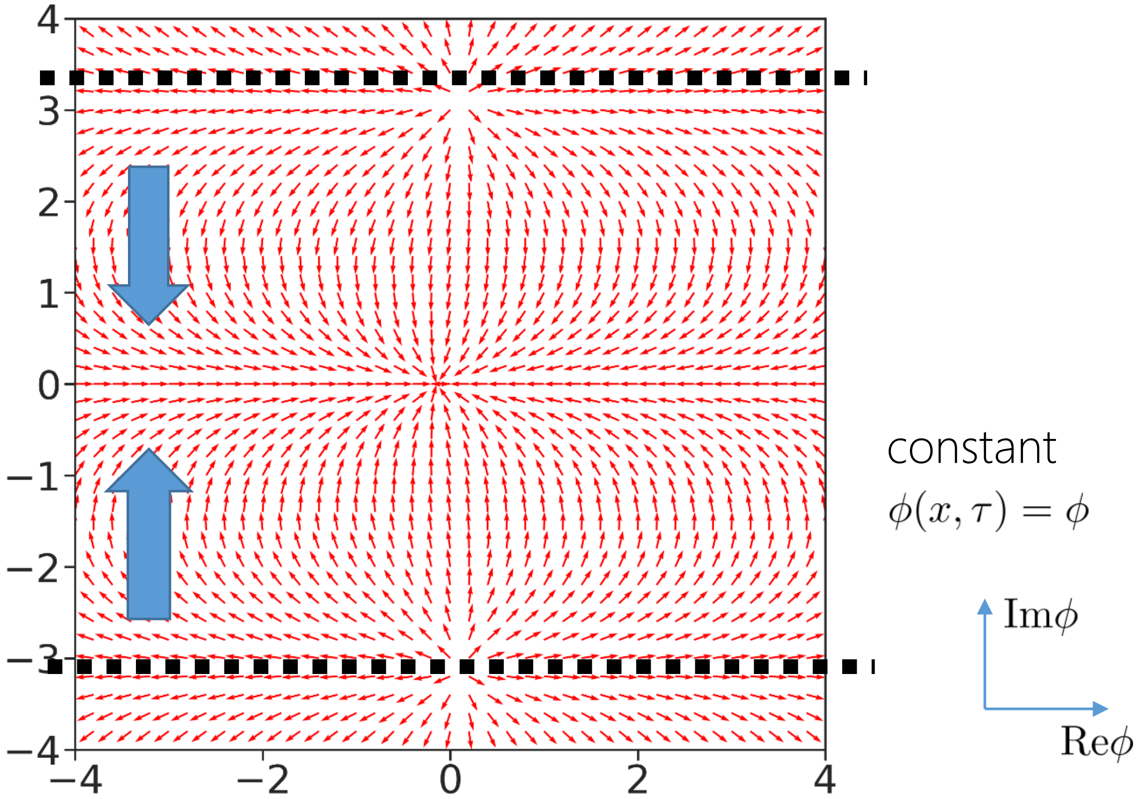
- Non positive definite fermion determinant causes the sign problem

◆ Complex Langevin (theory and application)

- In our setup (1D, attractive, $\beta h \neq 0$), complex Langevin is reliable
- We calculate temperature dependence of polaron energy
- Consistent with exact result at T=0

Appendix

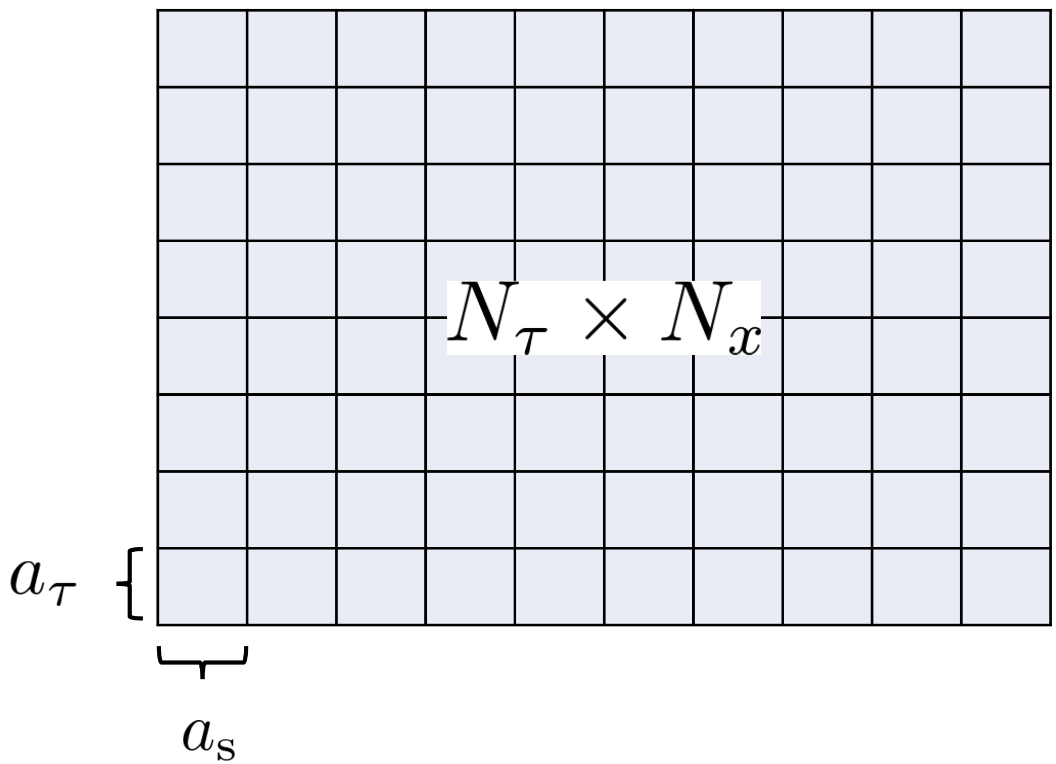
Flow of the drift term



Application

Our setup:

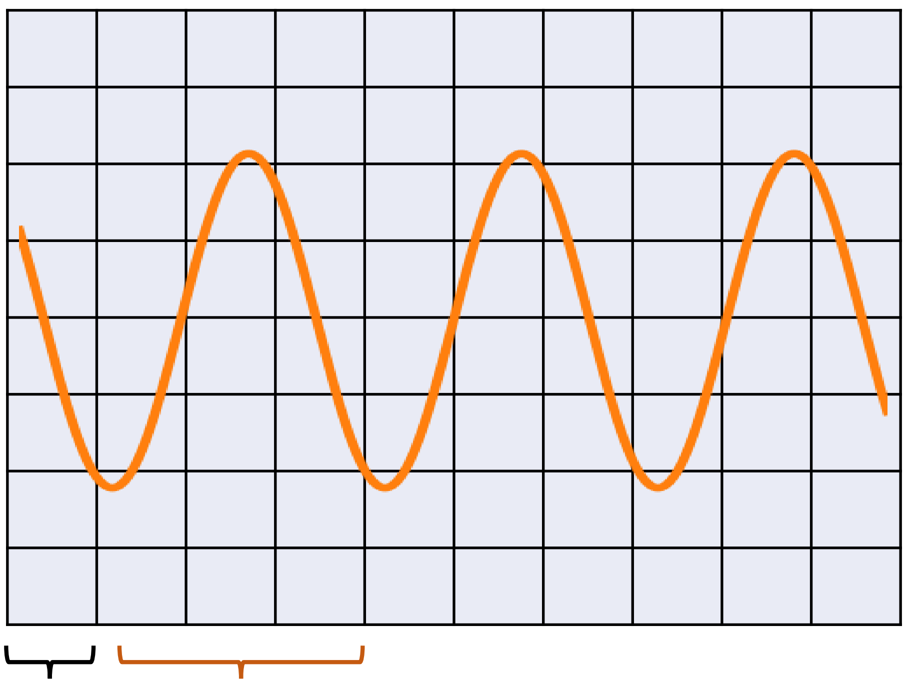
- Two-component Fermion ($\sigma = \uparrow, \downarrow$)
- Attractive contact interaction ($g > 0$)
- 1D
- Lattice regularization



Application

Our setup:

- Two-component Fermion ($\sigma = \uparrow, \downarrow$)
- Attractive contact interaction ($g > 0$)
- 1D
- Lattice regularization

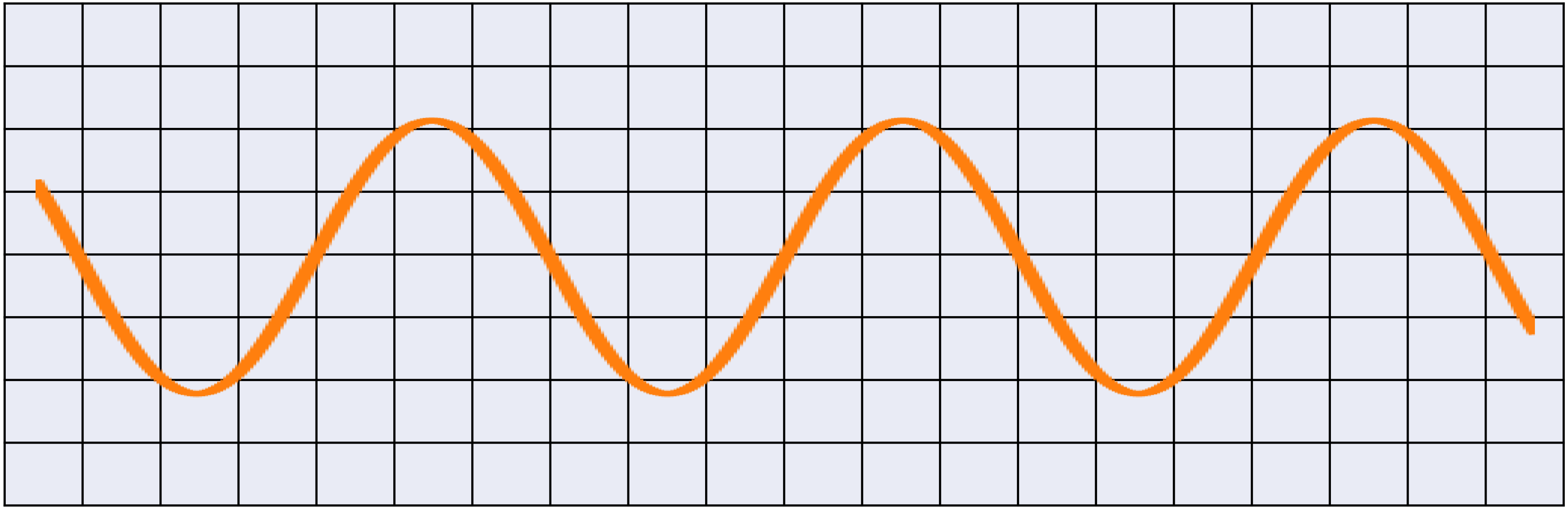


$a_\mathrm{s} \ll \lambda_T = \sqrt{2\pi\beta}$ (thermal de Broglie length)

Application

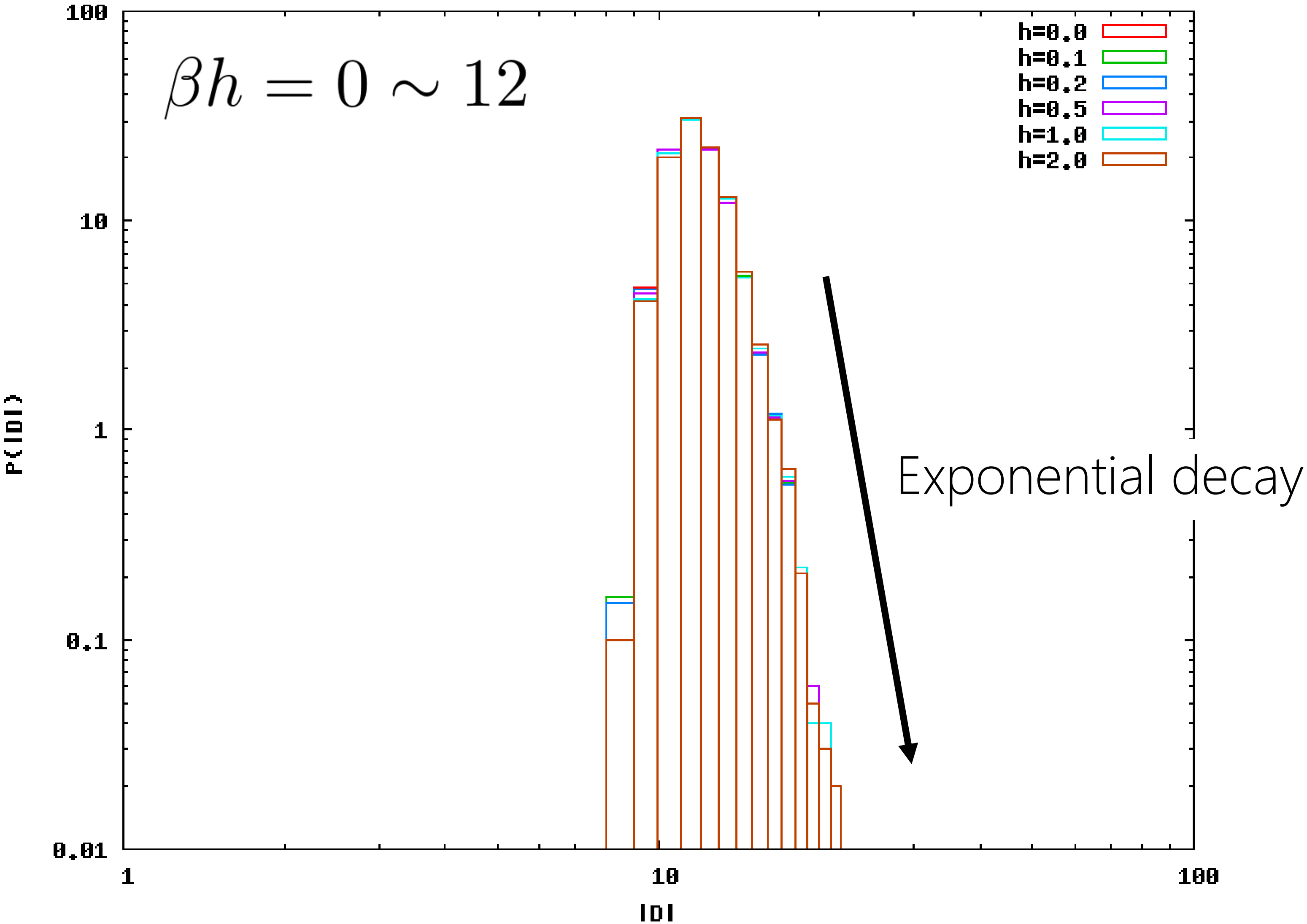
Our setup:

- Two-component Fermion ($\sigma = \uparrow, \downarrow$)
- Attractive contact interaction ($g > 0$)
- 1D
- Lattice regularization



Continuum limit: $a_\mathrm{s} \ll \lambda_T = \sqrt{2\pi\beta} \to \infty$

Complex Langevin works !



$N_x = 60, N_\tau = 40, r = 0.2, \beta\mu = 2, \lambda = 2$

Extracting the polaron energy

$$
\begin{aligned}
G(\tau) &= \langle 0|\psi_\downarrow(\tau)\psi_\downarrow{}^\dagger(0)|0\rangle \\
&= \langle 0|\mathrm{e}^{\hat{H}\tau}\psi_\downarrow(0)\mathrm{e}^{-\hat{H}\tau}\psi_\downarrow{}^\dagger(0)|0\rangle \\
&= \langle 0|\psi_\downarrow(0)\mathrm{e}^{-\hat{H}\tau}\psi_\downarrow{}^\dagger(0)|0\rangle \\
&= \sum_n \langle 0|\psi_\downarrow(0)\mathrm{e}^{-\hat{H}\tau}|n\rangle\langle n|\psi_\downarrow{}^\dagger(0)|0\rangle \\
&= \sum_n A_n \mathrm{e}^{-E_n\tau} \\
&\to A_0\mathrm{e}^{-E_0\tau}
\end{aligned}
$$