Circumventing the sign problem with complex Langevin in lattice field theory

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Fermilab Theory Seminar

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Outline

- Rotating Superfluids
- The sign problem in quantum many-body systems
- The Complex Langevin (CL) method
- Progress on rotating bosonic systems
  - Virial coefficients can shed some light
  - Using high performance computing tools
- Where do we go from here?

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PSA

My work focuses on bosons, but let's all be good fermions for the time being…

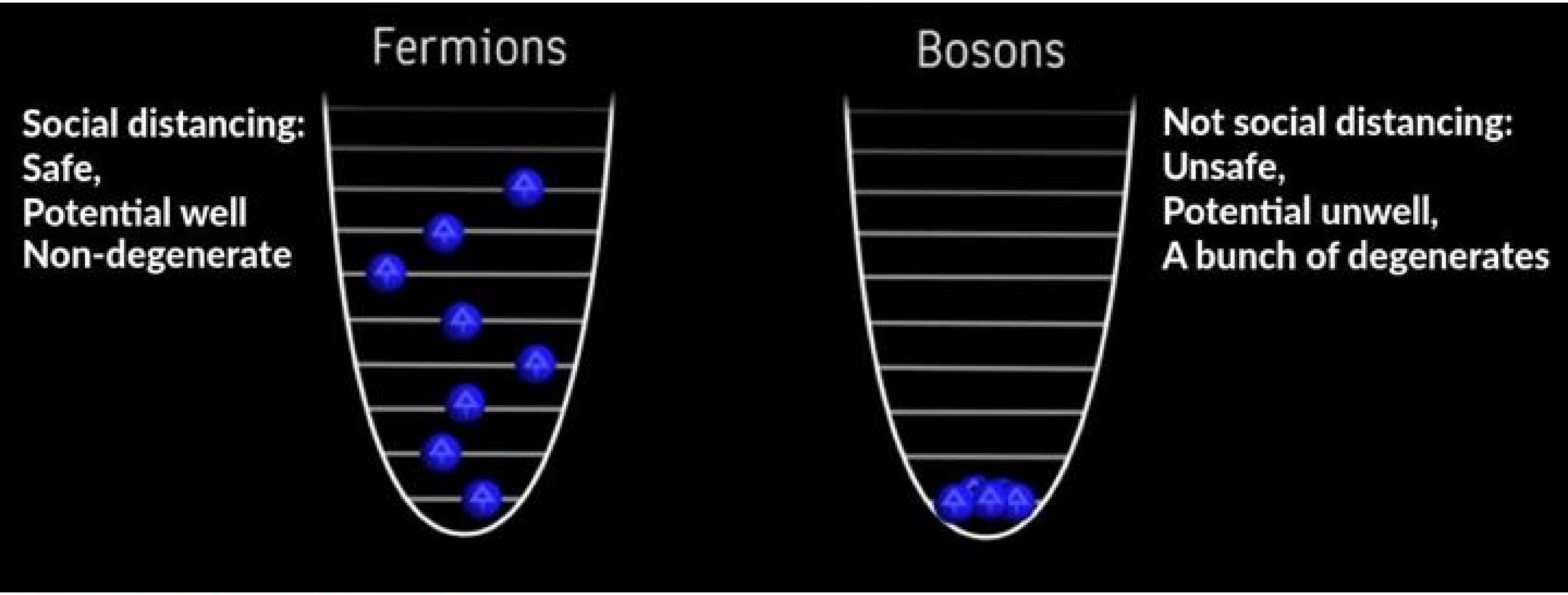


Photo credit: Shawn Westerdale

Superfluids

- Superfluids
  - Fluids which flow without friction
    - No loss of kinetic energy
  - Macroscopic quantum phenomenon like superconductivity
  - In nature:
    - Helium-4 and Helium-3
    - Neutron stars
  - In experiment:
    - Ultracold atoms

- Frictionless velocity flow leads to lots of interesting behavior

Rotating Superfluids

- Adding rotation to superfluids
  - Superfluids have irrotational velocity field (related to lack of friction)

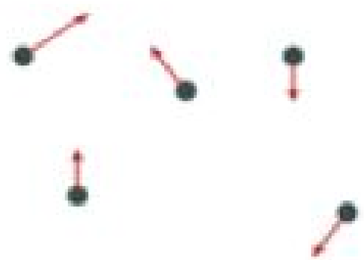
$$\vec{v}_s = \frac{\hbar}{m}\vec{\nabla}\phi$$
$$\vec{\nabla}\times\vec{v}_s = \frac{\hbar}{m}\vec{\nabla}\times\vec{\nabla}\phi$$

  - Rotation induces localized singularities (vortices) to sustain angular momentum
  - Angular momentum exists at the boundaries of the vortices
  - Circulation around a vortex is quantized

$$\oint_C \vec{v}_s \cdot d\vec{l} = \frac{\hbar}{m}(2\pi n)$$

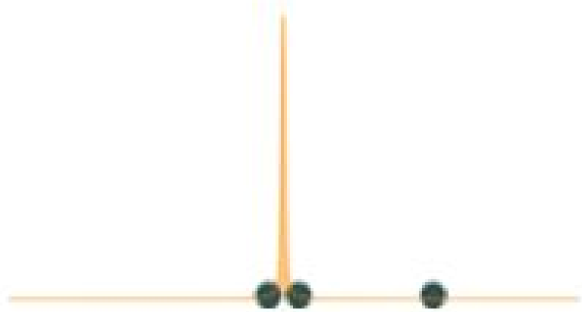
Rotating Superfluids

- What makes a rotating superfluid?

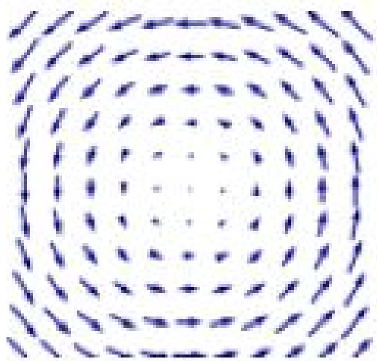


Non-relativistic dispersion

Trapped in a harmonic well



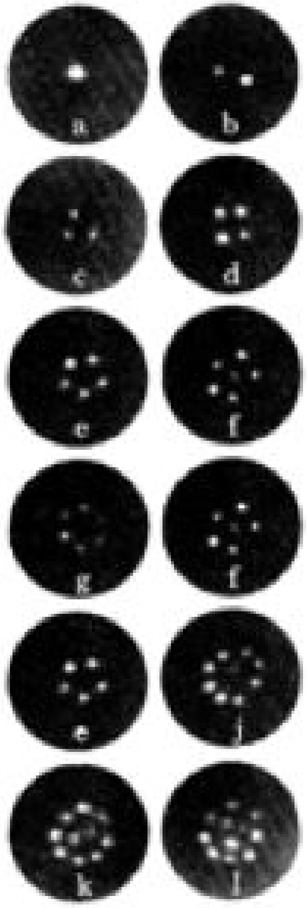
Interacting at short range

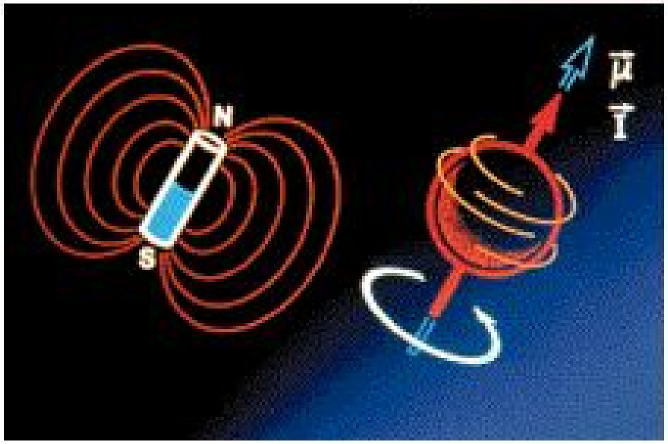


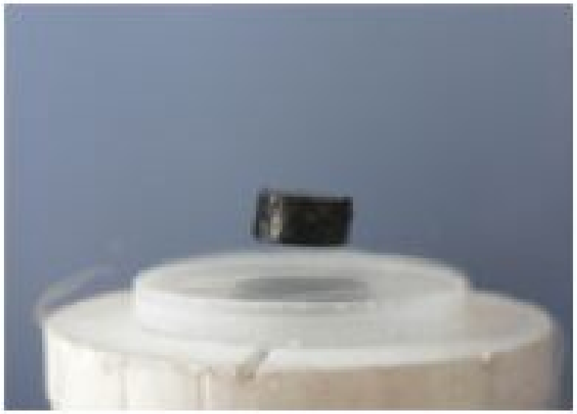
Rotating

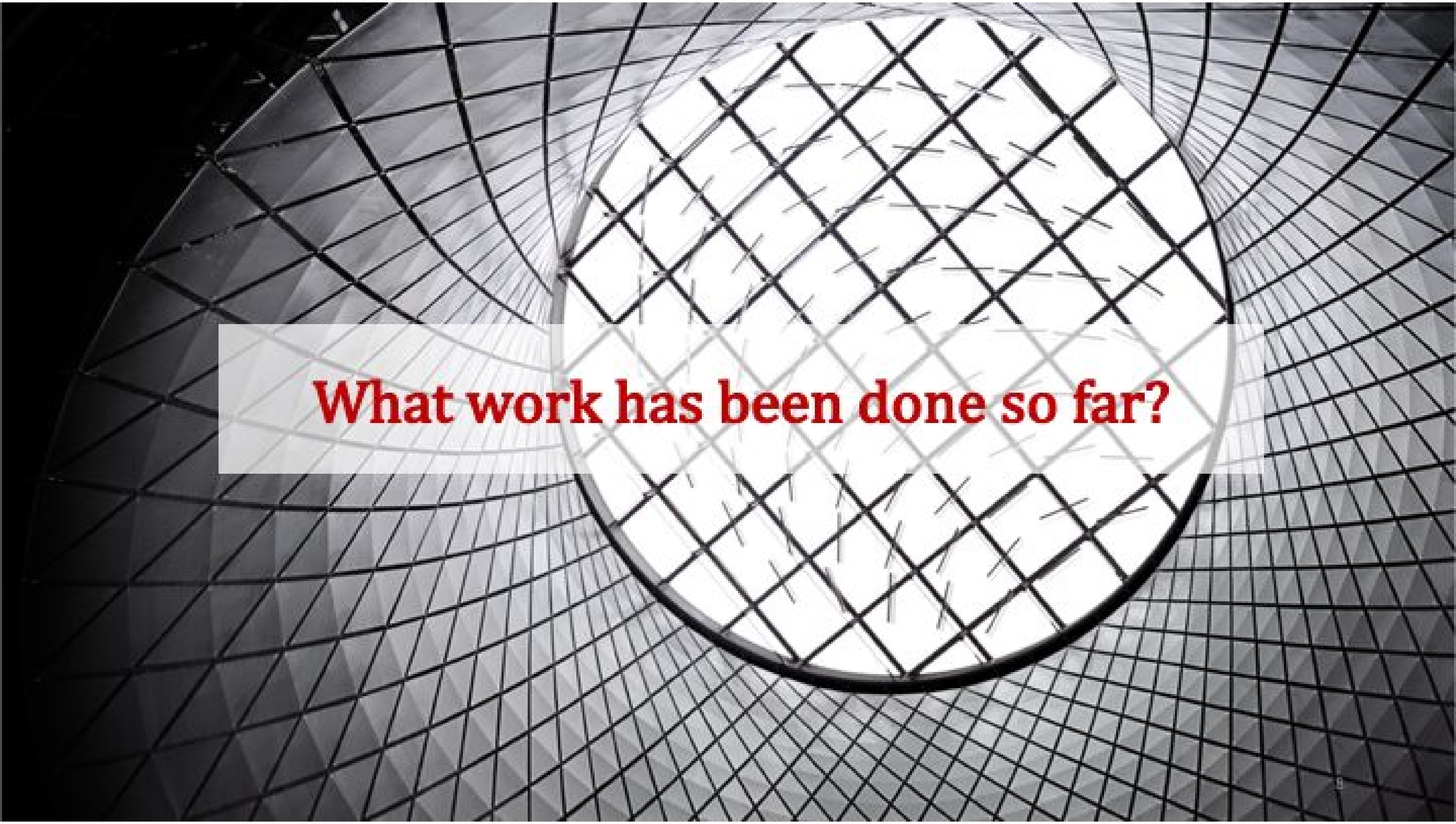
Rotating Superfluids

- Relevant physical systems
  - Superconductor in a magnetic field
  - Pulsars
  - Rotating nuclei
  - Rotating superfluid
  - Rotating dilute atomic gas





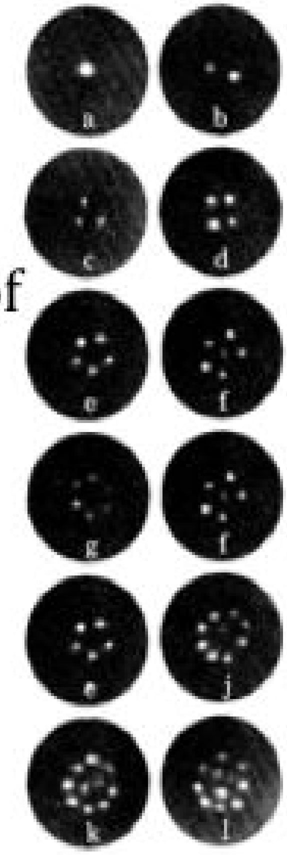



What work has been done so far?

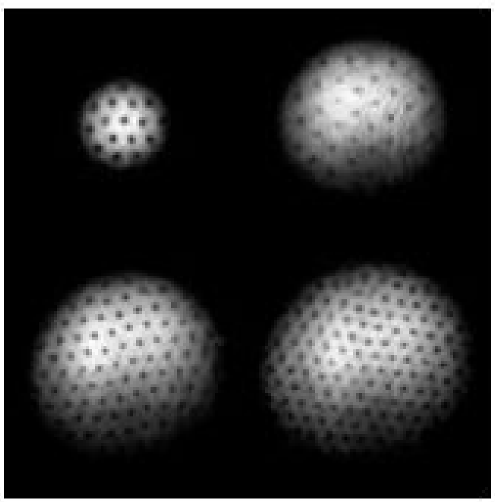
Rotating Superfluids

1949: Onsager predicts rotating superfluids will form vortices

1979: First observation of vortices in rotating ^4He



Phys. Rev. Lett. **4** 14 (1979)

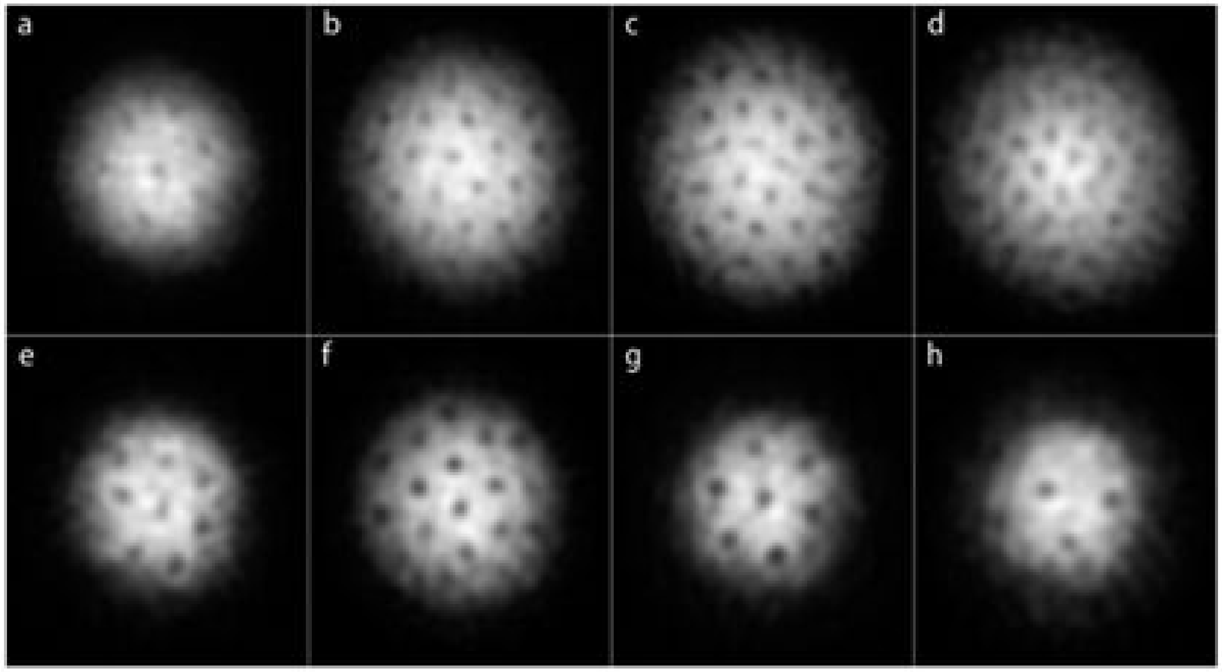


Science **292** 5516 (2001)

1990s-2000s: rotating BECs in ^4He and dilute atomic gases

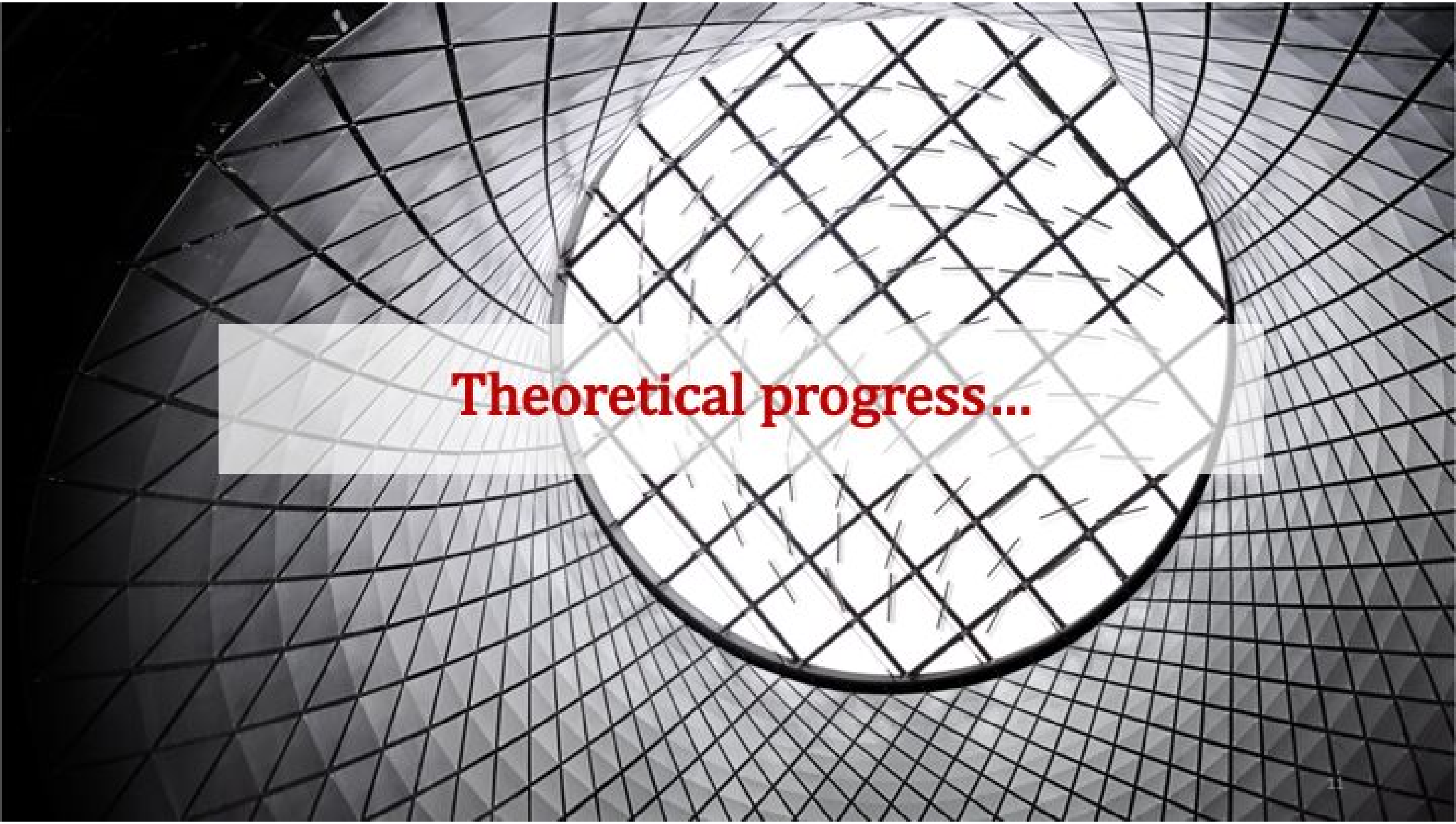
Rotating Superfluids

- This behavior has also been seen in fermions
- Cooper pairing leads to superfluidity and vortex formation under rotation



- Fundamentally bosonic behavior

Nature **435**, 1047-1051 (2005)



Theoretical progress…

Theoretical Progress

- Theoretical progress has stalled
- Many-body quantum systems → Quantum Monte Carlo (QMC)
- Path-integral formulation for QM allows us to compute observables

$$\mathcal{Z} = \int \mathcal{D}\phi e^{-S[\phi]}$$

- S encodes the dynamics of the system

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi e^{-S[\phi]} \mathcal{O}[\phi] = \int \mathcal{D}\phi \mathcal{P}[\phi] \mathcal{O}[\phi]$$

- QMC lets us evaluate stochastically, with $\mathcal{P}[\phi] = \frac{1}{\mathcal{Z}} e^{-S[\phi]}$

Quantum Monte Carlo (QMC)

- Simple action:

$$S[\phi] = a\phi^2$$

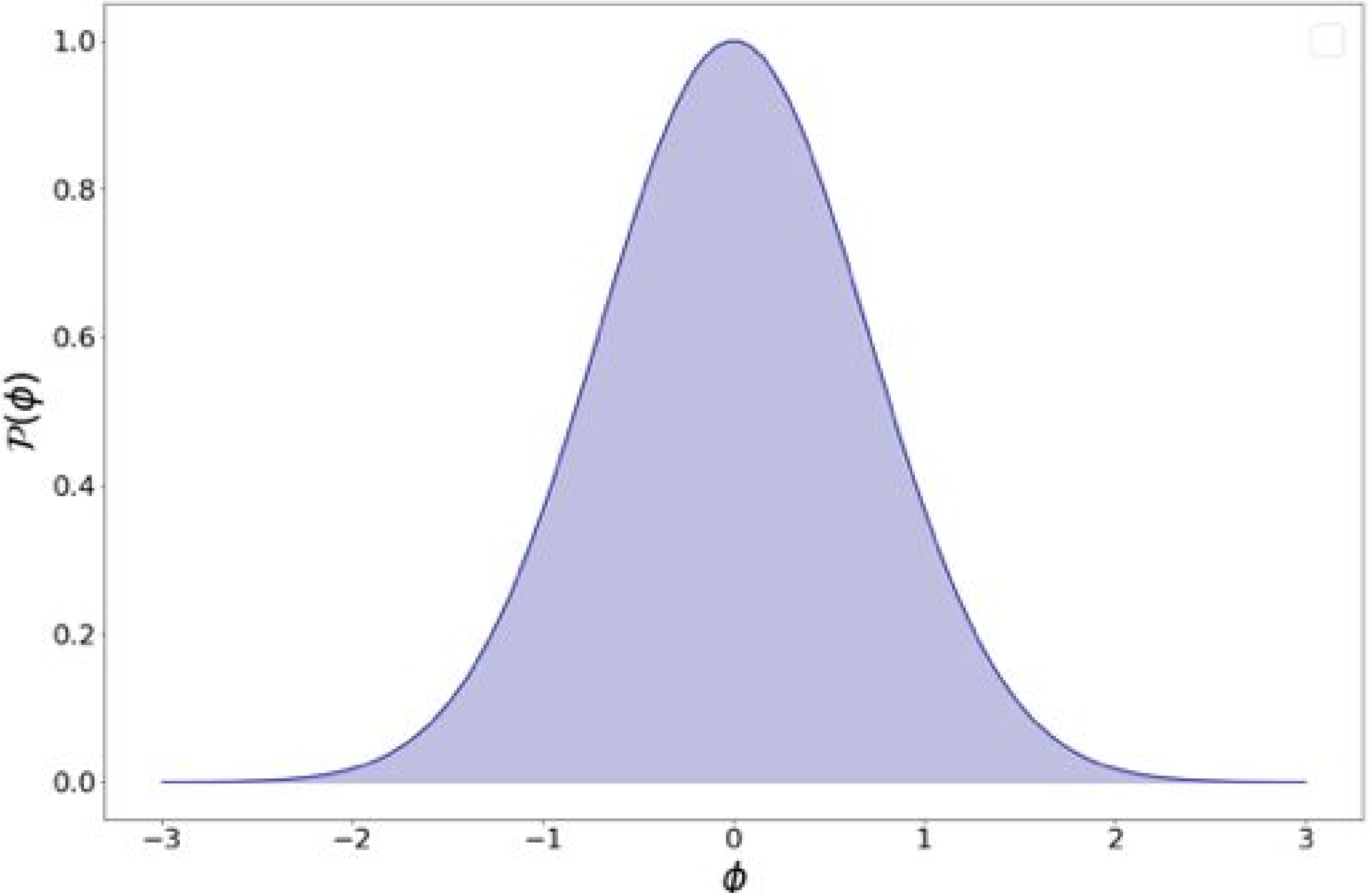
- Probability distribution:

$$\mathcal{P}[\phi] = \frac{1}{\mathcal{Z}} e^{-a\phi^2}$$

- Calculating an observable:

$$\begin{aligned} \mathcal{O}[\phi] &= a\phi^2 \\ \langle \mathcal{O} \rangle &= \sum \mathcal{O}[\phi]\mathcal{P}[\phi] \end{aligned}$$

Quantum Monte Carlo



The Sign Problem

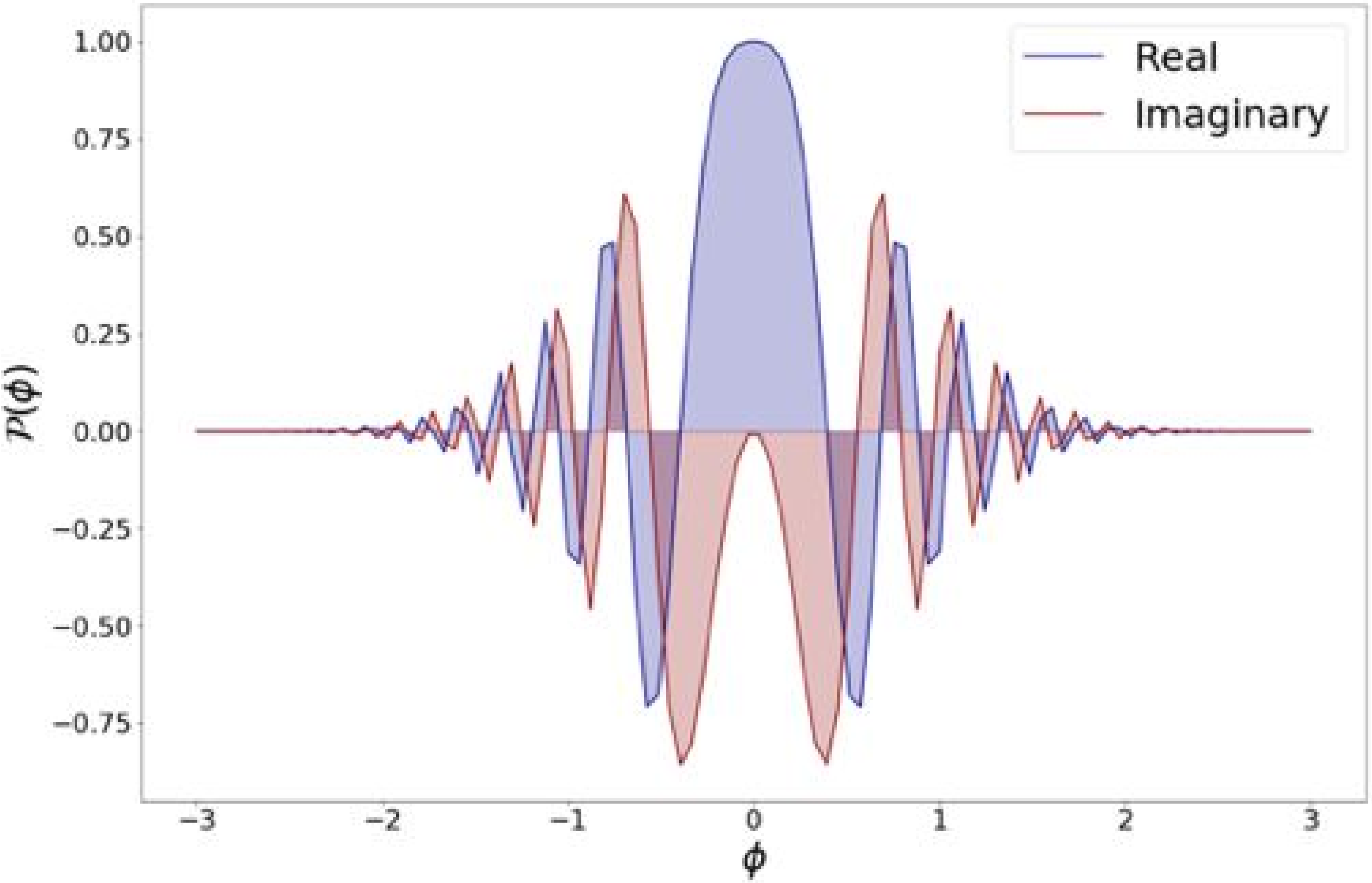
- Problem:
  what if our probability distribution is not well-defined?

- Simple example: $S[\phi] = a\phi^2 + ib\phi^2$

- Probability distribution:

$$\begin{aligned}\mathcal{P}[\phi] &= \frac{1}{\mathcal{Z}} e^{-a\phi^2 - ib\phi^2} \\ &= \frac{1}{\mathcal{Z}} \left(e^{-a\phi^2} (\cos b\phi^2 + i \sin b\phi^2) \right)\end{aligned}$$

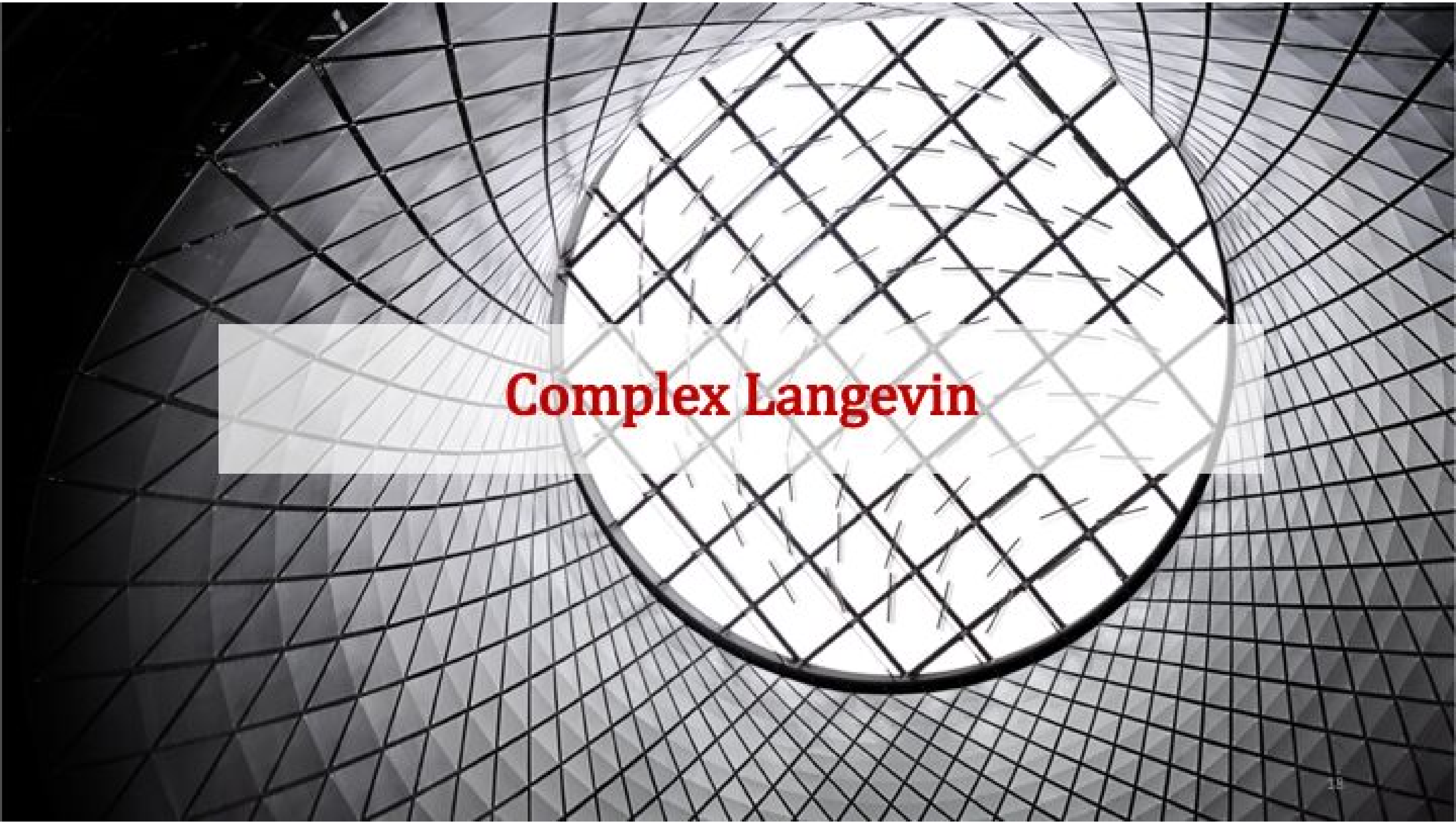
The Sign Problem



QMC: Limitations

- Certain systems are not accessible with standard QMC
- Problems arise when the action can be complex – the "sign problem"
  - Condensed matter (the Hubbard Model)
  - Nuclear physics (ab initio nuclear calculations)
  - Astrophysics (neutron stars)
  - QCD (quark matter)
  - Ultracold Atomic Gases
- The sign problem is NP-hard!
  - No *generic* polynomial-time solution expected to exist
  - Need to work *around* it

Complex Langevin



The Langevin method

- Goal: compute observables

$$\langle \mathcal{O} \rangle = \int \mathcal{D}\phi \mathcal{P}[\phi]\mathcal{O}[\phi]$$

- The Langevin equation evolves the fields in "fictitious" time

$$d\phi = -S'[\phi]dt_L + dW(t_L)$$

- Obeys the Fokker-Planck equation

$$\frac{d\mathcal{P}(\phi;t_L)}{dt_L} = \left(\partial_\phi^2 S[\phi] + \partial_\phi^2\right)\mathcal{P}(\phi;t_L)$$

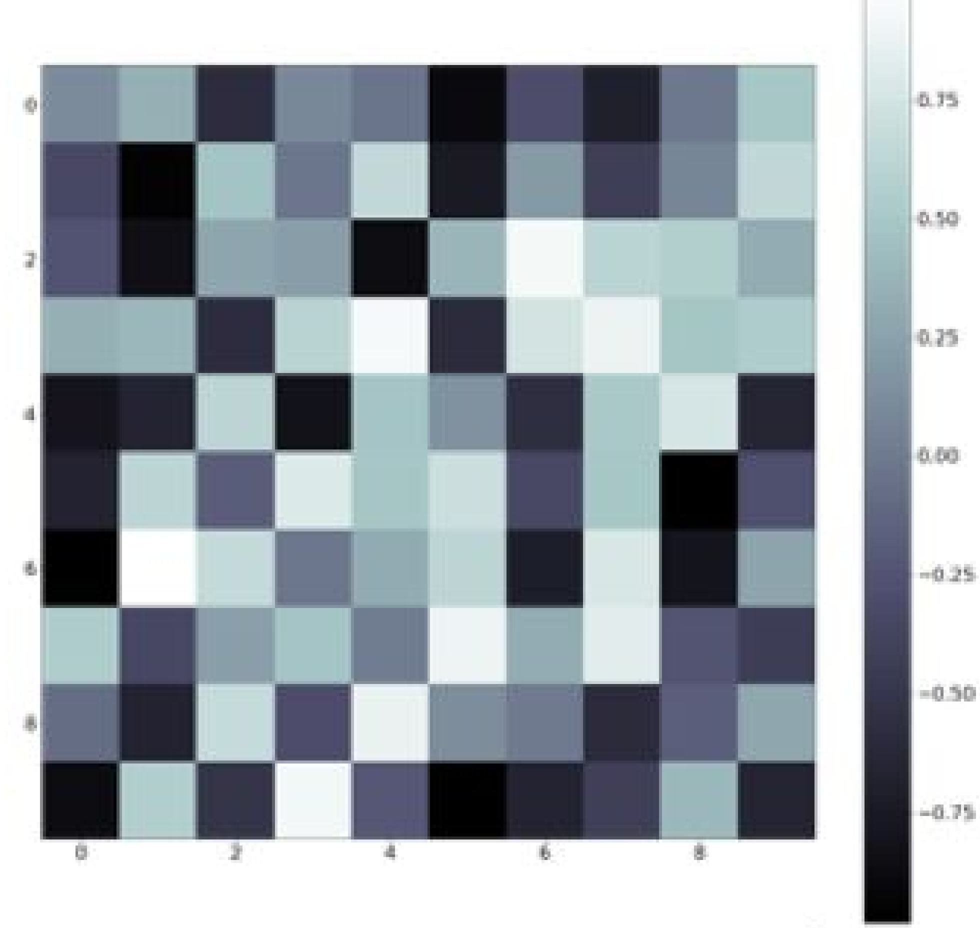
- Long time evolution produces sets of solutions distributed as e^{-S}

$$\langle \mathcal{O}[\phi] \rangle \approx \frac{1}{T}\int_{t_{th}}^{t_{th}+T} d\tau \mathcal{O}[\phi_\tau]$$

Where does our lattice come in?

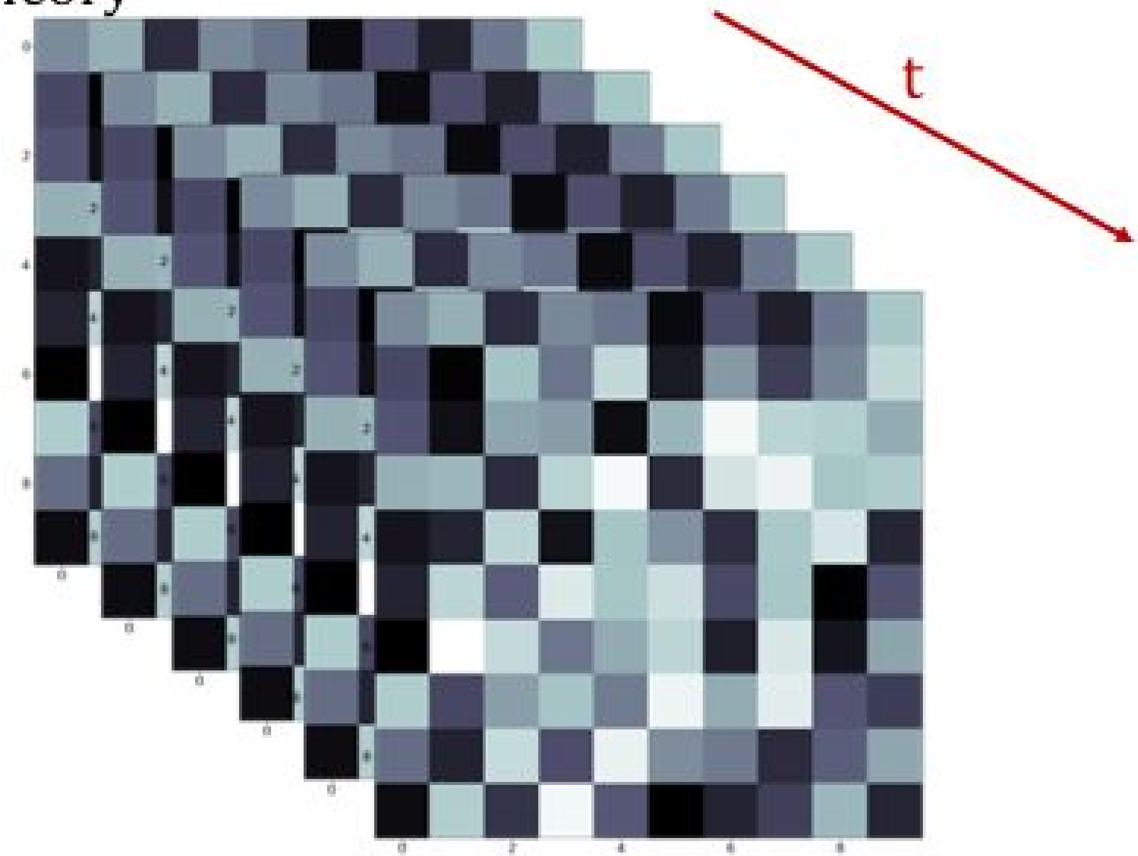
Putting the problem in discrete space

- Represent space and time as a finite lattice



Putting the problem in discrete space

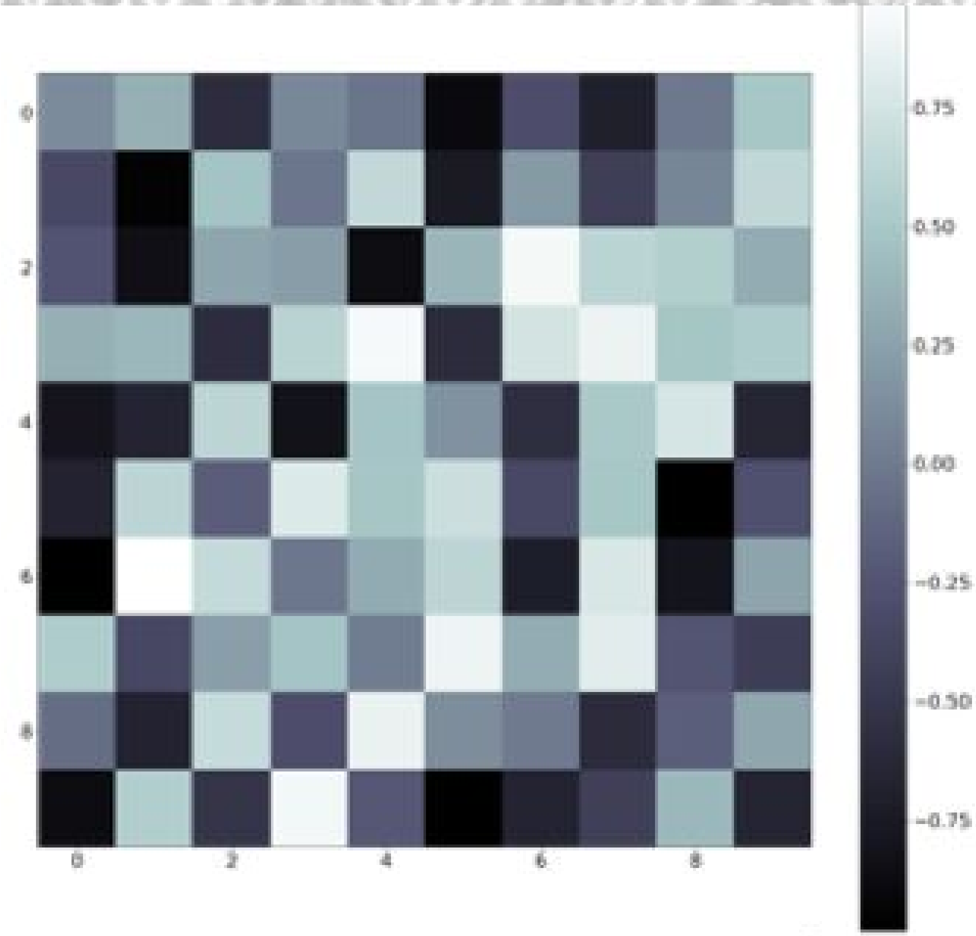
- Time and temperature are inversely related in nonrelativistic lattice field theory



$$t \sim \beta \sim 1/T$$

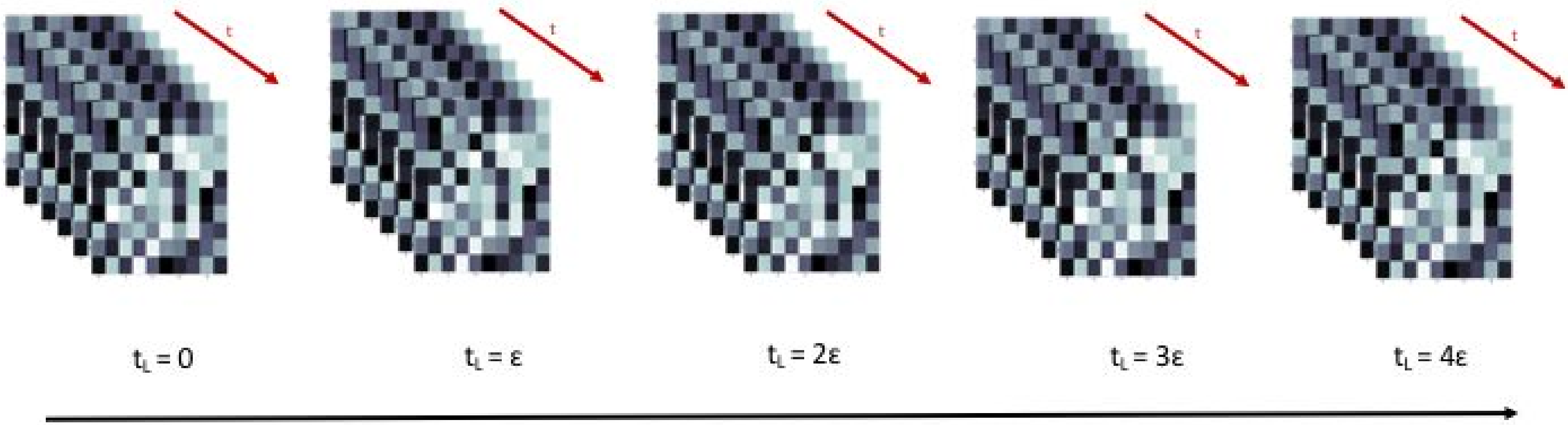
Putting the problem in discrete space

- Represent space and time as a finite lattice
- Evolve the fields at each spacetime site on the lattice
  - Using discrete steps in fictitious (Langevin) time



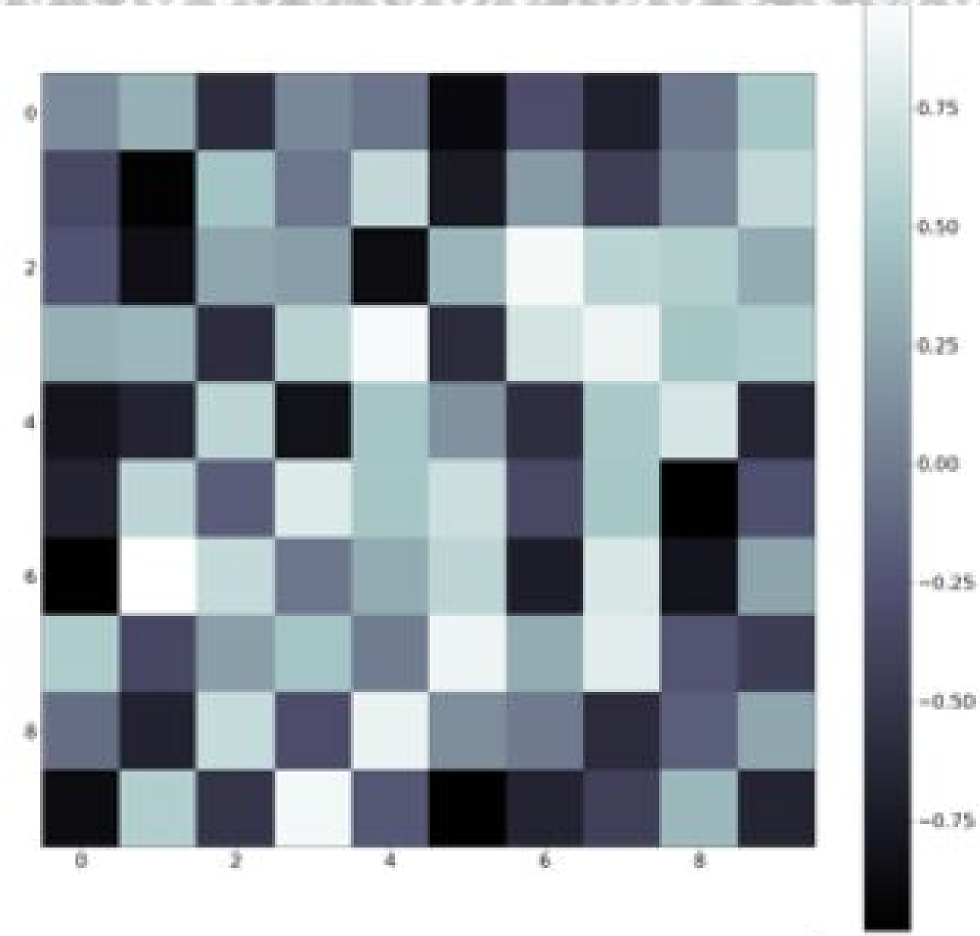
Putting the problem in discrete space

The entire spacetime lattice is updated at each point in Langevin time



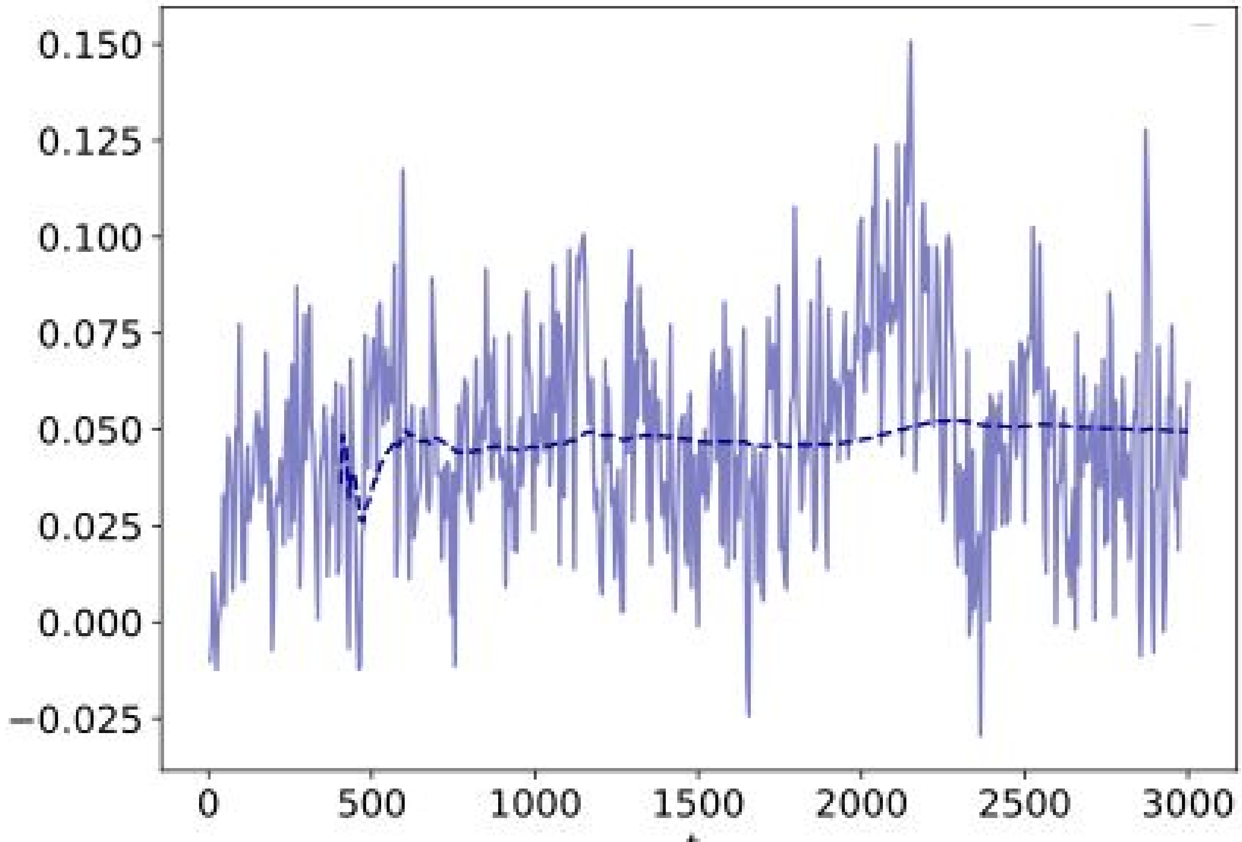
Putting the problem in discrete space

- Represent space and time as a finite lattice
- Evolve the fields at each spacetime site on the lattice
  - Using discrete steps in fictitious (Langevin) time
- Calculate observables from field values at each step
- Repeat until we have taken many samples (long time evolution)



Langevin evolution

- Long Langevin evolution of the fields



What happens when we have complex numbers?

Complex Langevin

- Complex Langevin extends this to a complex field

$$\phi(x) \rightarrow \phi^R(x) + i\phi^I(x)$$

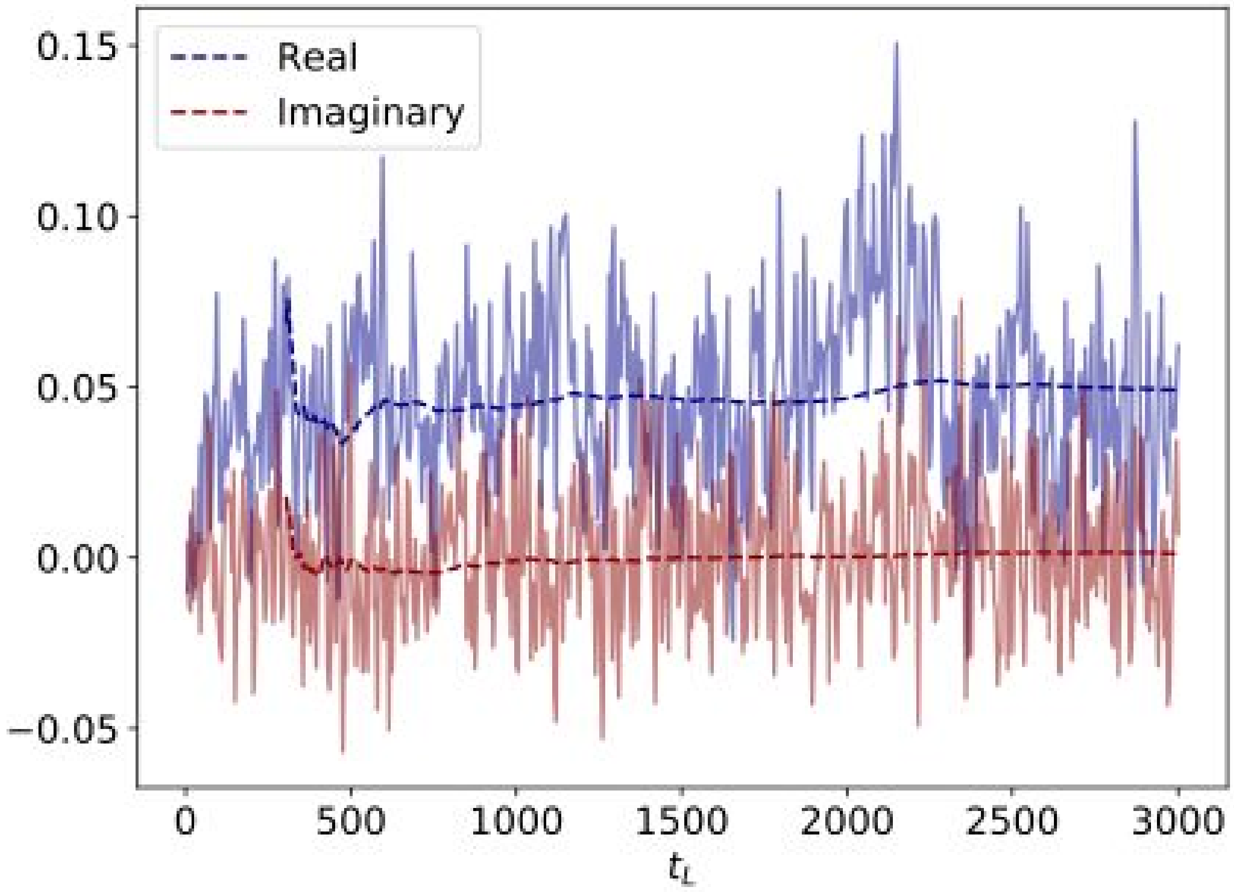
$$S[\phi(x)] \rightarrow S[\phi^R(x) + i\phi^I(x)] = \mathrm{Re}[S] + i\mathrm{Im}[S]$$

- Leading to a set of coupled stochastic differential equations

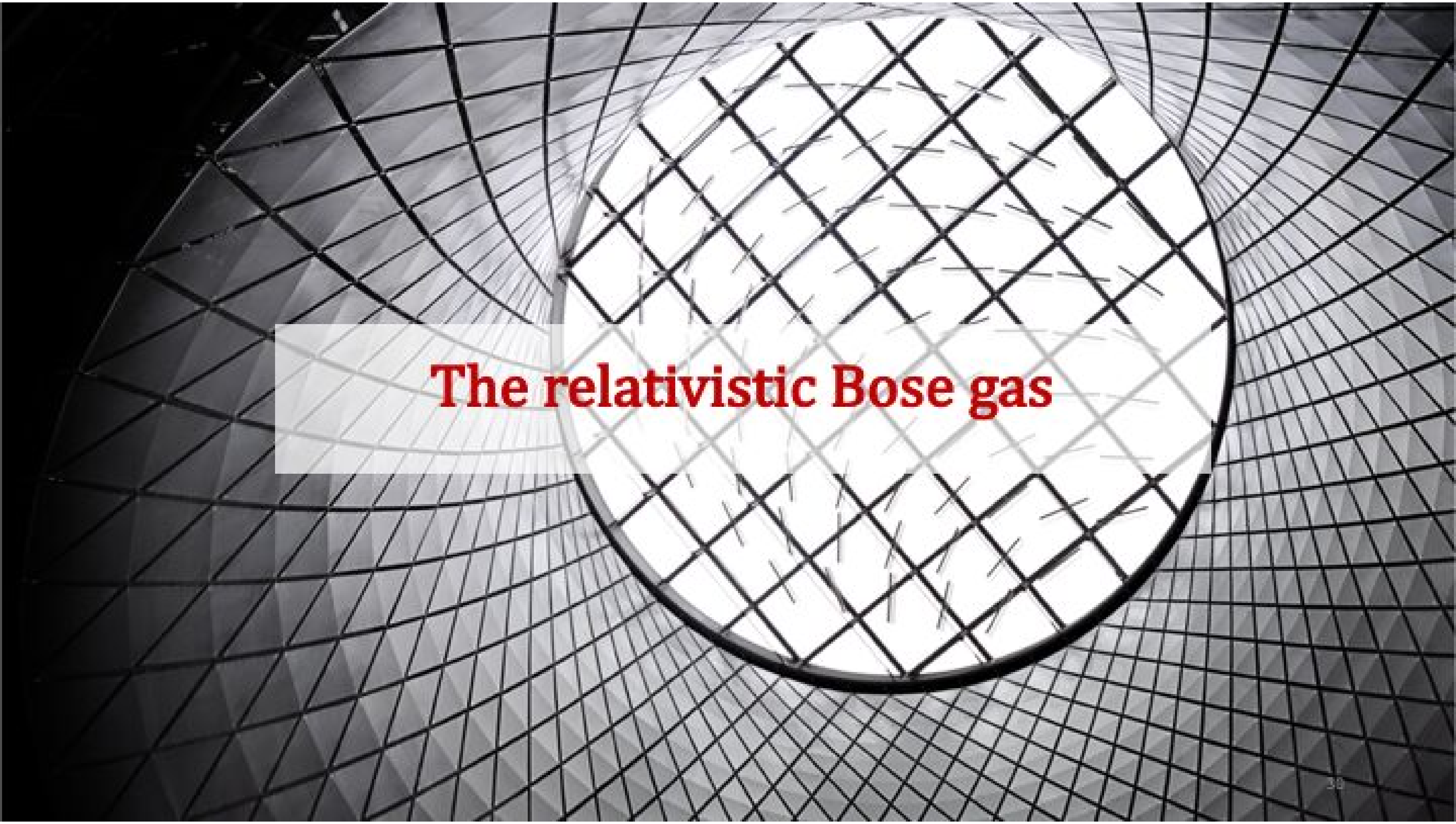
$$\begin{aligned} d\phi^R(x) &= K^R dt_L + \eta(t_L) \\ K^R &= -\mathrm{Re}\left[\frac{\delta S[\phi]}{\delta\phi}\right] \\ d\phi^I(x) &= K^I dt_L \\ K^I &= -\mathrm{Im}\left[\frac{\delta S[\phi]}{\delta\phi}\right] \end{aligned}$$

Complex Langevin evolution

- We do the same long-time evolution for both fields



The relativistic Bose gas



The relativistic Bose gas: action

- Action for the relativistic Bose gas

$$S = \int d^4x \left(|\partial_\nu \phi|^2 + (m^2 - \mu^2)|\phi|^2 + \mu(\phi^* \partial_4 \phi - \partial_4 \phi^* \phi) + \lambda |\phi|^4 \right)$$

- This suffers from a sign problem when $\mu > 0$

$$S^*(\mu) = S(-\mu)$$

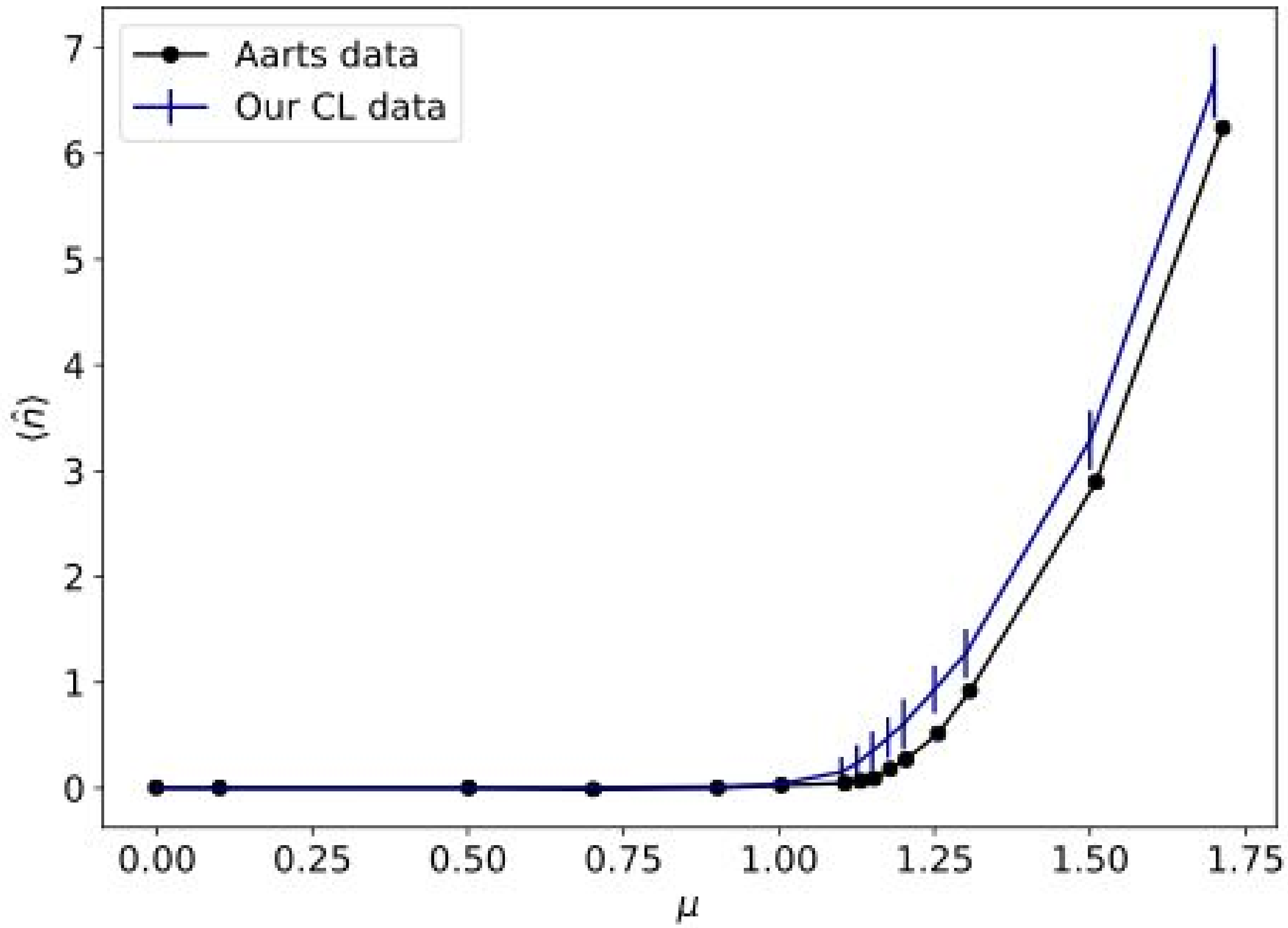
- Discretized action to use CL on the lattice:

$$\begin{aligned} S \;\; = \;\; \sum_x \Bigg(& \sum_{\nu=1}^{4} (m^2 + 2)\phi_x^* \phi_x + \lambda (\phi_x^* \phi_x)^2 \\ & - \sum_{\nu=1}^{4} (\phi_x^* e^{-\mu \delta_{\nu,4}} \phi_{x+\nu} + \phi_{x+\nu}^* e^{\mu \delta_{\nu,4}} \phi_x) \Bigg) \end{aligned}$$

The relativistic Bose gas: results

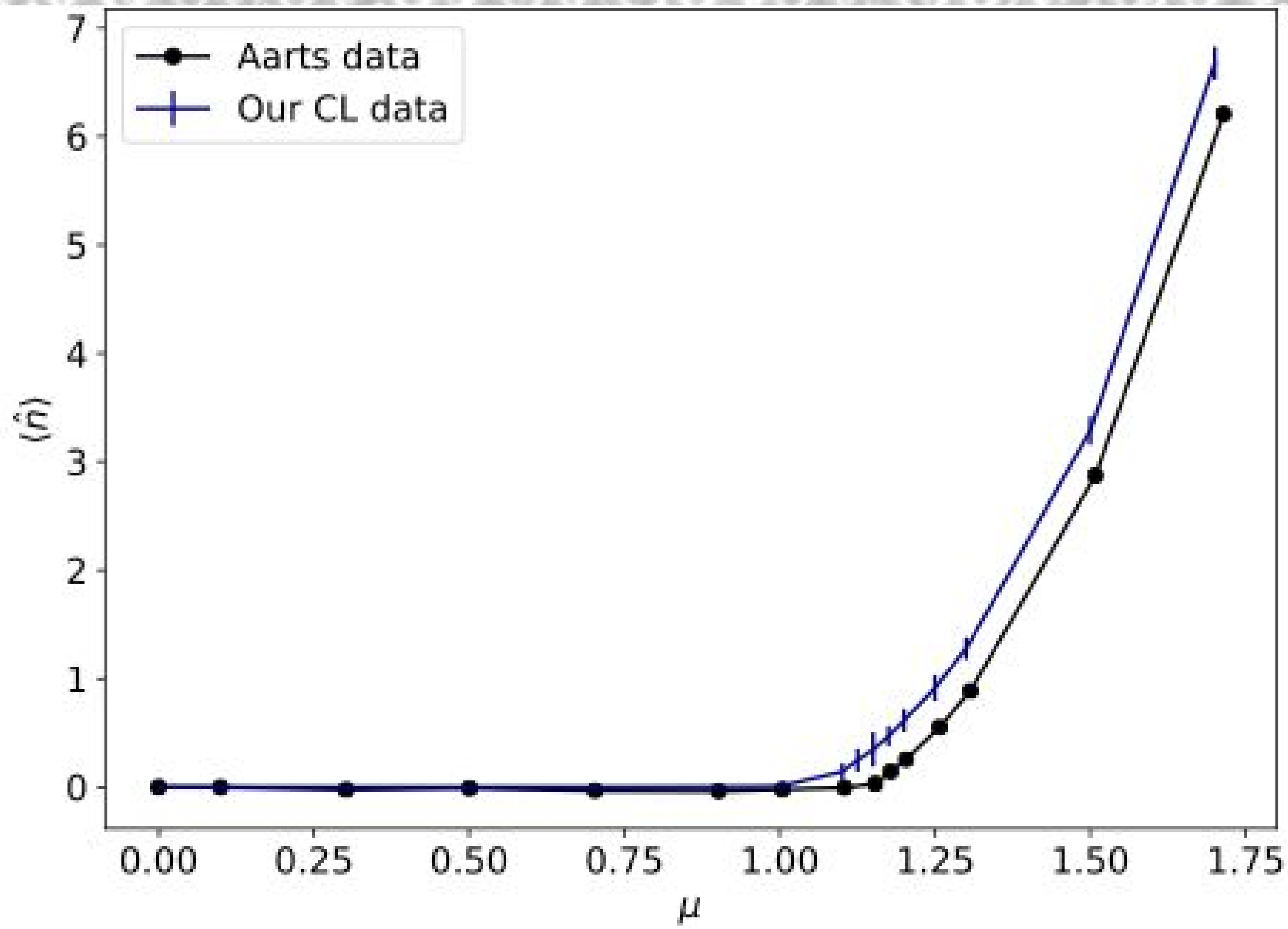
- Density
- $N_x = N_t = 4$

Phys. Rev. Lett. **102**, 131601 (2009)

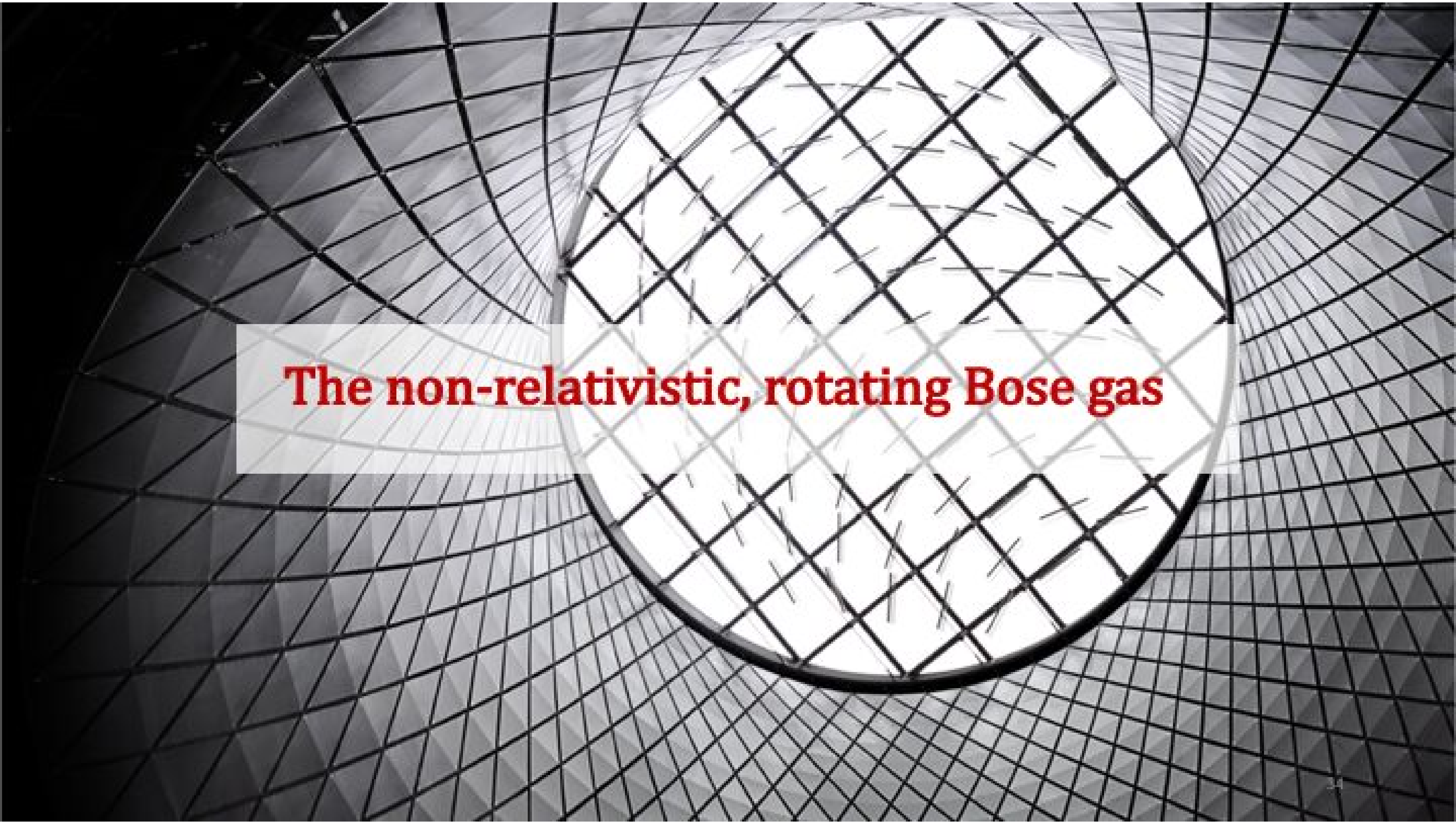


The relativistic Bose gas: results

- Density
- $N_x = N_t = 6$



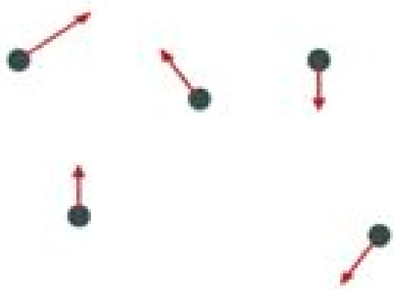
Phys. Rev. Lett. **102**, 131601 (2009)



The non-relativistic, rotating Bose gas

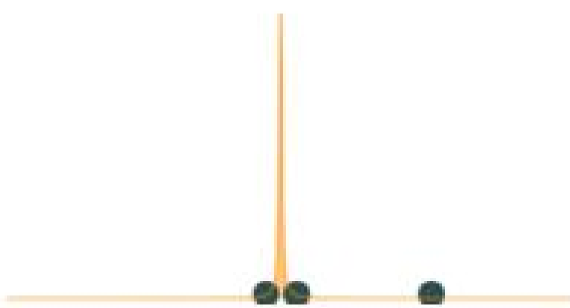
Rotating bosons: the action

$$S = \int dx\ dy\ d\tau \left[\phi^* \left(\mathcal{H} - \mu - \frac{m}{2}\omega_{\text{trap}}^2(x^2 + y^2) - \omega_z L_z\right)\phi + \lambda(\phi^*\phi)^2\right]$$

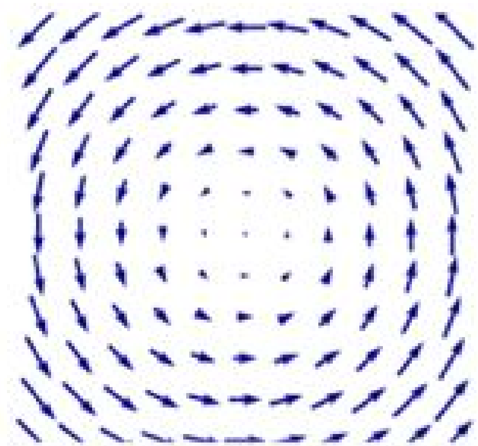


Non-relativistic dispersion

Trapped in a harmonic well



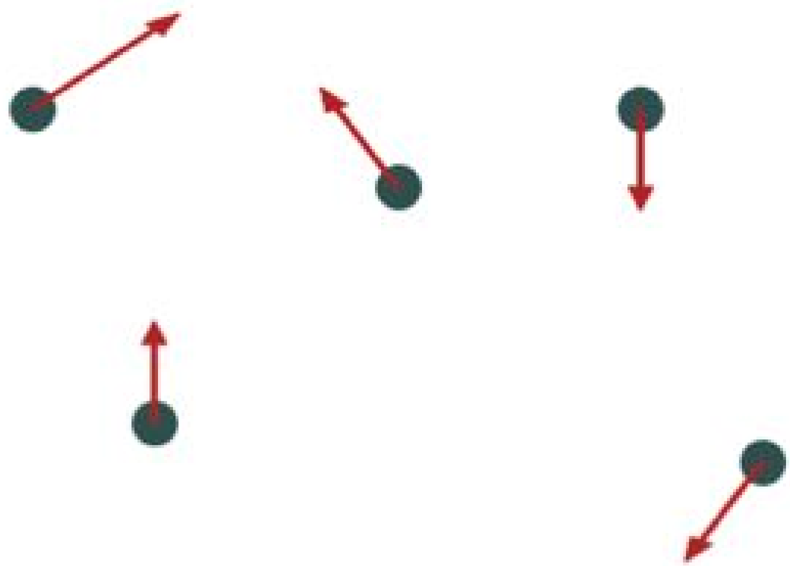
Interacting at short range



Rotating

Testing: the free Bose gas

- Exactly solvable: no interaction, rotation, or external potentials



Testing: the free Bose gas

- Start with S in 0+1 dimensions

$$S^{0+1} = \int \phi^*(\partial_\tau - \mu)\phi$$

$$S^{0+1}_{\text{lat}} = \sum_{x,\tau} \phi^*_{x,\tau}(\phi_{x,\tau} - e^{d\tau\mu}\phi_{x,\tau-1})$$

- Nonrelativistic time derivative is not symmetric
- Sign problem emerges in nonrelativistic bosonic systems the moment we complexify the fields

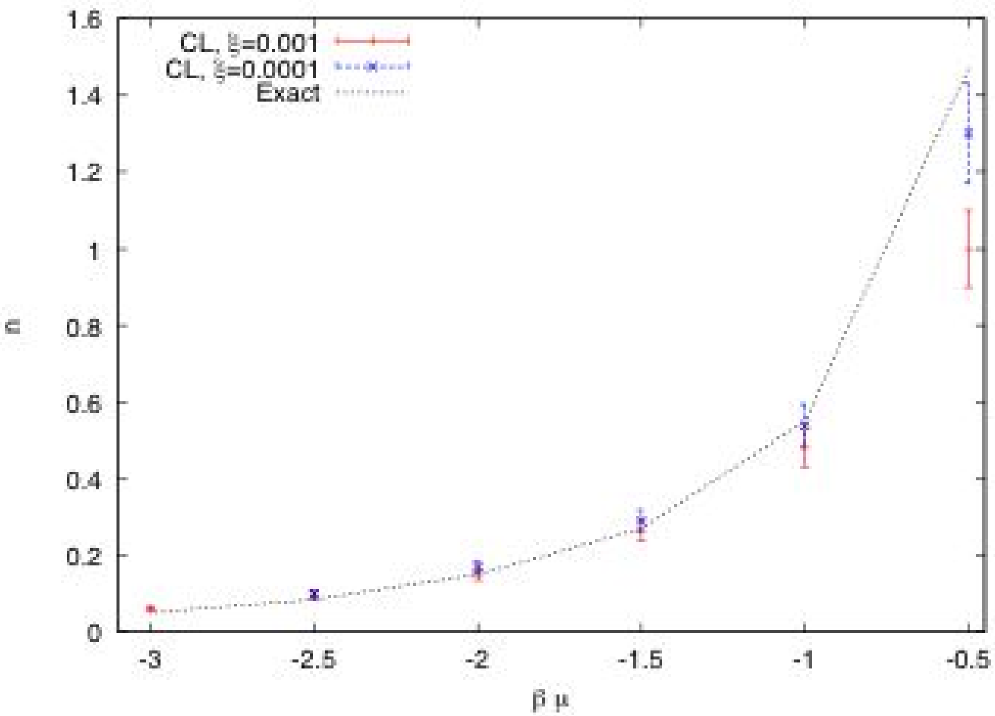
$$S^{0+1}_{\text{lat}} = \sum_{x,\tau} \phi^*_{x,\tau} M_{x,\tau,x',\tau'}\phi_{x',\tau'})$$

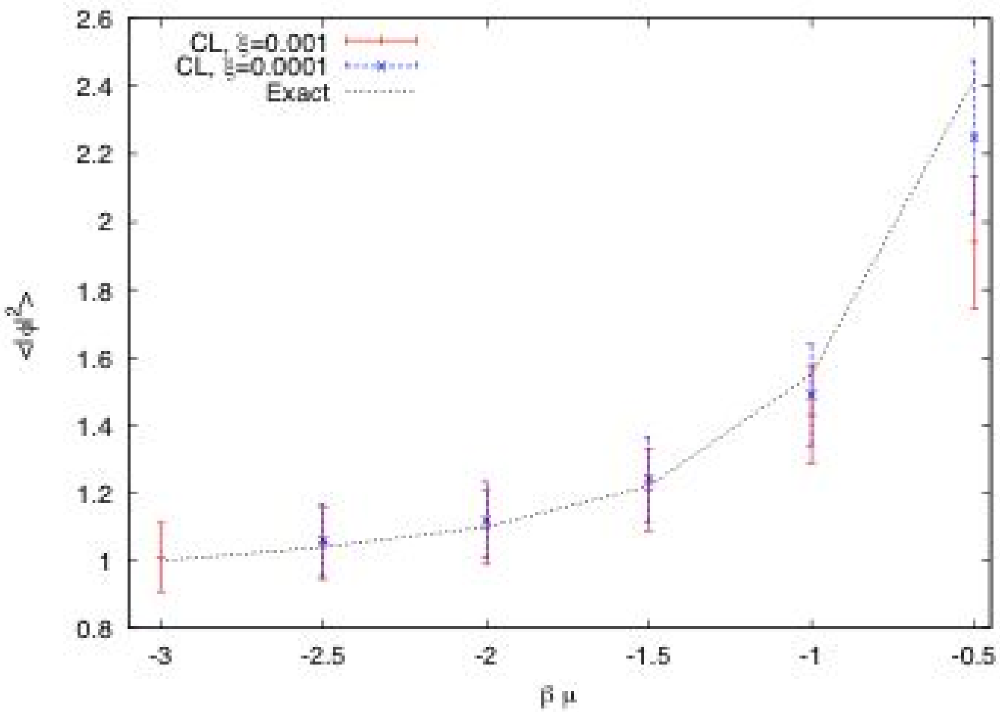
$$M \neq M^T$$

- Only occurs with nonrelativistic **bosons** – not an issue with fermions

Testing: the free Bose gas

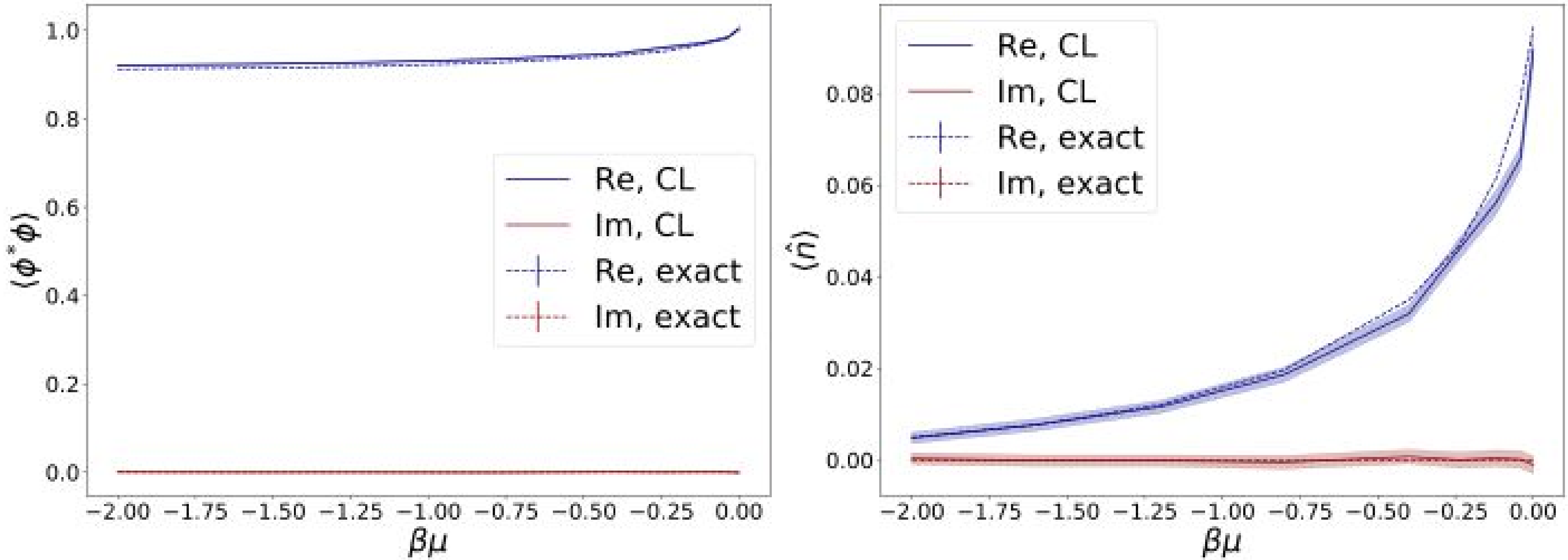
- Free Bose Gas, 0+1 dimensions





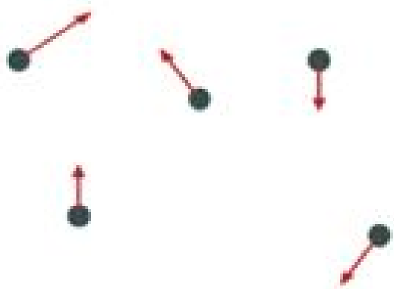
Testing: the free Bose gas

- The free gas in 2+1 dimensions



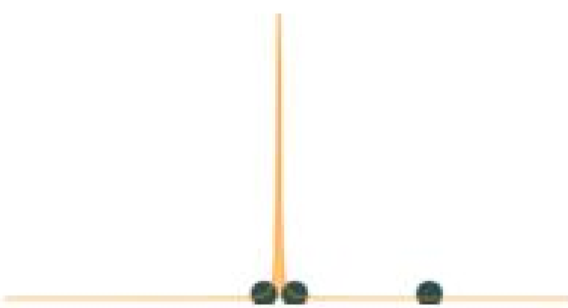
Now with rotation….

$$S = \int dx\ dy\ d\tau \left[\phi^* \left(\mathcal{H} - \mu - \frac{m}{2}\omega_{\text{trap}}^2(x^2 + y^2) - \omega_z L_z\right)\phi + \lambda(\phi^*\phi)^2\right]$$

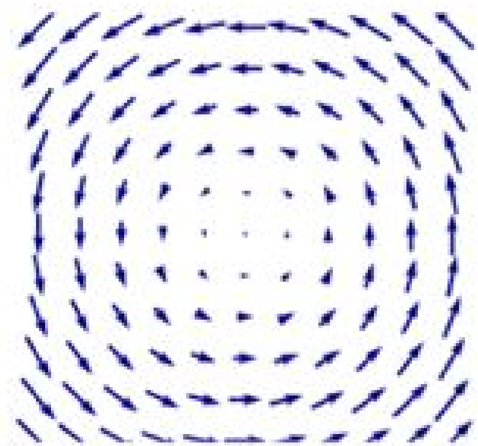


Non-relativistic dispersion

Trapped in a harmonic well



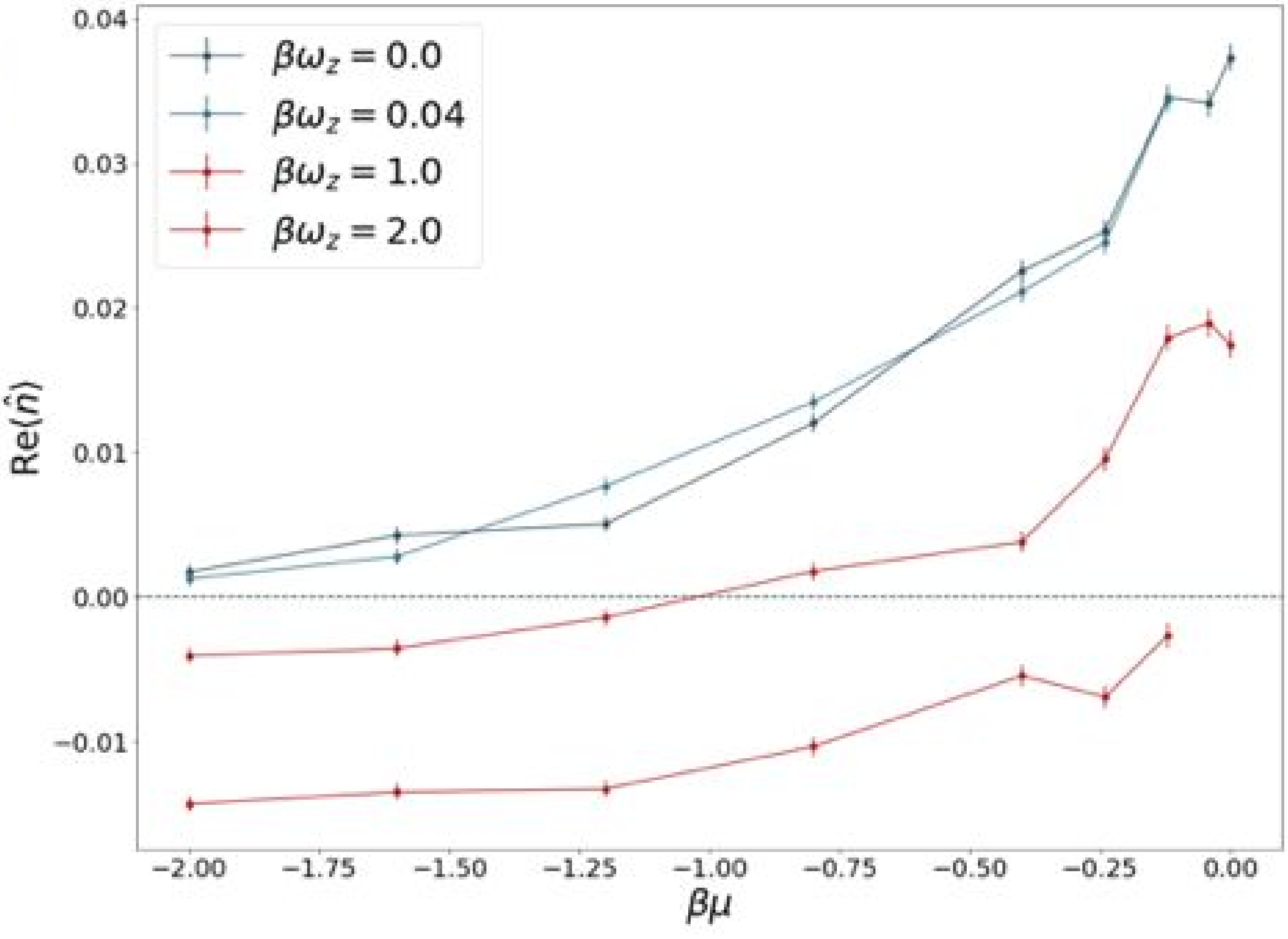
Interacting at short range



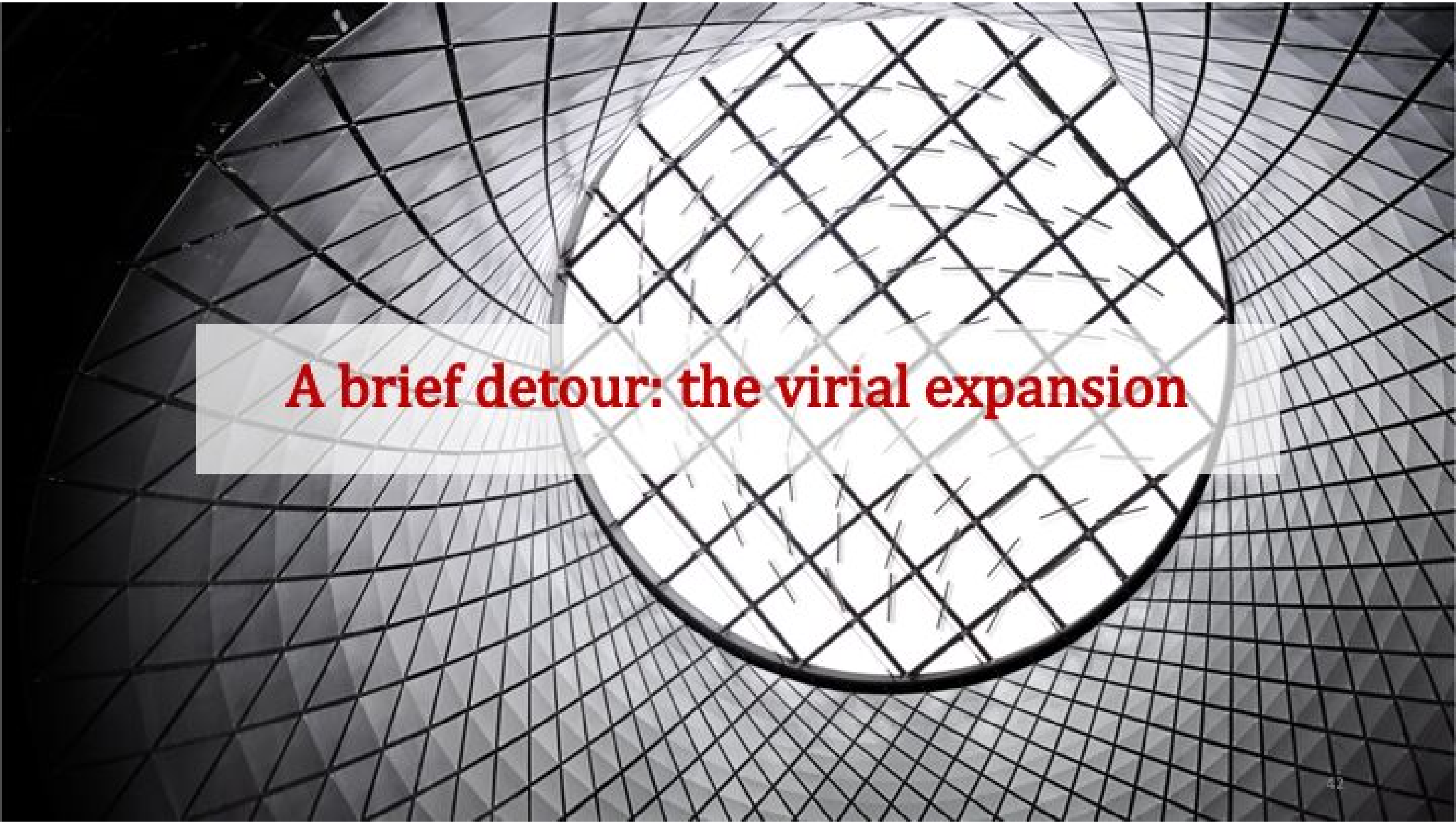
Rotating

Density calculation: rotating bosons

$$\beta\omega_{\mathrm{tr}} = 0.2$$



A brief detour: the virial expansion



A note on formalism

- So far, I have been using the Lagrangian formalism.
- Action

$$S = \int d^d x \; d\tau \left[\phi^* \left(\mathcal{H} - \mu - \frac{m}{2}\omega_{\text{trap}}^2 (x^2 + y^2) - \omega_z L_z \right) \phi + \lambda (\phi^* \phi)^2 \right]$$

- Path integral in terms of the action

$$\mathcal{Z} = \int \mathcal{D}\phi e^{-S[\phi]}$$

- Observables from path integral

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi e^{-S[\phi]} \mathcal{O}[\phi]$$

A note on formalism

- For this method, I use the Hamiltonian formulation.

$$\hat{H} = \int d^d x \left[\sum_{s=1,2} \hat{\psi}_s^\dagger(\mathbf{x}) \left(-\frac{\hbar^2 \nabla^2}{2m} \right) \hat{\psi}_s(\mathbf{x}) + \frac{1}{2} m \omega_{\text{tr}}^2 \mathbf{x}^2 \left(\hat{n}_1(\mathbf{x}) + \hat{n}_2(\mathbf{x}) \right) \right.$$
$$\left. + i \sum_{s=1,2} \hat{\psi}_s^\dagger(\mathbf{x}) \left(x\partial_y - y\partial_x \right) \hat{\psi}_s(\mathbf{x}) - g \hat{n}_1(\mathbf{x}) \hat{n}_2(\mathbf{x}) \right]$$

- Grand canonical partition function in terms of the Hamiltonian

$$\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta(\hat{H} - \mu \hat{N})} \right]$$

- Calculate observables from the partition function

$$\langle \mathcal{O} \rangle = \frac{\partial}{\partial \xi} \ln \mathcal{Z}$$

- There is a correspondence between these formalisms, where time and inverse temperature play the same role (see earlier discussion of our time lattice)

The virial expansion

- Expand the log of the partition function in the fugacity $z = e^{\beta\mu}$:

$$-\beta\Omega = \ln \mathcal{Z} = Q_1 \sum_{n=1}^{\infty} b_n z^n$$

- Coefficients can be calculated in terms of N-body partition functions

$$\mathcal{Z} = \sum_{N=0}^{\infty} z^N Q_N$$

$$b_1 = 1,\ b_2 = \frac{Q_2}{Q_1} - \frac{Q_1}{2!},\ b_3 = \frac{Q_3}{Q_1} - b_2 Q_1 - \frac{Q_1^2}{3!}$$

- Approximate solutions for thermodynamics via derivatives of Z
- Valid for small z (high-temperature/low density)

Calculating N-body partition functions

- The one-body partition function can be computed exactly

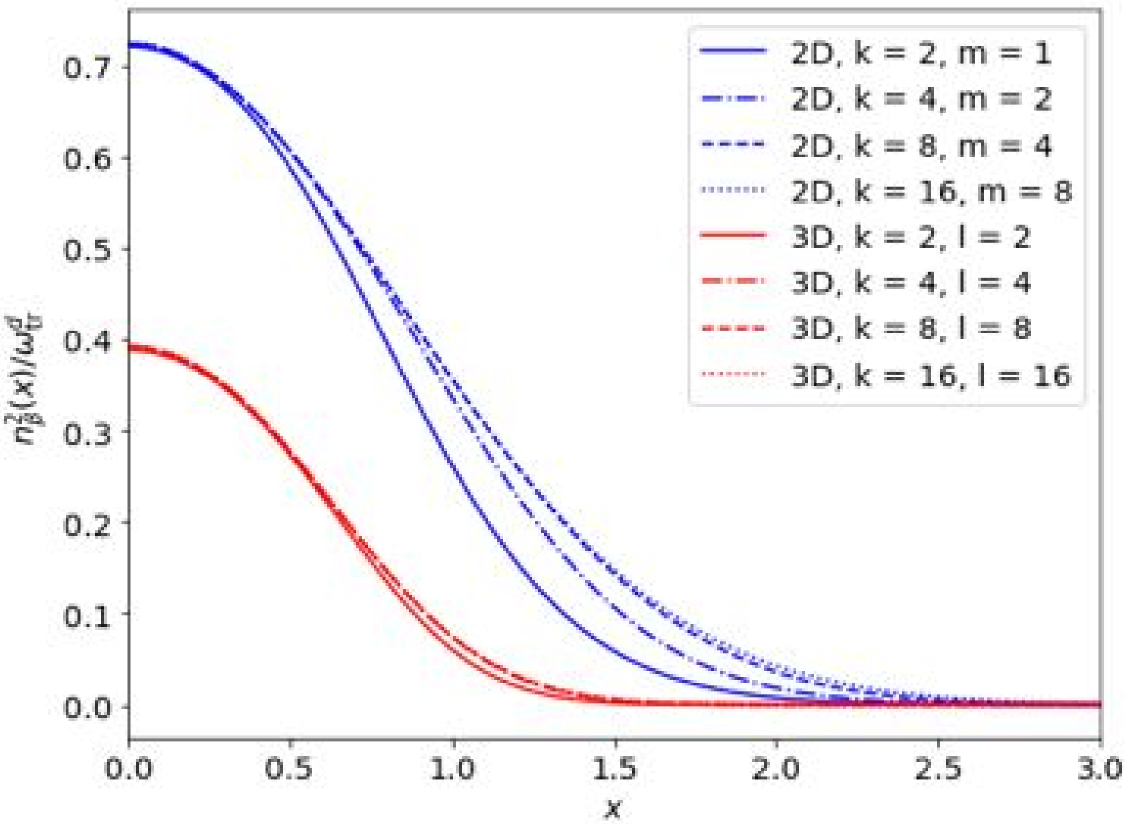
$$Q_1 = \sum_{\mathbf{k}} e^{-\beta E_{\mathbf{k}}}$$

- Many-body partition functions require truncating the sum

$$\begin{aligned} Q_{1,1} &= \mathrm{Tr}_{1,1}\left[e^{-\beta \hat{H}_0} e^{-\beta \hat{V}_{\mathrm{int}}}\right] \\ &= \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{x}_1,\mathbf{x}_2} \langle \mathbf{k}_1\mathbf{k}_2 | e^{-\beta \hat{H}_0} | \mathbf{x}_1\mathbf{x}_2 \rangle \langle \mathbf{x}_1\mathbf{x}_2 | e^{-\beta \hat{V}_{\mathrm{int}}} | \mathbf{k}_1\mathbf{k}_2 \rangle \\ &= \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{x}_1,\mathbf{x}_2} e^{-\beta (E_{\mathbf{k}_1} + E_{\mathbf{k}_2})} M_{\mathbf{x}_1,\mathbf{x}_2} |\langle \mathbf{k}_1\mathbf{k}_2 | \mathbf{x}_1\mathbf{x}_2 \rangle|^2 \end{aligned}$$

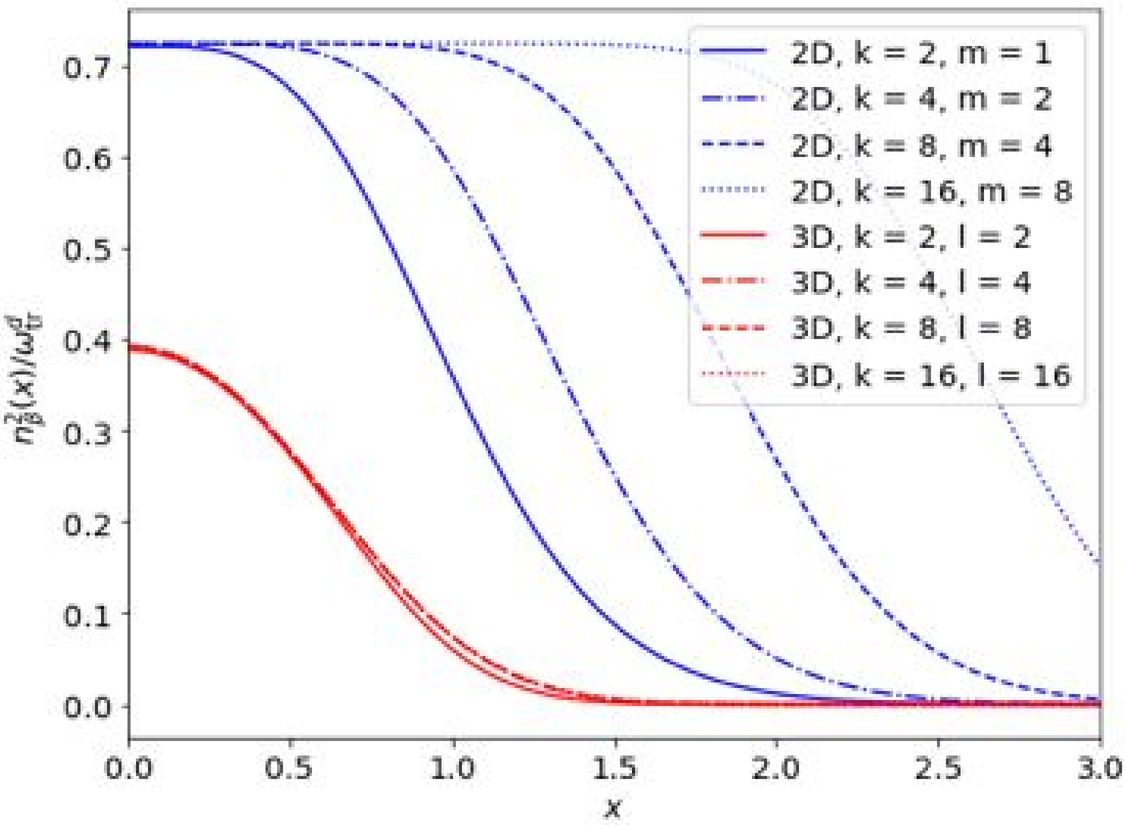
Calculating N-body partition functions

Truncation in spatial coordinates and quantum numbers can be done without large loss of accuracy



Calculating N-body partition functions

One exception: when our rotation exceeds our trap frequency



Noninteracting thermodynamics

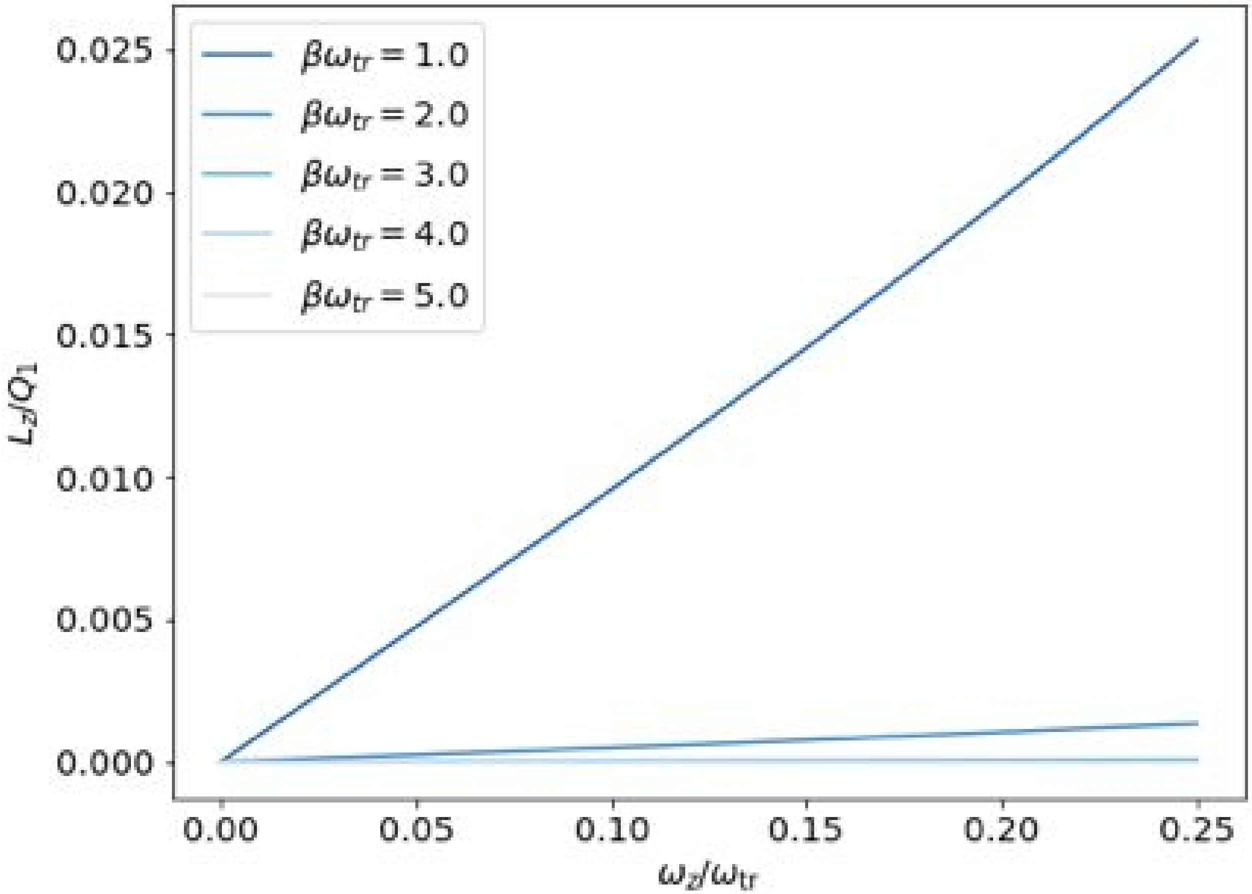
Angular momentum in virial expansion

$$\langle \hat{L}_z \rangle = -\frac{\partial \ln \mathcal{Z}}{\partial(\beta\omega_z)} = Q_1 \sum_{n=1}^{\infty} L_n z^n$$

$$L_n = n b_n \frac{e^{-n\beta\omega_+} - e^{-n\beta\omega_-}}{(1 - e^{-n\beta\omega_+})(1 - e^{-n\beta\omega_-})}$$

Noninteracting thermodynamics

Results of rotation on angular momentum (noninteracting, 2D)



Interacting thermodynamics

Interacting angular momentum to third order in virial expansion

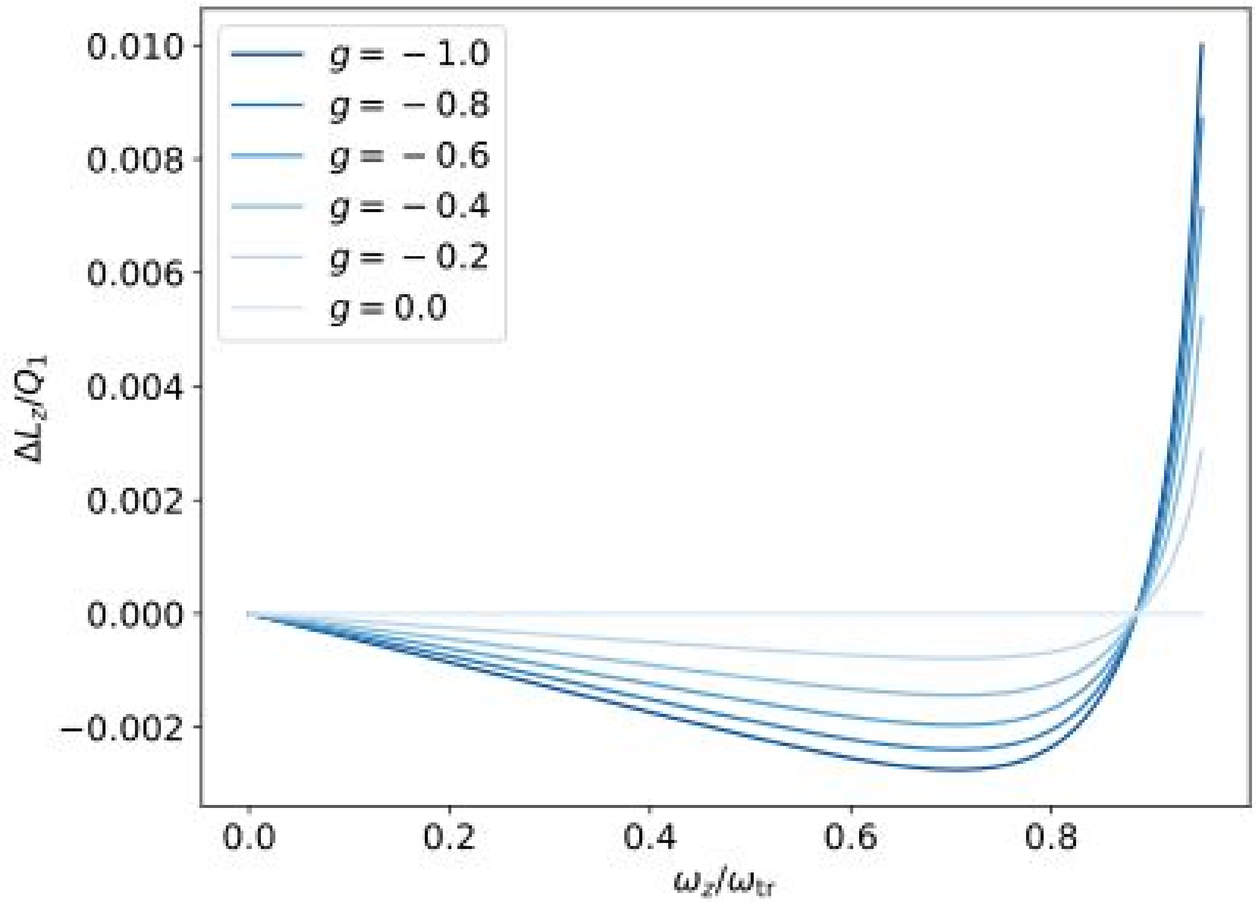
$$\frac{\Delta \langle L_z \rangle}{Q_1} = \Delta L_2 z^2 + \Delta L_3 z^3 + O(z^4)$$

$$\Delta L_n = \frac{1}{Q_1} \frac{\partial \left(Q_1 \Delta b_n\right)}{\partial(\beta \omega_z)} = \frac{\partial \left(\Delta b_n\right)}{\partial(\beta \omega_z)} + \Delta b_n \frac{\partial \left(\ln Q_1\right)}{\partial(\beta \omega_z)}$$

Interacting thermodynamics

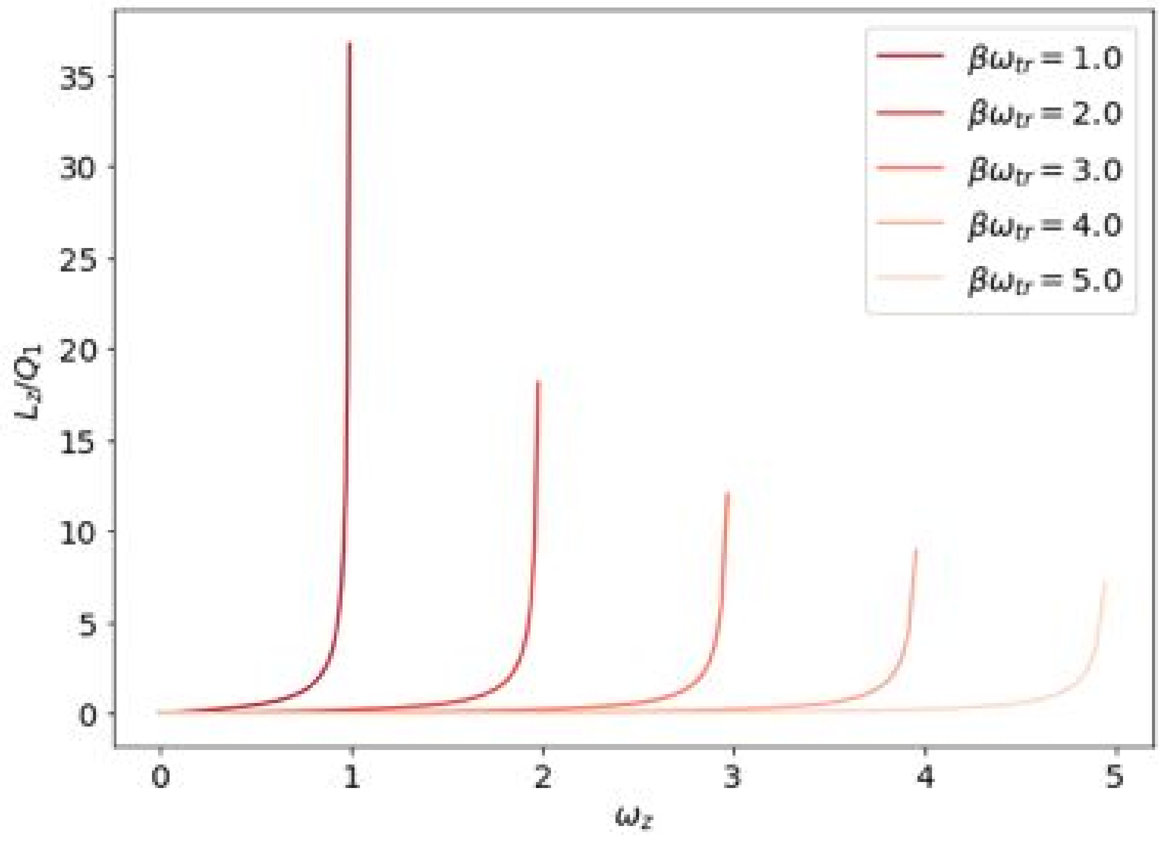
Results of interaction on angular momentum (rotating, 2D)

$$\beta\omega_{\mathrm{tr}} = 1$$



Noninteracting thermodynamics

The system experiences an instability when the rotation frequency meets or exceeds the trapping potential



Density can also be calculated with the virial expansion

Approximate solution using virial coefficients:

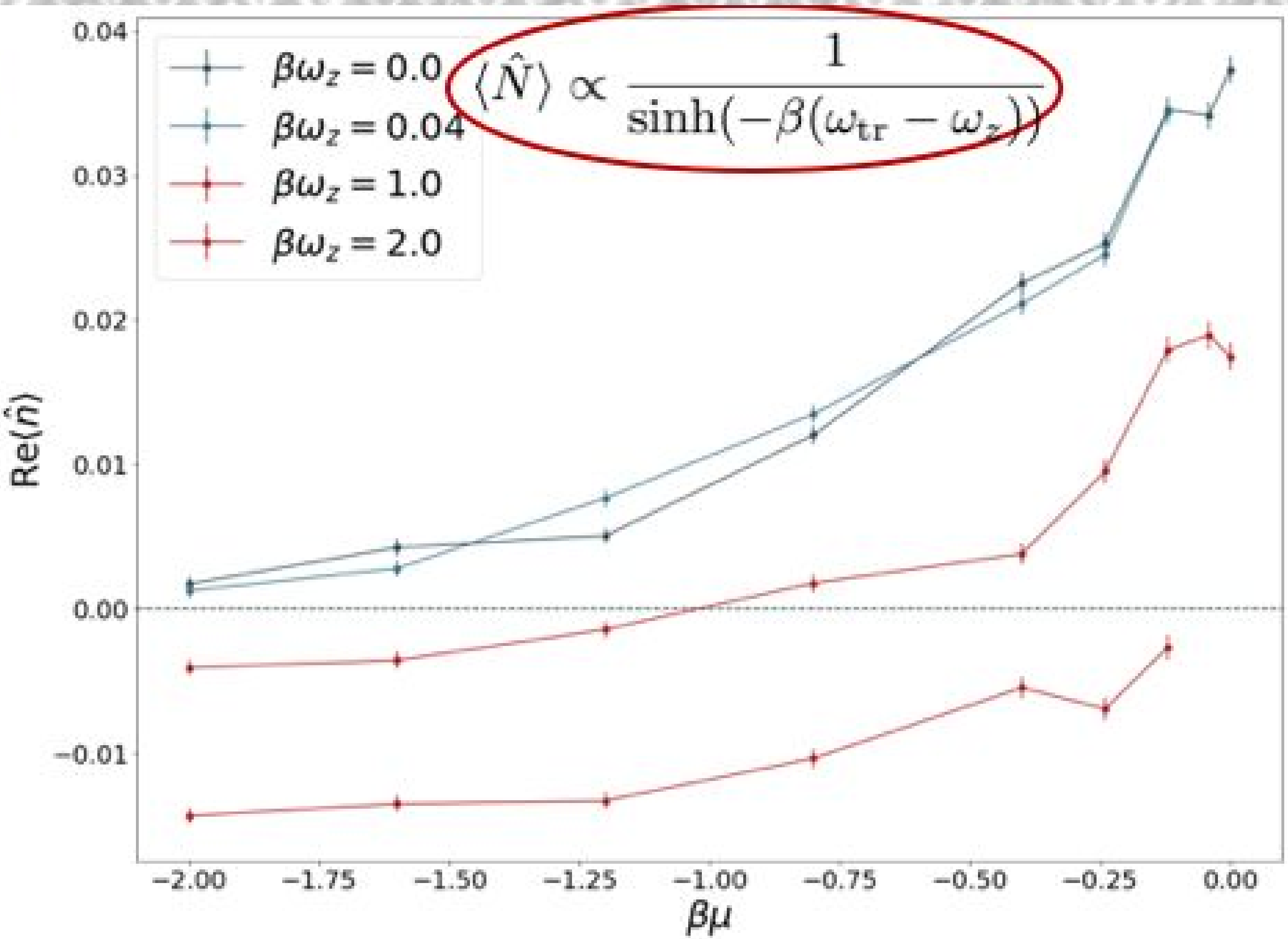
$$\langle \hat{N} \rangle = -\frac{\partial \ln \mathcal{Z}}{\partial(\beta\mu)}$$

$$\ln \mathcal{Z} = -\beta\Omega = Q_1 \sum_{n=1}^{\infty} b_n z^n$$

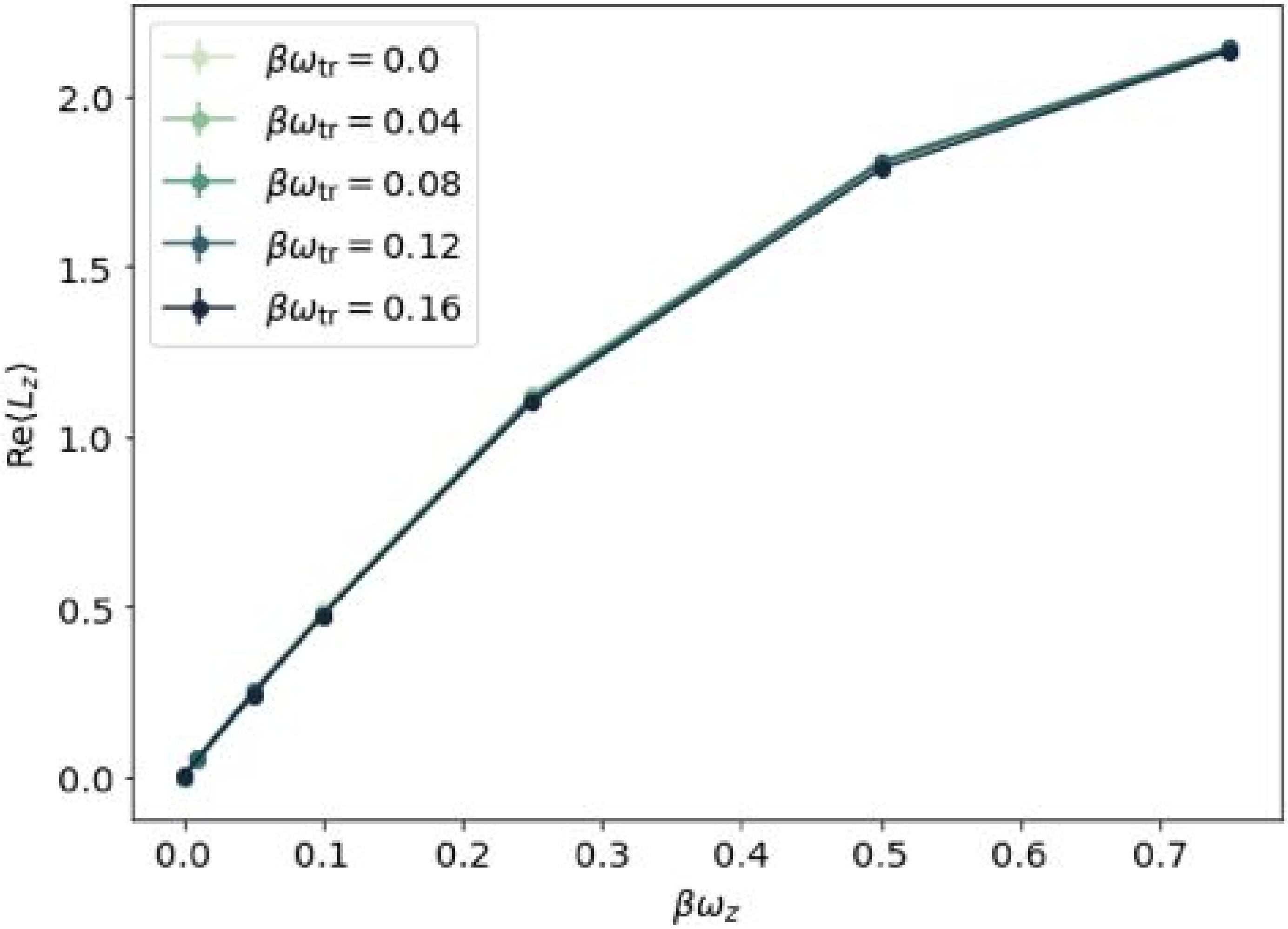
$$Q_1 b_n \propto \frac{-1}{\sinh(\beta(\omega_{\mathrm{tr}} - \omega_z))}$$

Balancing rotation and trapping potential

$\beta\omega_{\text{tr}} = 0.2$



Angular momentum: preliminary results



What might be going wrong?

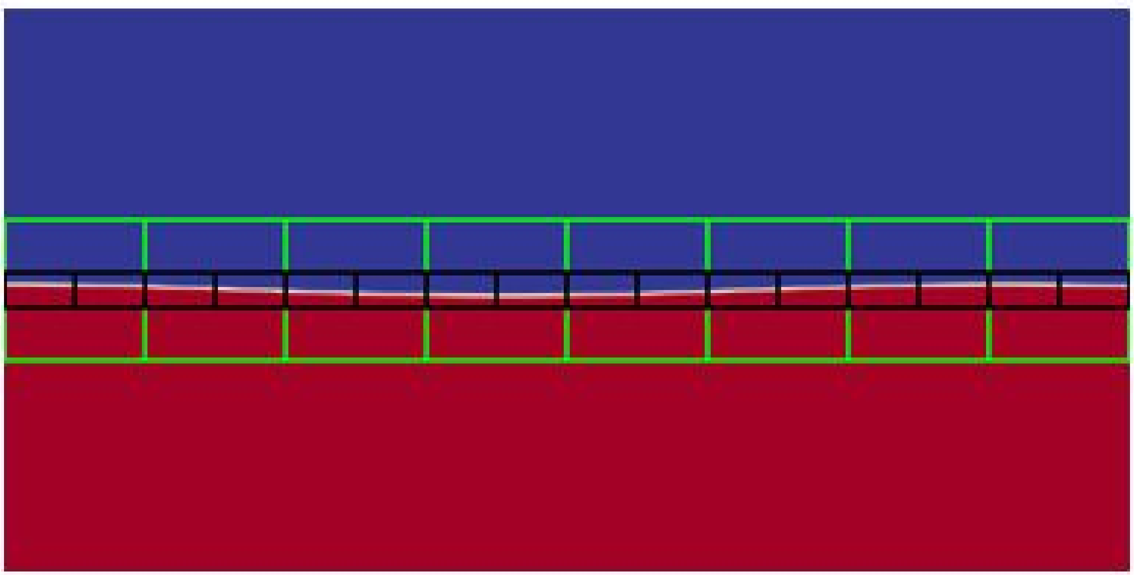
- Temperature might still be too high
  - Lower temperatures = larger lattices
  - We are already using $N_\tau = 160$
  - Need to improve computational efficiency
- Parameters are very sensitive to each other
  - Tuning trap strength, interaction, and rotation frequency is very delicate
  - May also be a factor of lattice size
- This problem needs much greater computing resources

AMReX

- Block-structured adaptive mesh refinement (AMR) software framework
- Part of the Exascale Computing Project's co-design center
- Supports CPU and GPU parallelism – MPI, MPI+ (MPI with OpenACC, OpenMP, CUDA, or some combination)
- See more at: https://amrex-codes.github.io/amrex/

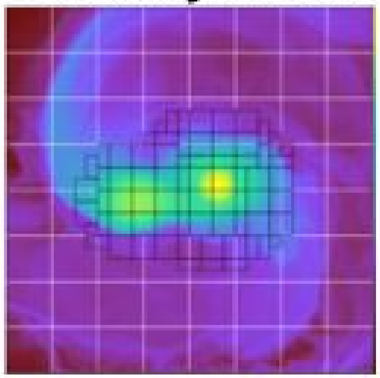
AMReX

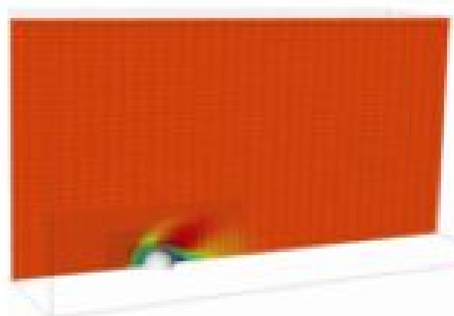
- What is "block-structured adaptive mesh refinement (AMR)"
- Focuses computational resources in areas of interest using a mix of fine and coarse grids.
- No parent-child relationship – the grid structure adapts dynamically

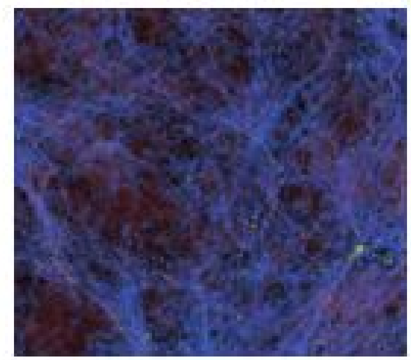


AMReX

- Established success in astrophysics, cosmology, combustion physics, fluid dynamics, and more…







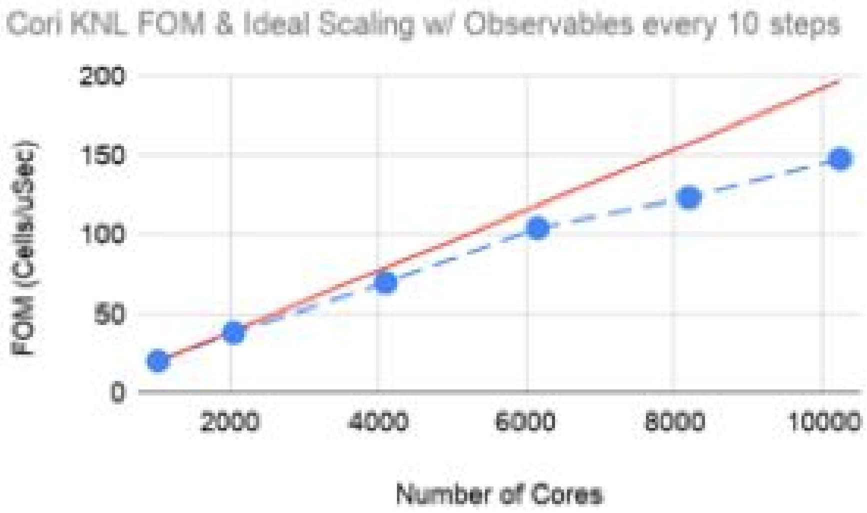
- All images come from: https://amrex-codes.github.io/amrex/gallery.html and https://amrex-astro.github.io/

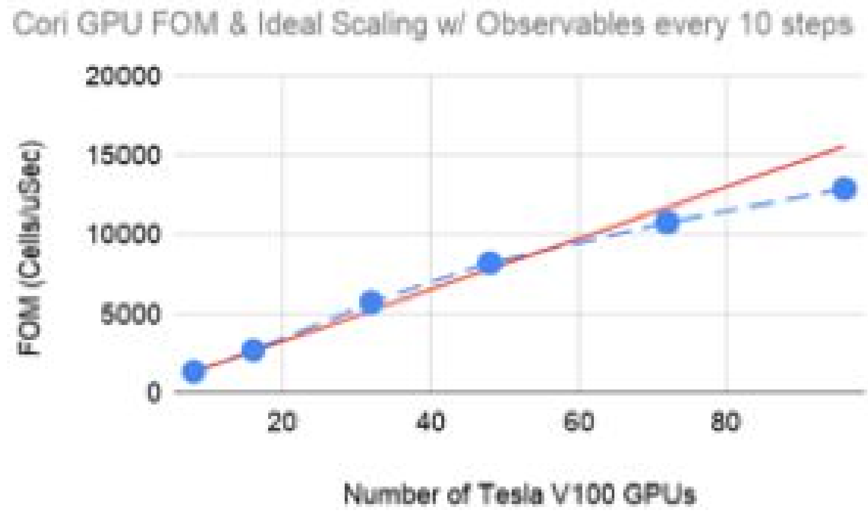
AMReX and rotating superfluids

- Concentrate our fine grids at the center of the trap, where we expect vortices to first appear
- Allows us to scale up our lattice size greatly to approximate continuum physics without a corresponding increase in computational cost
- We hope this will allow us to observe vortex formation in the density profiles as well as give us enough room to vary our lattice parameters within appropriate limits

AMReX and rotating superfluids

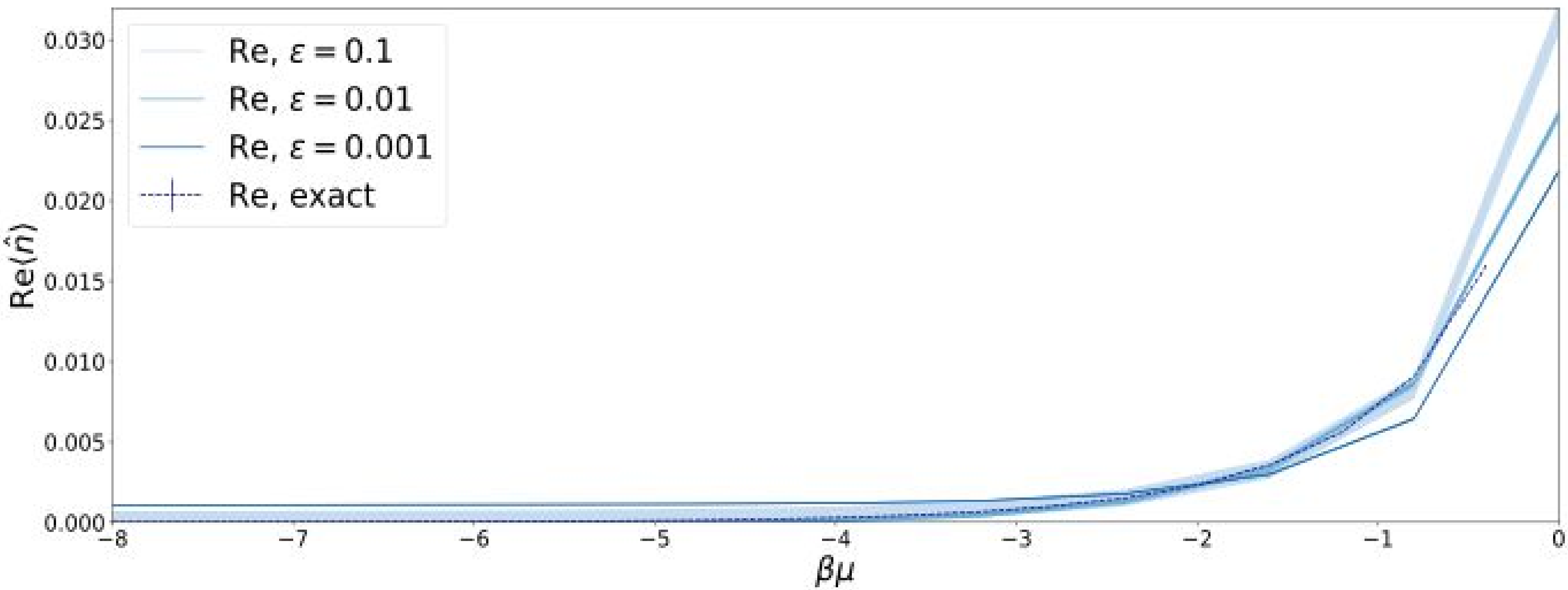
- Goal: utilize the adaptive mesh refinement to concentrate our computational power in areas of interest
- Early results:
  - We're seeing massive speedup in our algorithm using AMReX's parallelization
  - This is even before applying the adaptive mesh





AMReX and rotating superfluids

- Tuning the Langevin evolution

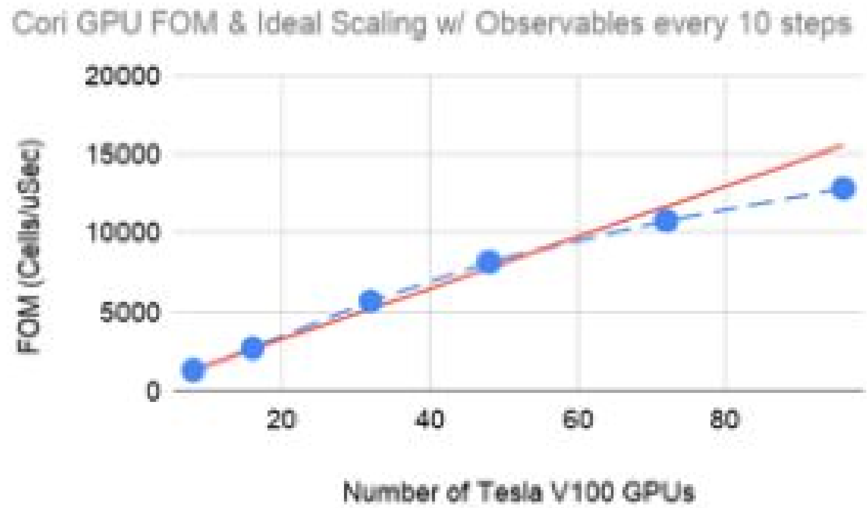


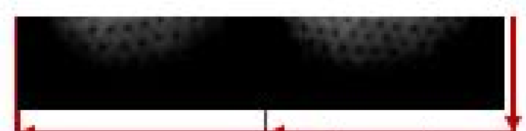
Future directions

- Decrease temperature and increase spatial lattice
  - AMReX will allow us to do this without sacrificing computational resources
- Density should show triangular
- Look for discontinuities in the c

$$\Gamma[l] \quad = \quad \frac{1}{2\pi} \oint_{l\times l} dx \left(\theta_{\tau,x} \right.$$

$$\theta_{\tau,x} \quad = \quad \tan^{-1} \left(\frac{\mathrm{Im}[\phi_{\tau,x}}{\mathrm{Re}[\phi_{\tau,x}]} \right)$$





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Summary

- Complex Langevin is a very useful method
- Rotating superfluids are proving to be a much more complicated system, extremely sensitive to the parameters
- Additionally, to get to lower temperatures, we need much larger lattices, which results in greater computational time needed
- Current work includes a collaboration with AMReX to maximize efficiency and scale up lattices
- We're not there yet, but we've learned a lot about this system that will help us crack it one day!

Want to know more about complex Langevin?

"Complex Langevin and other approaches to the sign problem in quantum many-body physics"

C.E. Berger, L Rammelmüller, A.C. Loheac, F. Ehmann, J. Braun, J.E. Drut

arXiv 1907.10183

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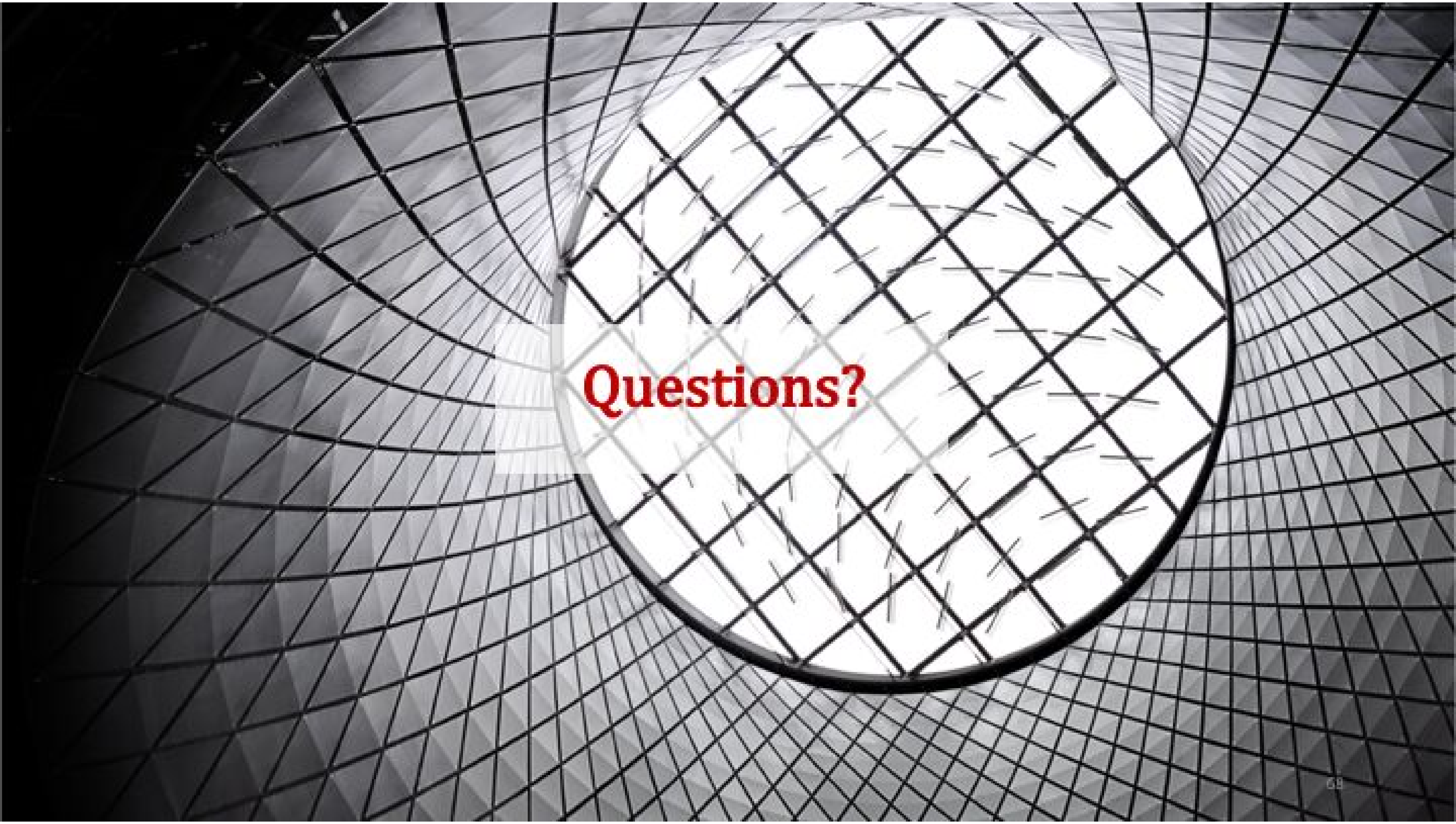
SILENCE IS VIOLENCE www.caseyeberger.com/social-justice.html

EXASCALE COMPUTING PROJECT

BOSTON UNIVERSITY

UNC THE GRADUATE SCHOOL Royster Society of Fellows

DOE CSGF


Questions?

Imaginary noise

- Why does our complex Langevin evolution only have noise in the real term?

$$d\phi^R(x) = -\mathrm{Re}\left[\frac{\delta S[\phi]}{\delta\phi}\right] dt_L + \eta(t_L)$$
$$d\phi^I(x) = -\mathrm{Im}\left[\frac{\delta S[\phi]}{\delta\phi}\right] dt_L$$

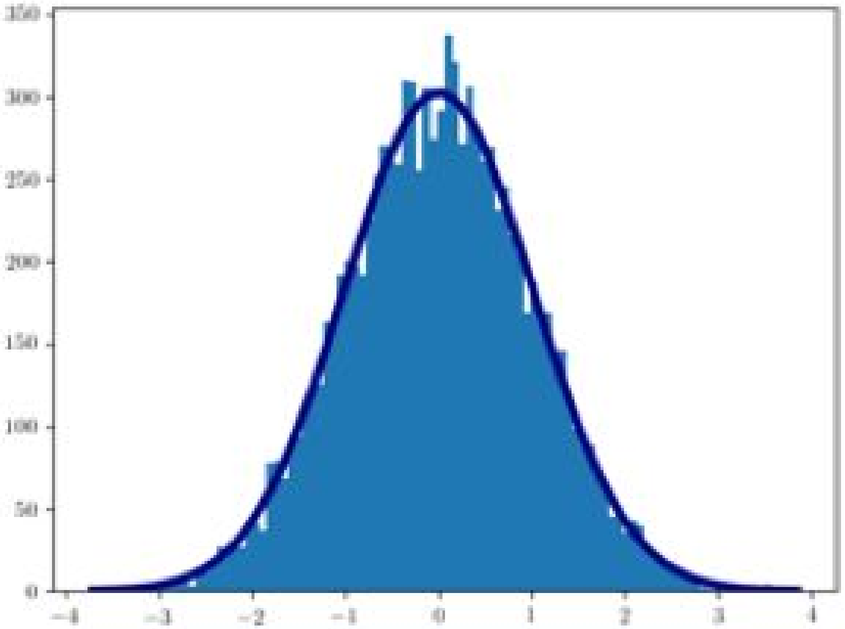
- Use of real noise only still satisfies the mathematical definition of Gaussian white noise

$$\langle\eta_R^2\rangle = 2N_R dt_L, \quad \langle\eta_R^2\rangle = 2N_R dt_L$$
$$N_R - N_I = 1, \quad \langle\eta_R\rangle = \langle\eta_I\rangle = 0$$

- Introducing imaginary noise tends to result in more excursion problems – removing it is a way to control excursions in the imaginary direction and encourage convergence

dW and Gaussian noise

- dW is white noise which obeys a set of conditions
- These conditions are met by using Gaussian-distributed white noise



$$dW(t_L) \quad = \quad \int_{t_L}^{t_L+dt_L} d\tau \eta(\tau)$$

$$\langle dW(t_L)^2 \rangle \quad = \quad \int_{t_L}^{t_L+dt_L} d\tau \int_{t_L}^{t_L+dt_L} d\tau' \langle \eta(\tau)\eta(\tau') \rangle = 2dt_L$$

CL Evolution

Update the fields using the discrete complex Langevin equations

$$\begin{aligned}\phi^R_{a,x}(n+1) &= \phi^R_{a,x}(n) - \epsilon K^R_{a,x}(n) + \sqrt{\epsilon}\eta_{a,x} \\ \phi^I_{a,x}(n+1) &= \phi^I_{a,x}(n) - \epsilon K^I_{a,x}(n)\end{aligned}$$