# Quantum Monte Carlo in momentum space and on the Lefschetz thimble

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Advances in quantum Monte Carlo techniques for non-relativistic many-body systems, INT, Seattle



# Collaborators

- Configuration interaction Monte Carlo
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  - Francesco Pederiva (U. Trento)
  - Alessandro Roggero (U. Trento)

    *AM & Y. Alhassid, arXiv:1304.1645 (2013)*

    *A. Roggero, AM & F. Pederiva, arXiv:1304.1549 (2013)*

    *A. Roggero, AM & F. Pederiva, in preparation*
- Lefschetz thimble Monte Carlo
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  - Marco Cristoforetti (ECT*)
  - Francesco di Renzo (U. Parma)

    *M. Cristoforetti, F. di Renzo & L. Scorzato, PRD (2012)*

    *M. Cristoforetti, F. di Renzo, AM & L. Scorzato, arXiv:1303.7204 (2013)*

    *AM, M. Cristoforetti & L. Scorzato, in preparation*

# Configuration Interaction Monte Carlo

- QMC *a la* fixed-node DMC in CI/k-space
  QMC with non-local ($\chi$ EFT) forces

- Variational energies from CC wave functions
  Standard CC theory is non-variational

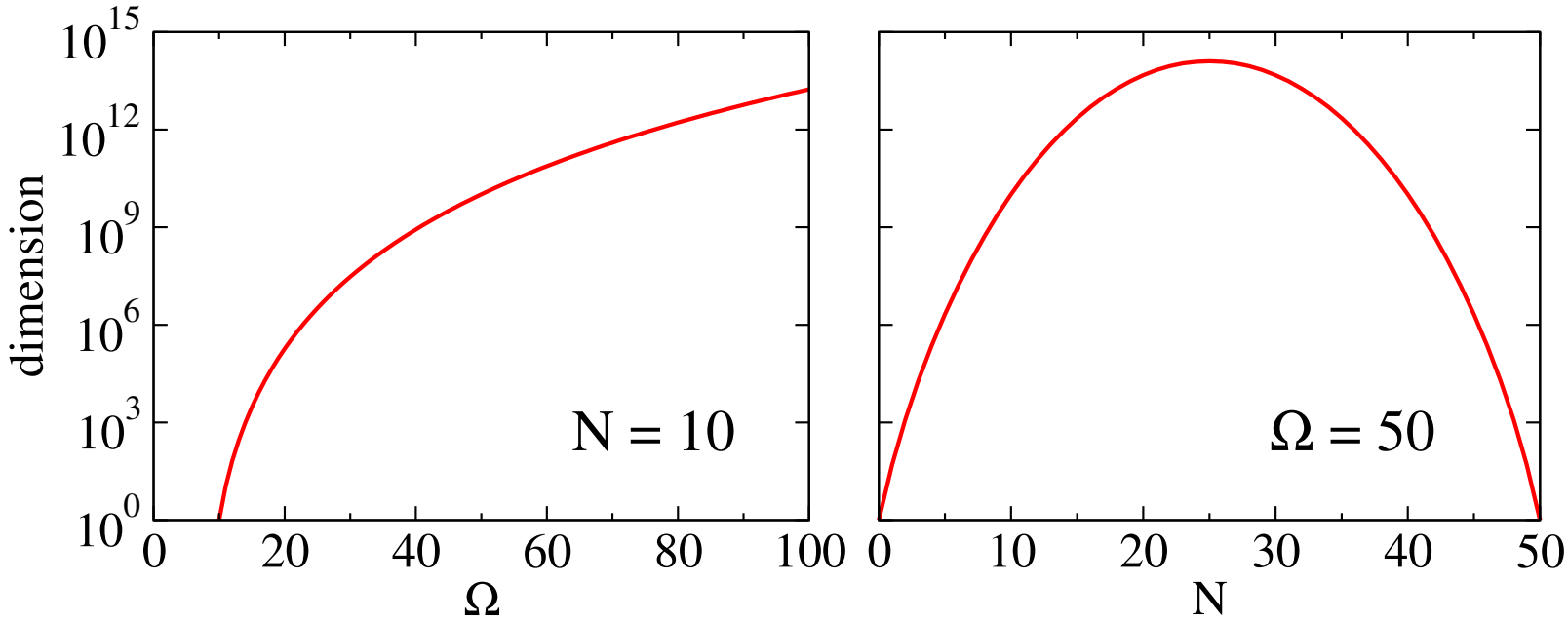
- Momentum distribution in QMC

# The rise of second quantization

We want to solve:

$$H = \sum_{i}^{\Omega} \varepsilon_i a_i^\dagger a_i + \sum_{ijkl}^{\Omega} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k + \dots$$

Full-CI diagonalization possible only for small systems



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- A general $V_{ijkl}$ leads to a non-local interaction in $r$-space
- Cannot apply standard $r$-space fixed-node DMC
- Formulate DMC in CI space?

# Configuration interaction Monte Carlo

- Use the power method

$$|\Psi_{\text{Ground State}}\rangle = \lim_{N\to\infty} \mathcal{P}^N |\Psi_{\text{Initial State}}\rangle$$

  - Occupation number basis : $|\mathbf{n}\rangle = |\ldots 0101\ldots\rangle$
  - Interpret $\mathcal{P}_{\mathbf{mn}}$ as transition probabilities

- Propagator
  - Simplest choice: $\mathcal{P} = (1 - \Delta\tau H)$
  - In reality we use more efficient propagators : $e^{-\Delta\tau(H-E_T)}$

# Configuration interaction Monte Carlo

$$\mathcal{P} = 1 - \Delta\tau H \rightarrow |\Psi_{\tau+\Delta\tau}\rangle = \mathcal{P}|\Psi_\tau\rangle$$

$$\Psi_{\tau+\Delta\tau}(\mathbf{m}) = \sum_{\mathbf{n}} \langle \mathbf{m}|\mathcal{P}|\mathbf{n}\rangle \Psi_\tau(\mathbf{n})$$

$$= \sum_{\mathbf{n}} \left( \frac{\langle \mathbf{m}|\mathcal{P}|\mathbf{n}\rangle}{\sum_{\mathbf{m}} \langle \mathbf{m}|\mathcal{P}|\mathbf{n}\rangle} \right) \left( \sum_{\mathbf{m}} \langle \mathbf{m}|\mathcal{P}|\mathbf{n}\rangle \right) \Psi_\tau(\mathbf{n})$$

$$= \sum_{\mathbf{n}} \underbrace{p(\mathbf{m},\mathbf{n})}_{\text{Transition probability}} \underbrace{w(\mathbf{n})}_{\text{Branching}} \Psi_\tau(\mathbf{n})$$

MC sampling not possible if $p(\mathbf{m},\mathbf{n}) < 0$

$\Longrightarrow \langle \mathbf{m}|H|\mathbf{n}\rangle > 0 \longrightarrow$ sign problem

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- There is a sign problem for the generic case
- We need to somehow construct non-negative propagators

Transition probability Branching

MC sampling not possible if $p(\mathbf{m}, \mathbf{n}) < 0$

$\implies \langle \mathbf{m}|H|\mathbf{n}\rangle > 0 \longrightarrow$ sign problem

# Non-negative propagator

How to choose a non-negative propagator?

Borrow from lattice-GFMC (discrete, finite Hilbert space)

*ten Haaf et al PRB (1995)*

- Use importance sampling to circumvent the sign problem

$$\mathcal{P} \longrightarrow \mathcal{P}_{\text{new}}(\Phi_G) \geq 0$$

- But there is a price

Variational upper bound

Exact GS energy

- Better $\Phi_G \implies$ tighter bound
- $E_{CIMC} \leq \langle \Phi_G | H | \Phi_G \rangle$

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How to choose the importance function $\Phi_G$?

Exact GS energy ~~bound~~

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# Good CI wave functions

The importance function should be:

- Accurate/Flexible: Should be able to include the major correlations in the system
- Calculable : Need a fast algorithm to calculate it on a computer (fast = at most polynomial in N and/or $\Omega$)

- Plenty of experience in r-space ($\sim 50$ years)
- Very little is CI/k-space
- 'Fourier' transform of r-space wave functions (e.g. Jastrow-Slater) does not work

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**Can we get known CI w.f.s to work with MC?**

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- Very little is CI/k-space
- 'Fourier' transform of r-space wave functions (e.g. Jastrow-Slater) does not work

# Antisymmetric geminal power

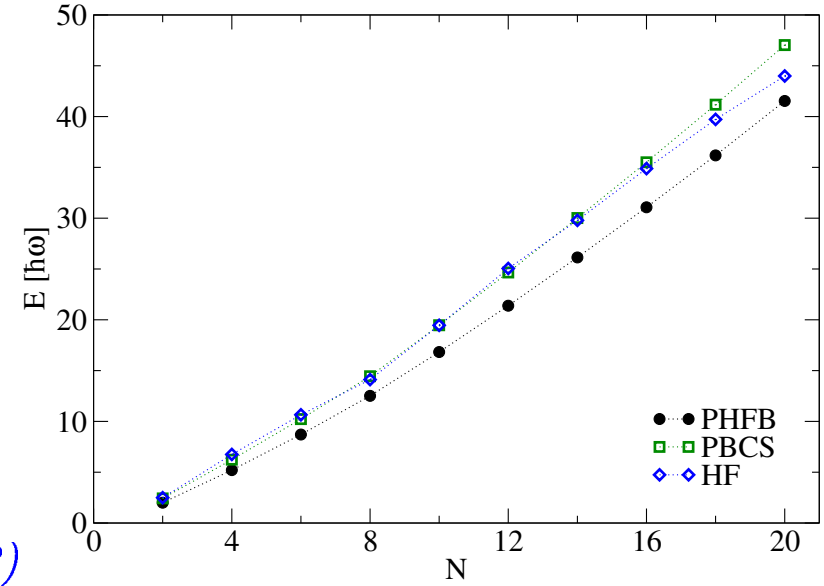
- For even N

$$|\Phi_{\mathrm{AGP}}\rangle = \left(\phi_{ij} a_i^\dagger a_j^\dagger\right)^{N/2} |0\rangle$$

- For odd N, we put the additional particle in a general sp orbital
- Fast algorithms : $\langle \mathbf{n}|\Phi_G\rangle$ is a Pfaffian ($\sim N^3$).
- Very flexible : can include different kinds of 2b correlations
- HFB, BCS, HF are special cases

# Trapped unitary fermi gas

- Atoms in a harmonic trap
- Contact interaction among $\uparrow$ and $\downarrow$ spins only
- In this case $\langle \mathbf{n} | \Phi_G \rangle$ is a determinant!

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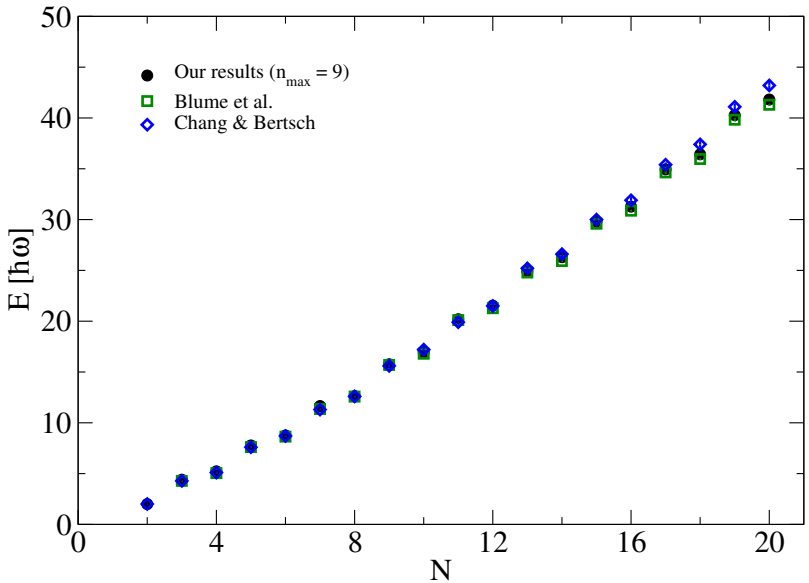


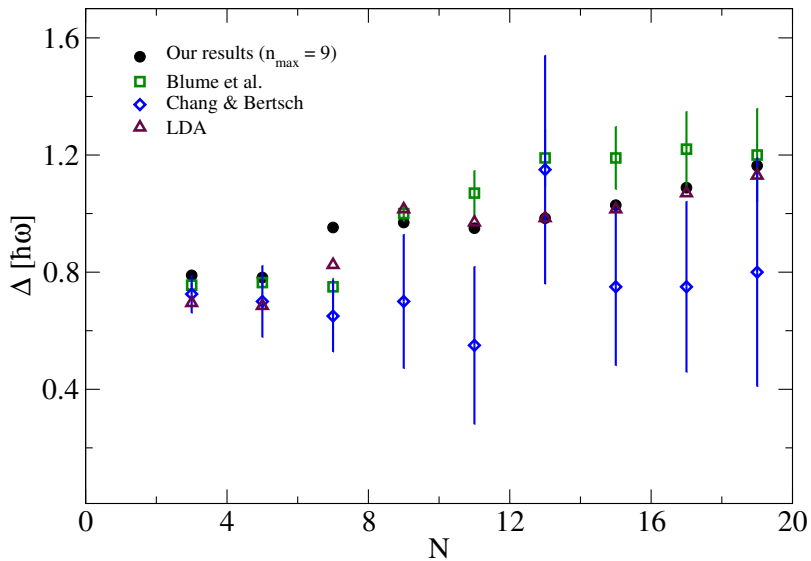

# Coupled Cluster wave functions

$$|\Phi_{CC}\rangle = e^{T}|\Phi_0\rangle$$

$$T = \sum t_i^a a_a^\dagger a_i + \sum t_{ij}^{ab} a_a^\dagger a_b^\dagger a_i a_j + \ldots$$

- Different truncations for T lead to different approximations CCD, CCSD, CCSDT ...
- Accurate: CCSD(T) is 'gold standard' in chemistry ✓
- Energies not variational in the standard approach ✗

Can we calculate $\langle n|\Phi_{CC}\rangle$ quickly?

# The magic formula

Start with Coupled Cluster Doubles (good for uniform systems):

$$\Phi^{m}_{CCD}\left(\begin{smallmatrix} p_1 p_2 \cdots p_m \\ h_1 h_2 \cdots h_m \end{smallmatrix}\right) = \Phi_{CCD}(\mathbf{n})$$

for

$$|\mathbf{n}\rangle = a^{\dagger}_{p_1} \ldots a^{\dagger}_{p_m} a_{h_1} \ldots a_{h_m} |\Phi_{HF}\rangle$$

Recursive formula:

$$\Phi^{m}_{CCD}\left(\begin{smallmatrix} \cdots \\ \cdots \end{smallmatrix}\right) = \sum_{\gamma=2}^{m} \sum_{\mu<\nu}^{m} (-)^{\gamma+\mu+\nu} t^{p_\mu p_\nu}_{h_1 h_\gamma} \Phi^{m-2}_{CCD}\left(\begin{smallmatrix} \cdots \\ \cdots \end{smallmatrix}\right)$$

*A. Roggero, AM & F. Pederiva, arXiv:1304.1549 (2013)*

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- Can be easily generalized to CCSD, CCSDT ...
- Scaling only with # ph
- No scaling with particle number or basis size!

*A. Roggero, AM & F. Pederiva, arXiv:1304.1549 (2013)*

# Results for 3DEG

- The 3d electron gas is the canonical long range Hamiltonian.
- Good benchmark, many calculations available

How to do CIMC?

- Lattice in momentum space
- Single particle basis = plane waves
- Include all sp states up to some $k^2 \leq k^2_{max}$

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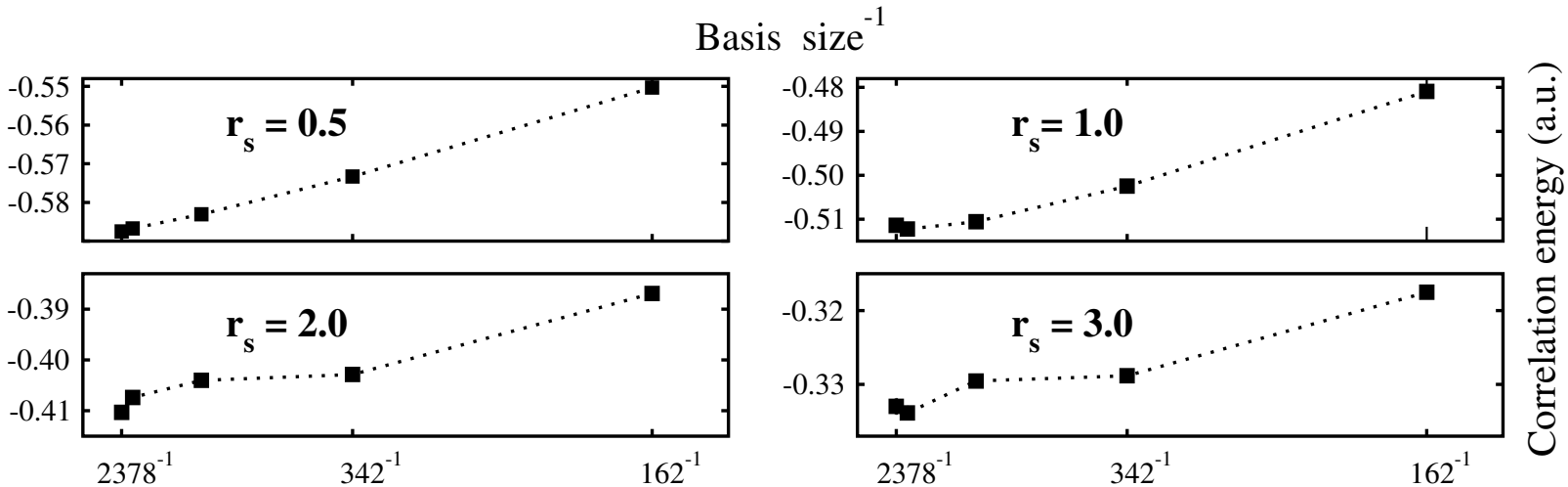


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- CCD + CIMC captures $\sim 95\%$ of the correlation energy
- No adjustable parameters in the wf
- Accuracy comparable to $r$-space MC
- Can improve systematically: CCDT, ...

*Roggero, AM & Pederiva, arXiv:1304.1549 (2013)*

# What have we acheived, so far?

- Formulated 'Fixed-node' DMC in CI/k-space ✓
- Shown how to use two well known classes of accurate wave functions as importance functions ✓
- Supervariational energies from CC wave functions
  Remember

$$E_{GS} \leq E_{CIMC} \leq \langle \Phi_G | H | \Phi_G \rangle$$

  when $\Phi_G \equiv \Phi_{CC}$

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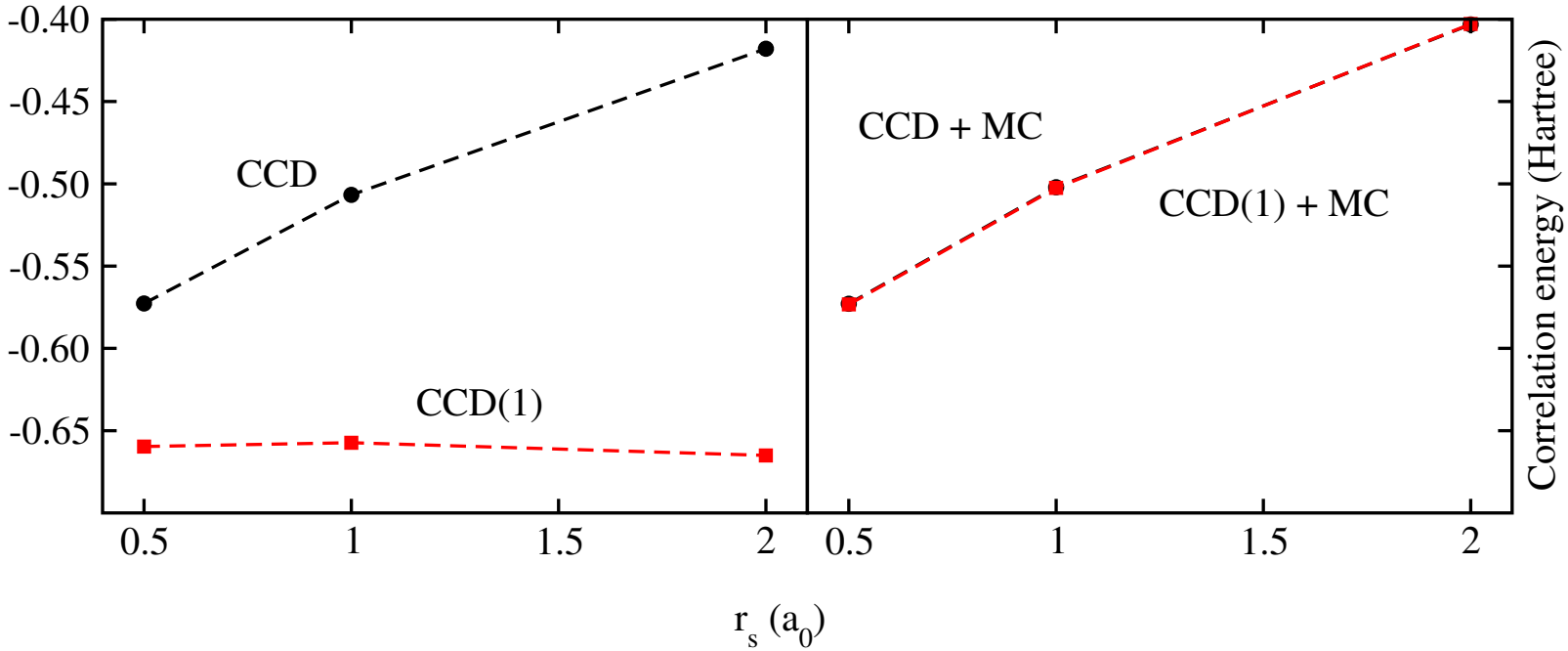
# But, we can do better ...

## Sign-structure important, not exact amplitudes




- CCD(1) = CCD wf with amplitudes taken from 2nd order perturbation theory
- Huge saving in computational time
- Can be very important for CCSD(T)

# Fringe benefits: momentum distribution

- Difficult in r-space MC
- However, its diagonal in k-space ✓
- We can even calculate pure estimators ✓
  - Typically in DMC/GFMC one calculates $\langle \Phi_G | \mathcal{O} | \Psi \rangle$
  - Not the same as $\langle \Psi | \mathcal{O} | \Psi \rangle$, if $[\mathcal{O}, H] \neq 0$
  - But in CIMC we can calculate $\langle \Psi | \mathcal{O} | \Psi \rangle$ using the Feynman-Hellmann theorem

$$\langle \Psi | n_k | \Psi \rangle = \left. \frac{\partial \langle H + \alpha n_k \rangle}{\partial \alpha} \right|_0 = \langle \Phi_G | n_k | \Psi \rangle - \text{const.} \times \text{cov}(E, n_k)$$

No need to calculate numerical derivatives! ✓

*Gaudin & Pitarke, PRL (2007)*
*Roggero, AM & Pederiva, in preparation*

# Fringe benefits: momentum distribution

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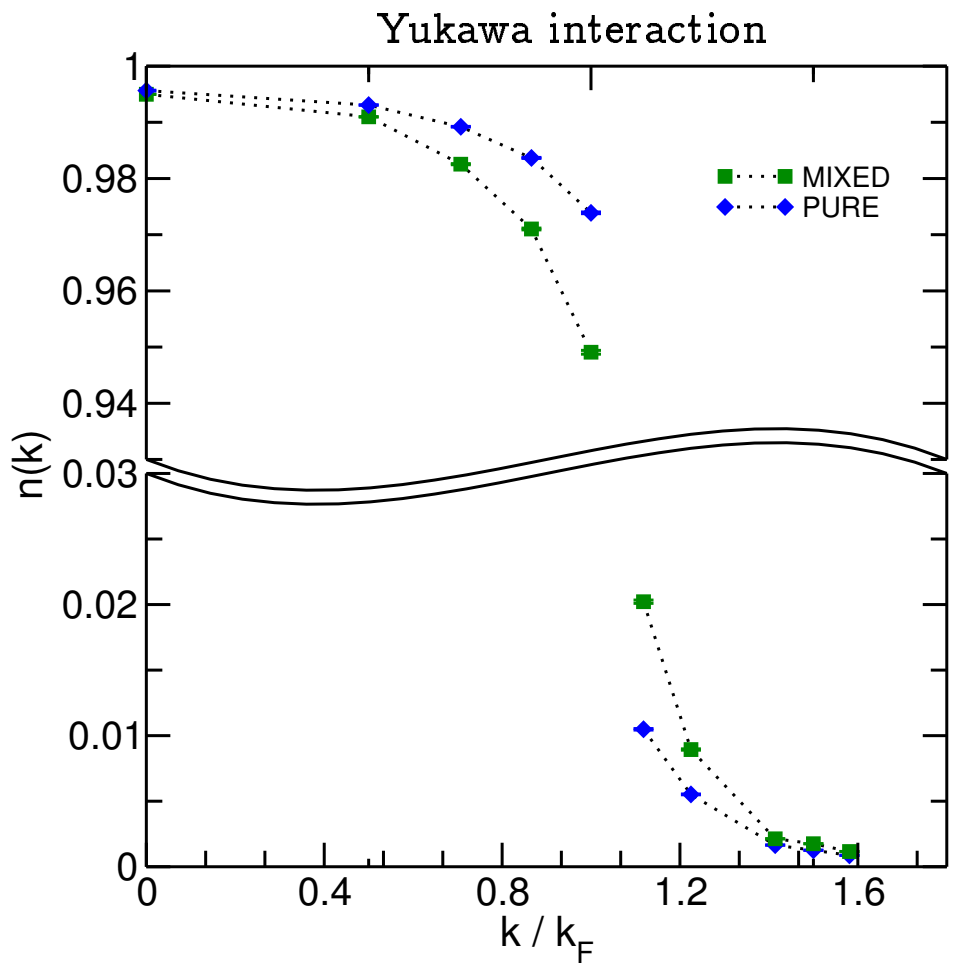


$|\mathcal{O}|\Psi\rangle$

the

$t.\times \mathrm{cov}(E, n_k)$

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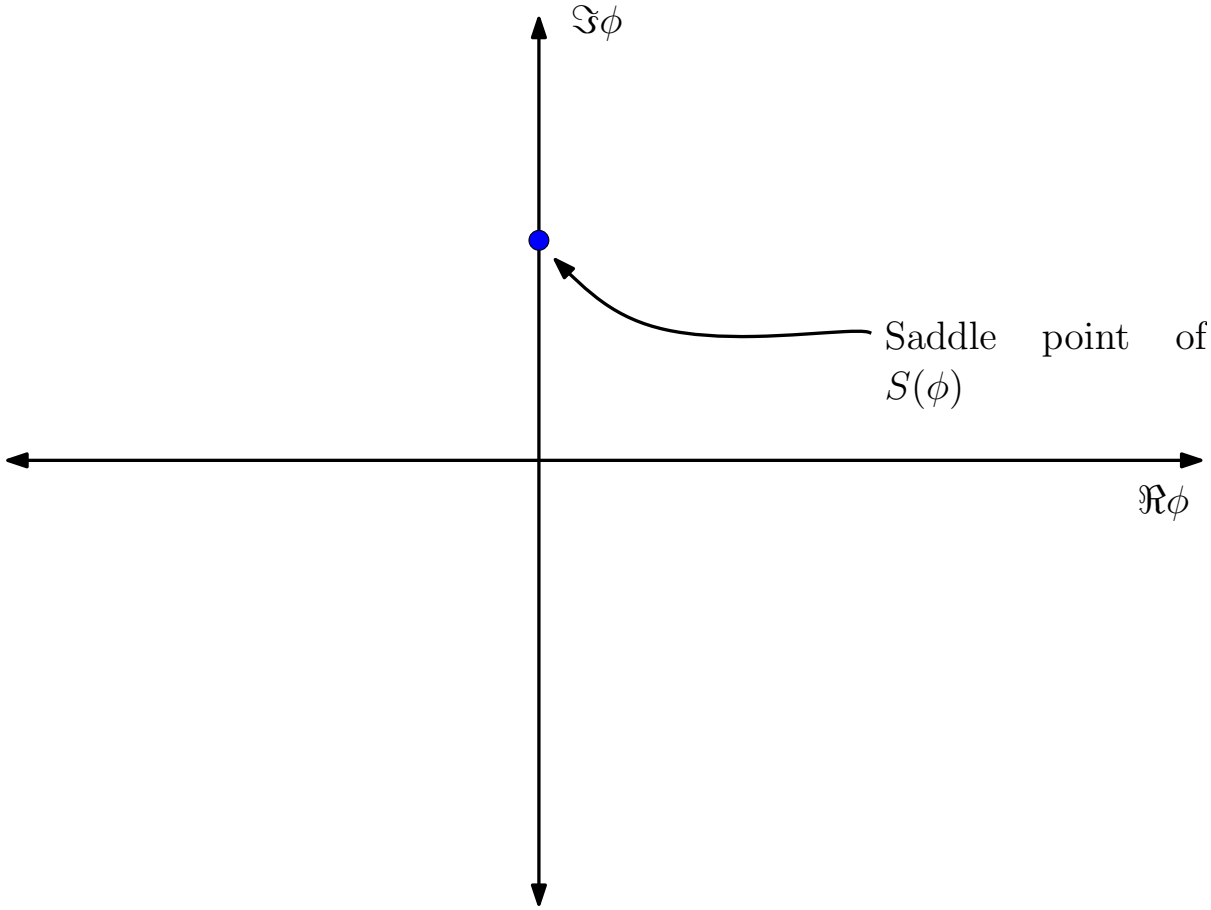
# Lefschetz thimble Monte Carlo

- We want to calculate quantities like this

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathbb{R}^n} d\phi \mathcal{O}(\phi) e^{-S(\phi)}}{\int_{\mathbb{R}^n} d\phi e^{-S(\phi)}}$$

- If $S(\phi)$ is not real, we have a sign problem.
- Can we do better by letting $\phi$ venture into the complex plane?

# Successive complexification of life



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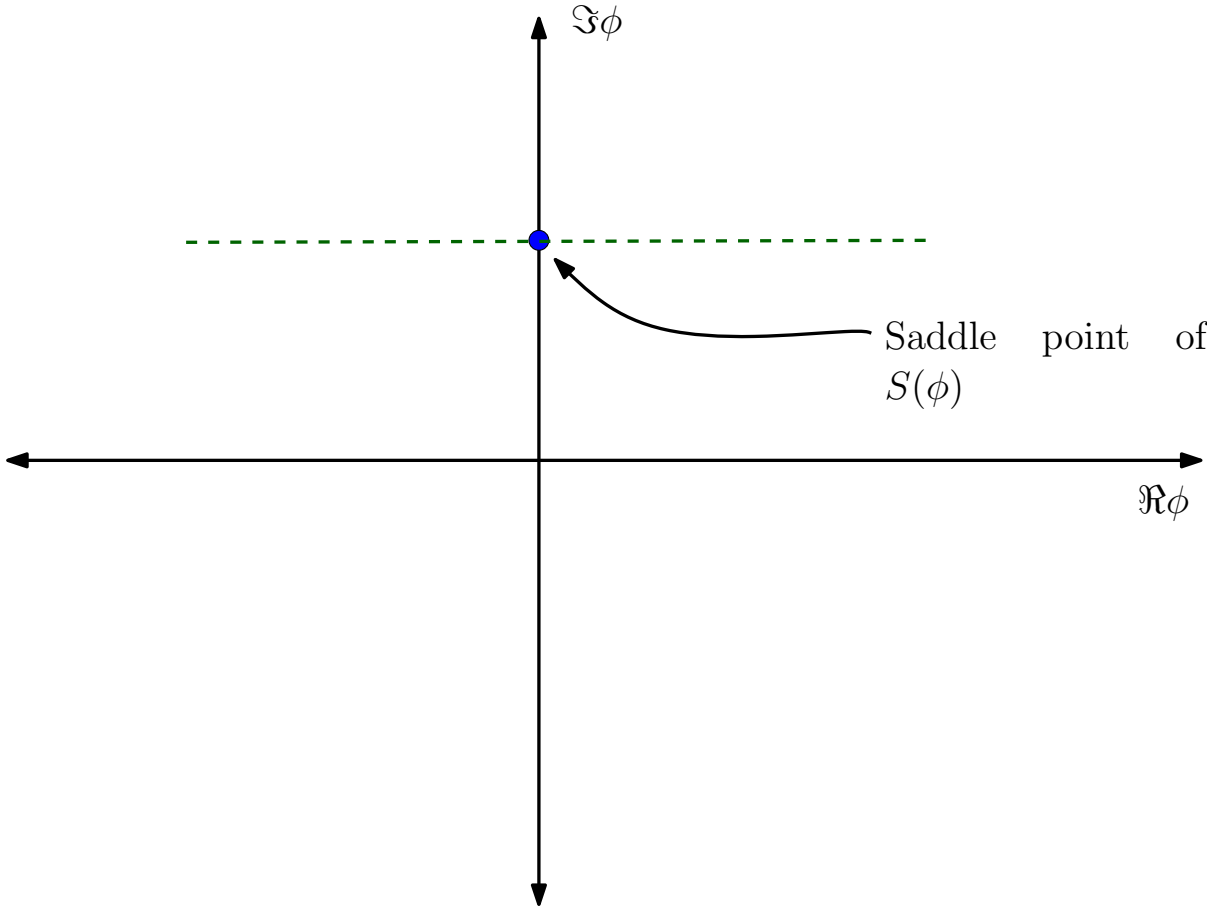

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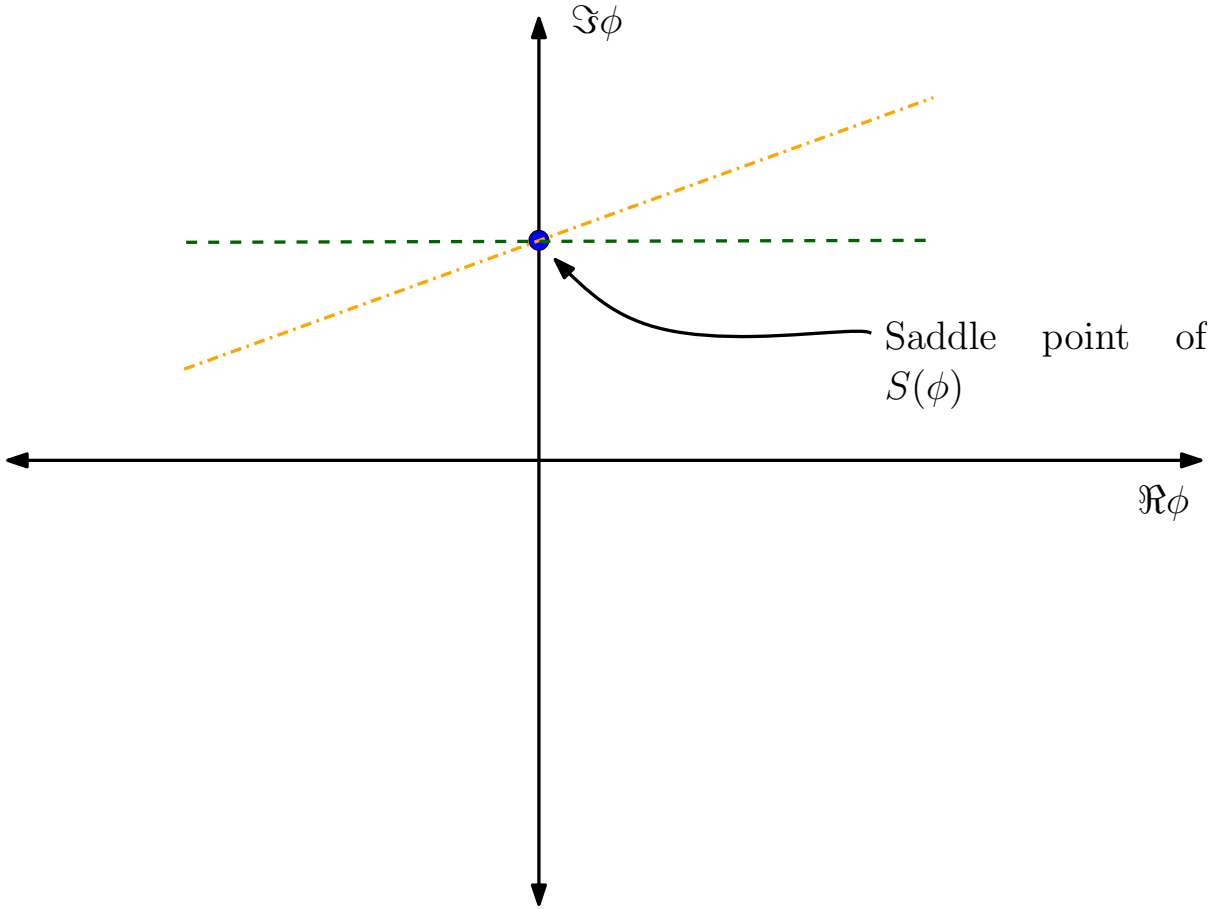

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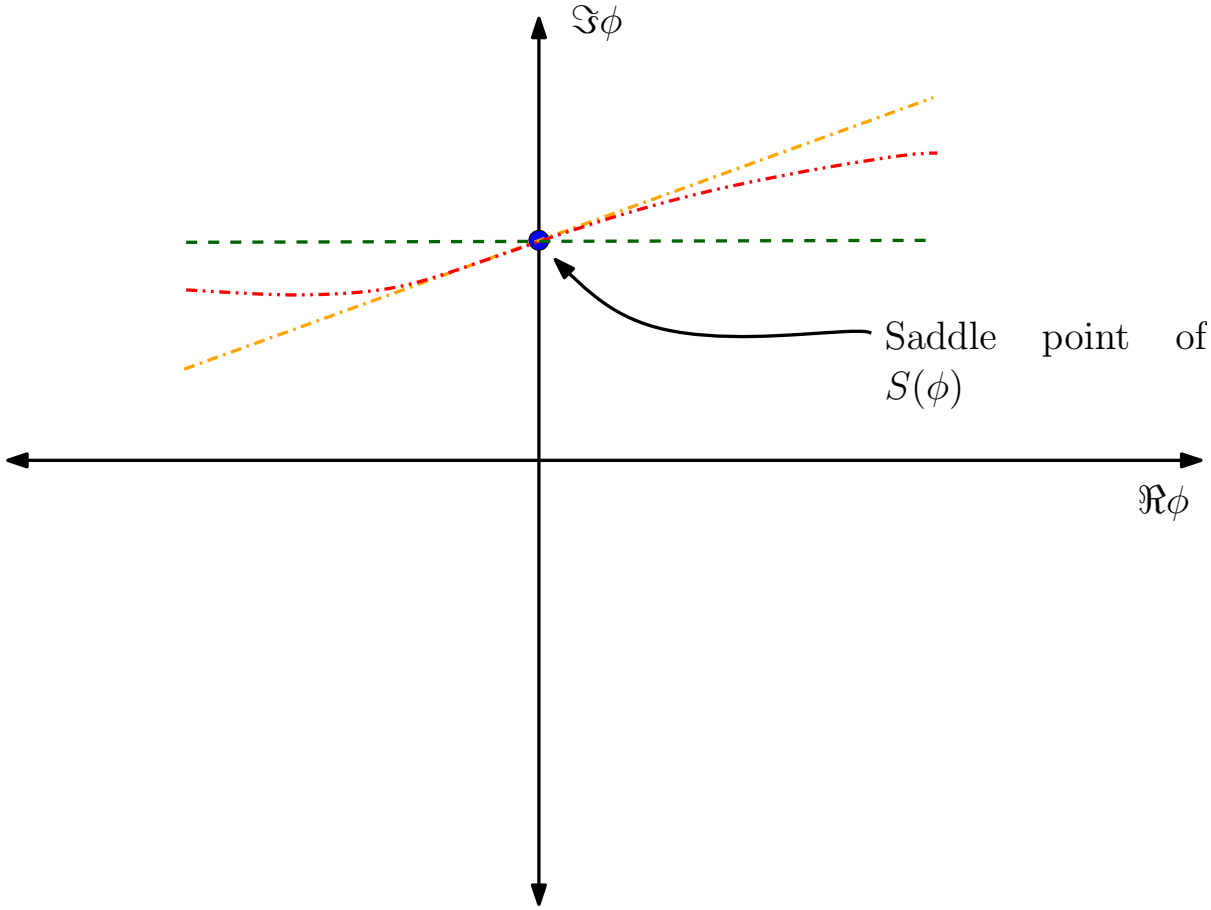

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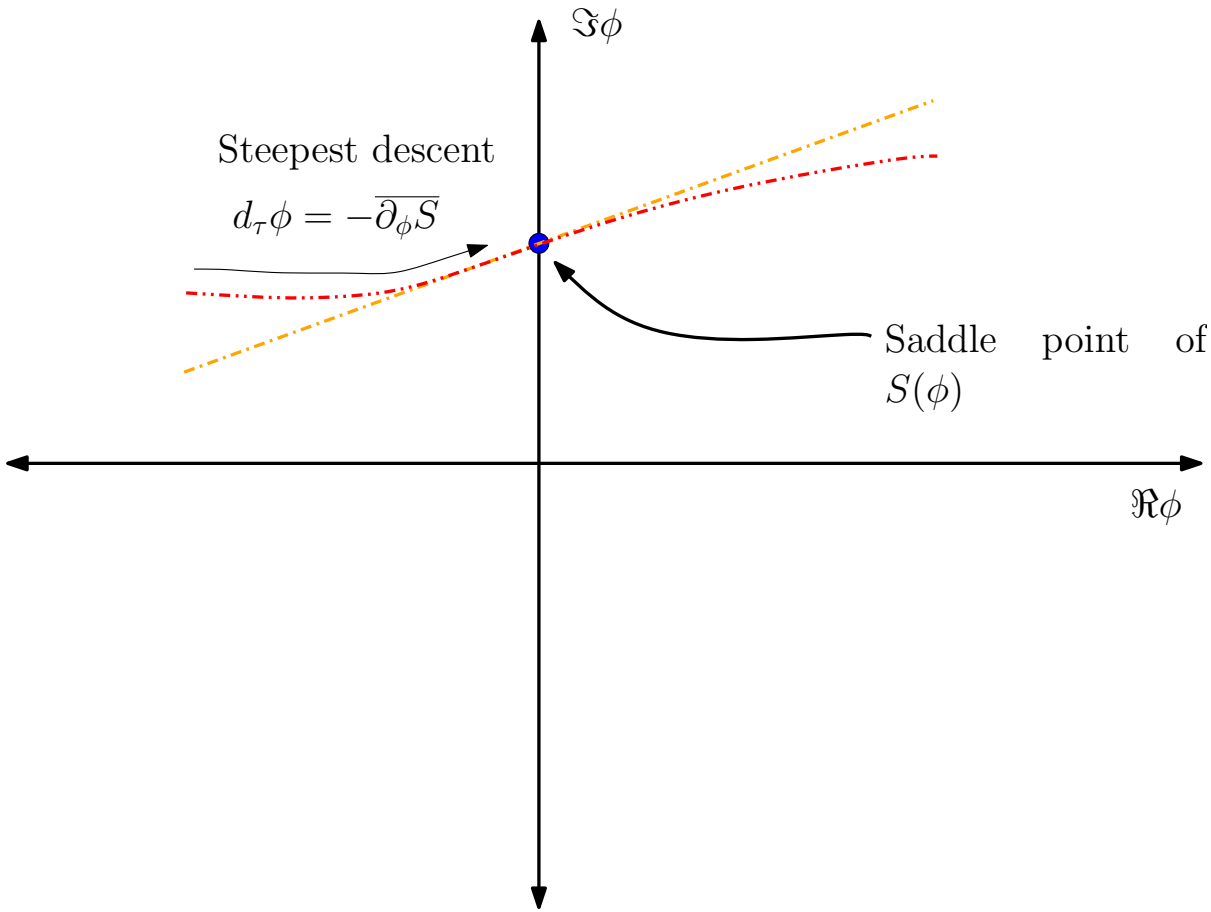

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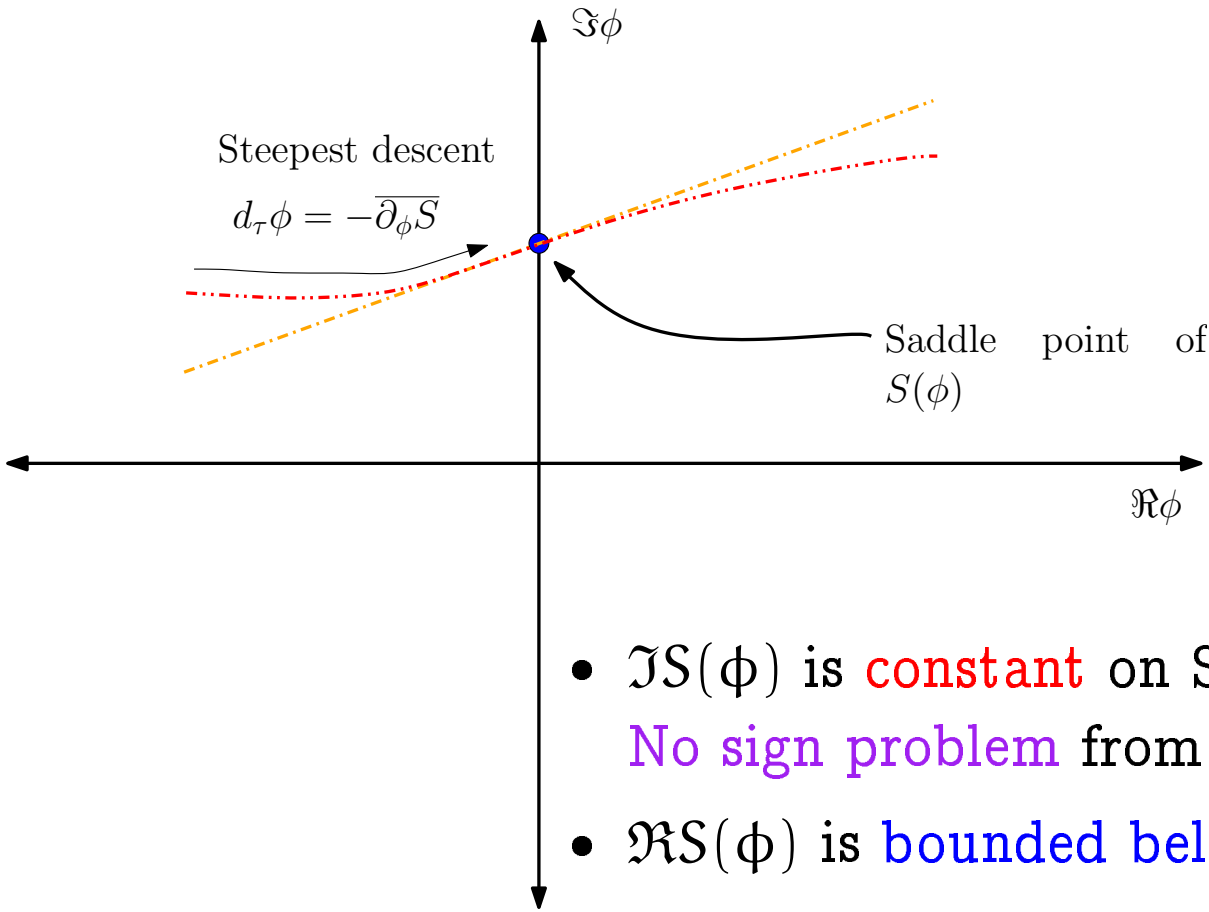



- $\Im S(\phi)$ is constant on SD path
  No sign problem from the action! ✓
- $\Re S(\phi)$ is bounded below on SD path ✓

# Life and times on the Lefschetz thimble

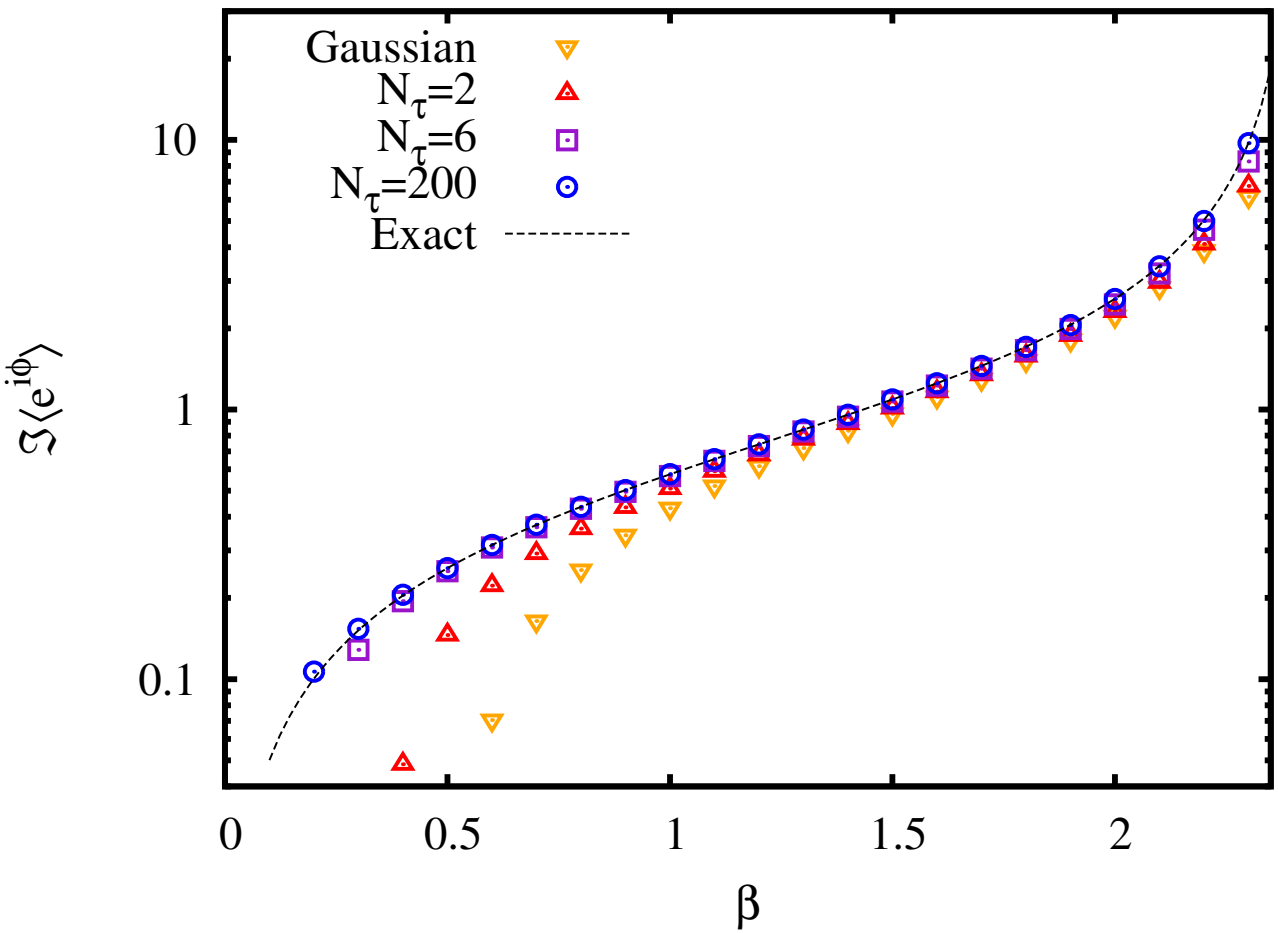
- A Lefschetz thimble is a many dimensional generalization of the paths of steepest descent
- It is the union of all paths of steepest descent which end at the saddle point at $\tau \to \infty$
- It is a n-dimensional object ✓
- On the Lefschetz thimble

$$\langle \mathcal{O} \rangle = \frac{e^{-i\Im S} \int_{\mathcal{J}} d\phi \mathcal{O}(\phi) e^{-\Re S(\phi)}}{e^{-i\Im S} \int_{\mathcal{J}} d\phi e^{-\Re S(\phi)}}$$

Constant

Non-trivial measure

# One-link model: $S(\phi) = -i\beta\cos(\phi)$

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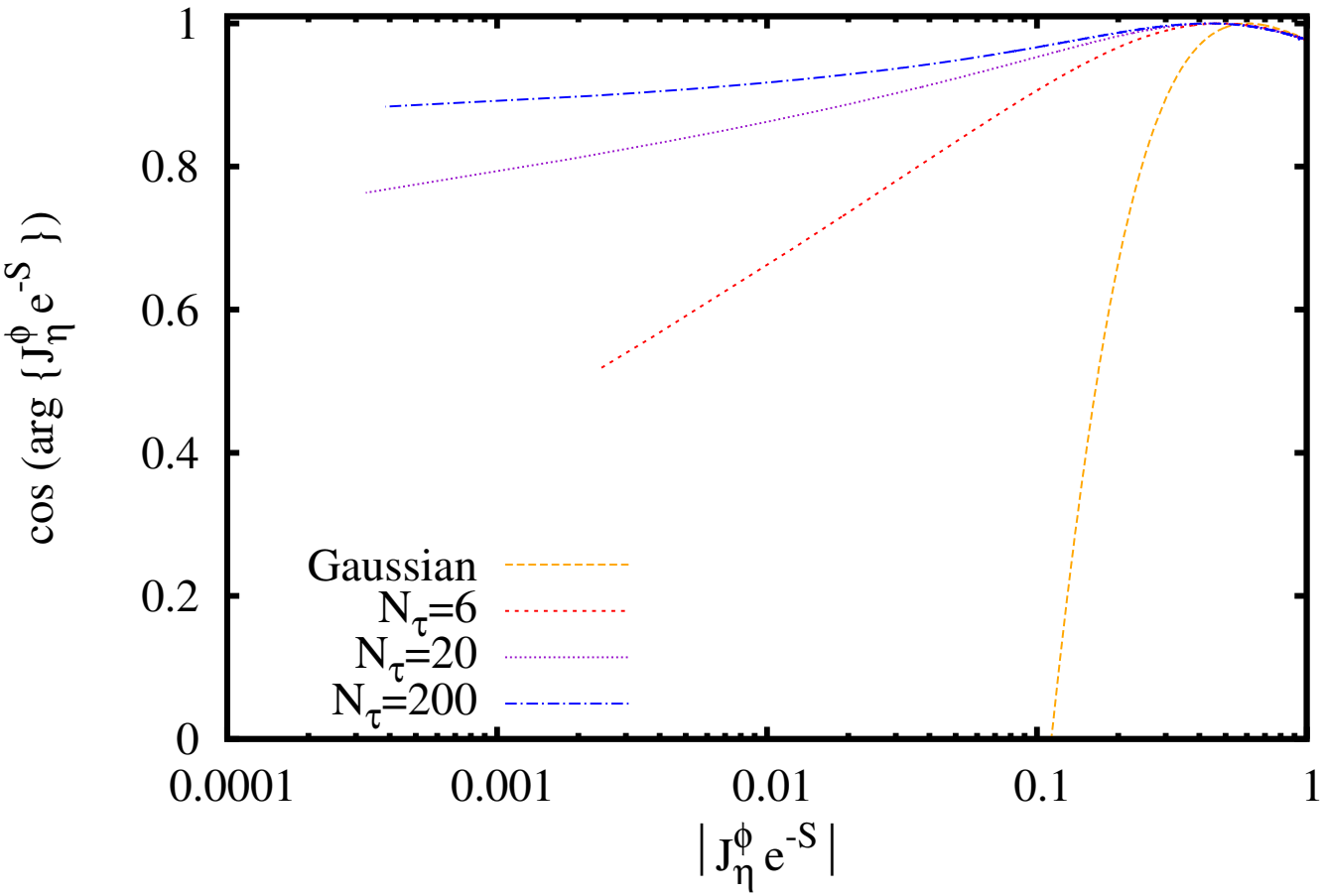


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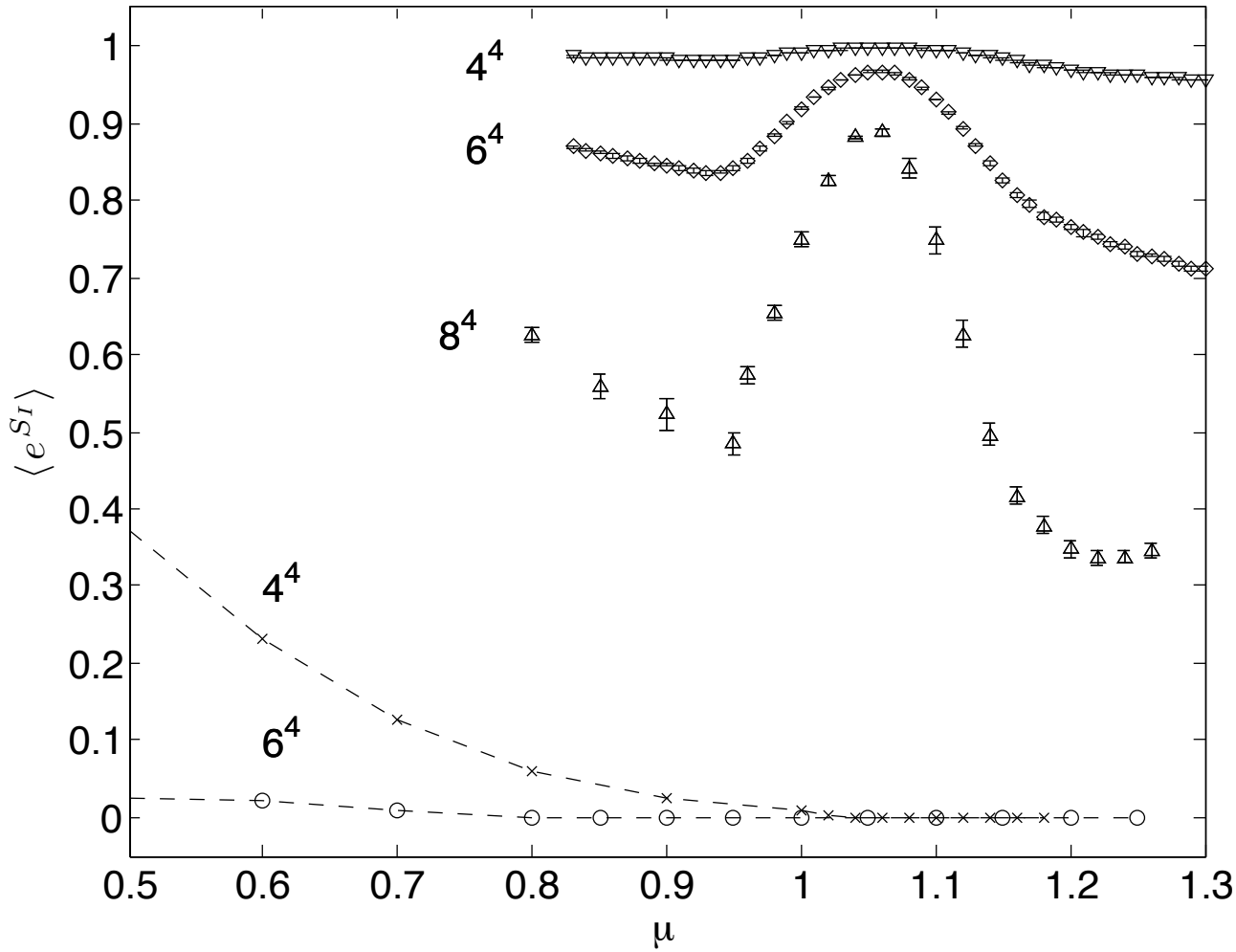
# Complex $\phi^4$ theory

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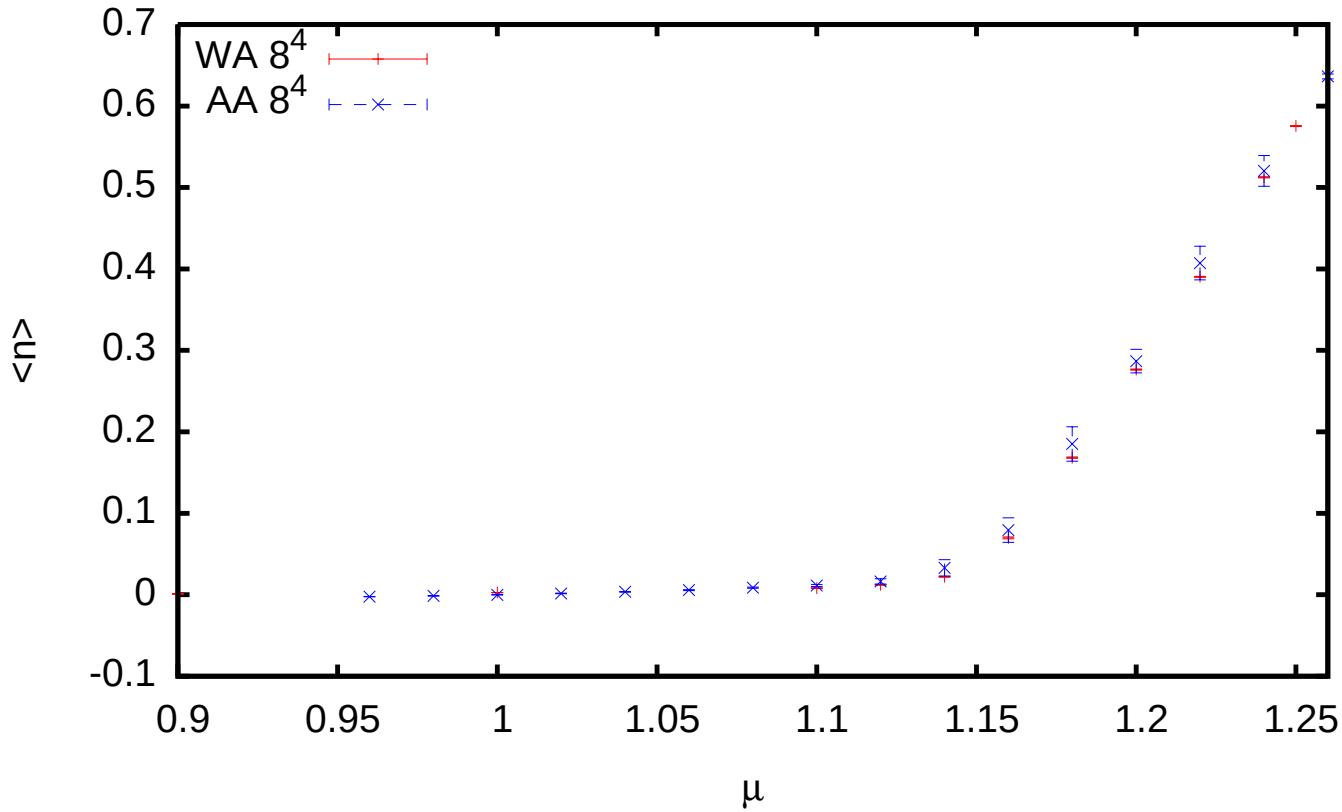


*M. Cristoforetti, F. di Renzo, AM & L. Scorzato, arXiv:1303.7204 (2013)*

# Details

Q How to sample on the Lefschetz thimble?

We have used two different algorithms

- Langevin dynamics, improved version in progress
- Mapping Lefschetz thimble $\rightarrow$ flat manifold + Metropolis

Q What about the measure?

Need to calculate the Jacobian of the tangent space

Q Does the measure lead to a sign problem?

We cannot prove that it does not, but

- Leading order $= 1$
- Fluctuations small where $e^{-\Re S}$ large

Q Enough to integrate on one (or a small #) thimble(s)?

Strong arguments in favor, but no rigorous proof

# THE END

# Fixing the sign problem in Fock space

- Comes from the Hamiltonian (if $H_{mn} > 0$ for $m \neq n$)
- Carrying walker sign leads to a null state
- No concept of 'continuity' in discrete Fock space
- Node fixing not possible 


Fixed 'sign' Hamiltonian

$$[\mathcal{H}_\gamma]_{mn} = \delta_{mn}\{H_{nn} + (1+\gamma) \sum_{s_{nn'}>0} \Phi_G(n') H_{n'n} \Phi_G(n)^{-1}\}$$
$$+ (1-\delta_{mn})\{\gamma\Theta(s_{mn}) + \Theta(-s_{mn})\}H_{mn}$$

where $s_{mn} = \text{sign}\{\Phi_G(m) H_{mn} \Phi_G(n)^{-1}\}$

# Fixing the sign problem in Fock space

$$[\mathcal{P}_\gamma]_{\mathbf{mn}} = \Phi_G(\mathbf{m}) \left\{ \delta_{\mathbf{mn}} - \Delta\tau \left( [\mathcal{H}_\gamma]_{\mathbf{mn}} - E_T \delta_{\mathbf{mn}} \right) \right\} \Phi_G^{-1}(\mathbf{n})$$

- $\mathcal{H}_{\gamma=-1} = H$
- $\mathcal{H}_{0\leq\gamma\leq1}$ has no sign problem by construction
- GS energies of $\mathcal{H}_{0\leq\gamma\leq1}$ provide upper bounds for the GS energy of H
- So does any linear extrapolation to $\gamma = -1$

  *ten Haaf et al., PRB (1995); Sorella & Capriotti, PRB (2000);*

  *Beccaria, PRB (2001)*
  *AM & Y. Alhassid, arXiv:1304.1645 (2013)*

Our tightest upper bound for GS energy of H is :

$$E_{CIMC} = \mathbf{2E}_{GS}[\mathcal{H}_{\gamma=\mathbf{0}}] - \mathbf{E}_{GS}[\mathcal{H}_{\gamma=\mathbf{1}}]$$