Worldline Approach to Few-Body Physics on the Lattice

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Few-body physics of contact interactions

- Nuclear physics (pionless effective field theory)
- Ultra-cold gases
- Trapped atoms

1D Systems

- Amazing experimental progress on ultra-cold atoms confined to 1D has renewed interest in 1D systems (Guan, Batchelor, and Lee 2013)
  - The effective 1D interaction strength can be tuned as desired through Feshbach resonances (Chin et al. 2010)
- Systems with effective $SU(N)$ internal symmetry
- Experiments with mixed species have given access to mass-imbalanced systems, such as ^{6}Li and ^{40}K (Trenkwalder et al. 2011)
- Analytic solutions (for example, (Yang 1967; Gaudin 1967)) are known for special configurations in 1D, but the general case of spin and mass-imbalanced is unsolved.

Sign problems in 1D system

- Traditional auxiliary field MC has sign problems even in 1D: Good testing ground for new approaches to solve sign problems.
- Examples:
  - (Alexandru et al. 2017): Thimble approach for 1D Thirring model
  - (Ayyar, Chandrasekharan, and Rantaharju 2018): Fermion bag approach for the 1D Thirring model
  - (Rammelmüller et al. 2017): Complex Langevin for mass-imbalanced non-relativistic fermions with repulsive interactions
- World-line formulations solves the sign problem for 1D systems in several cases (Wiese 1993; Evertz 2003)

The Hamiltonian: Continuum

$$H_{\text{continuum}} = -\sum_{\alpha=\uparrow,\downarrow} \int dx \frac{1}{2m_\alpha} \psi_\alpha^\dagger \nabla^2 \psi_\alpha + g \int dx \;\; \psi_\uparrow^\dagger \psi_\uparrow \psi_\downarrow^\dagger \psi_\downarrow \quad (1)$$

Parameters:

- Mass-imbalance

$$\bar{m} = \frac{m_\uparrow - m_\downarrow}{m_\uparrow + m_\downarrow}, \; m = \frac{m_\uparrow + m_\downarrow}{2} \quad (2)$$

- Coupling:

$$\gamma = g/n \quad (3)$$

  where $n = N/L$ is the number density.
- E_{FG}: Fermi-gas energy (mass-balanced).

The Hamiltonian: Lattice

- Lattice (spatial box size L_x, lattice spacing a):

$$H = -\sum_{\alpha} t_\alpha \sum_{\langle ij \rangle} \left(c^\dagger_{\alpha i} c_{\alpha j} + c^\dagger_{\alpha j} c_{\alpha i} - 2 c_{\alpha i} c^\dagger_{\alpha i} \right) + U \sum_i {c_{\uparrow i}}^\dagger c_{\uparrow i} {c_{\downarrow i}}^\dagger c_{\downarrow i} \tag{4}$$

  where $\alpha = \{\uparrow, \downarrow\}$ is the species label, i is the position index, and $t_\alpha = \frac{1}{2 m_\alpha a^2}$, $U = \frac{g}{a}$.
- *Goal:* compute the ground-state energies of Hamiltonian (4) in the $(N_\uparrow, N_\downarrow)$ particle sector for general masses $m_\uparrow \neq m_\downarrow$ with both attractive and repulsive interactions.

Worldline Formulation

- Traditional auxiliary field MC has positive weights only in the case of equally populated spin species and equal masses.
- The world-line formulation (almost) solves the sign problem for fermions in 1D!
- Sign problems for fermions only arise from boundary conditions.
- No sign problem in a trap or open boundary conditions. With periodic boundary conditions a sign problem can emerge but is mild. (Wiese 1993; Evertz 2003)

Worldline Formulation

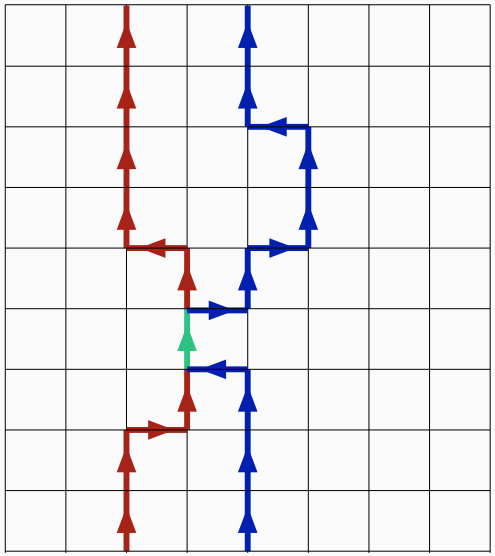
- The partition function:

$$Z = \mathrm{Tr}\, e^{-\beta \hat{H}} \tag{5}$$

$$= \mathrm{Tr} \sum_N \int_0^\beta dt_1 \cdots dt_N \prod_{k=1}^{N} e^{(t_k - t_{k_1})[\sum_x (2t_\uparrow - \mu_\uparrow)\hat{N}_{\uparrow x} - U\hat{N}_{\uparrow x}\hat{N}_{\downarrow x}]}\, \hat{H}_{\mathrm{hop}} \tag{6}$$

$$= \sum_{\mathcal{C}} W[\mathcal{C}] \tag{7}$$

where $\mathcal{C}$ are world-line configurations of the particles on a space-time lattice.

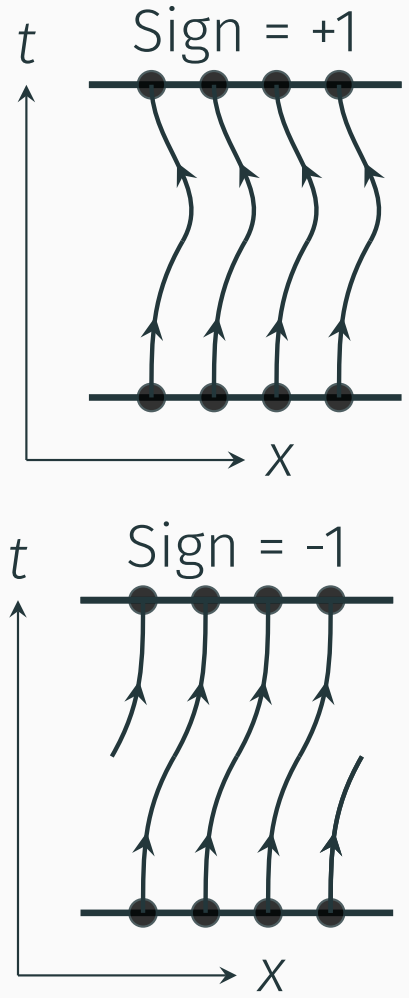


Wordline Formulation : Sign Problem in 1D

- Only nearest neighbor hops $\implies$ fermions effectively become *hardcore bosons*, up to a sign from cyclic permutations.
- With periodic boundary conditions (both space and time),

$$\mathrm{Sign}[\mathcal{C}] = (-1)^{(N_p-1)N_w} \quad (8)$$

- No sign problem for odd particle numbers!



Example of how the sign problem arises in the worldline formulation.

Worm Algorithm

- Very efficient way to generate uncorrelated configurations. (Prokof'ev and Svistunov 2001; Adams and Chandrasekharan 2003; Evertz 2003)
- Chemical potential allows to tune the average number of particles in the ground state.

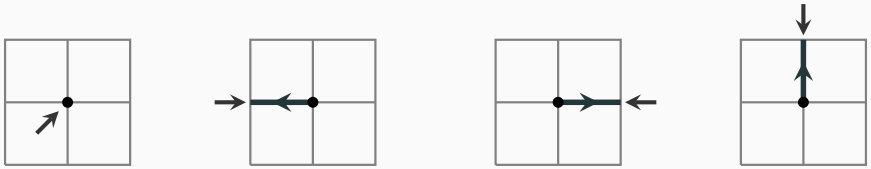
$$\hat{H}_\mu = \hat{H} - \mu_1 \hat{N}_1 - \mu_2 \hat{N}_2 \tag{9}$$

- Extension to higher dimensions is trivial

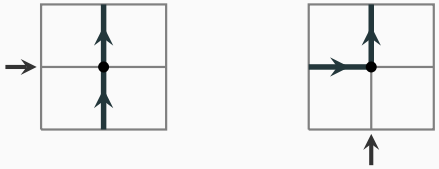
Worm Algorithm: Generating Configurations

Worm Algorithm: Generating Configurations

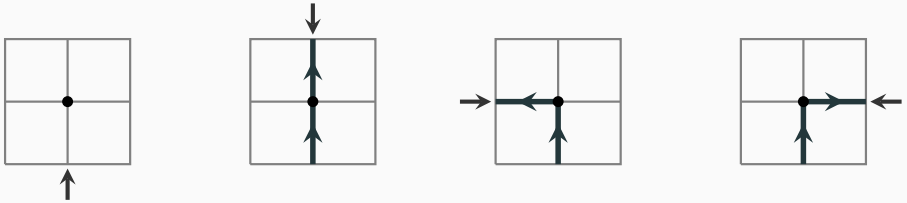
- Begin/End Updates:

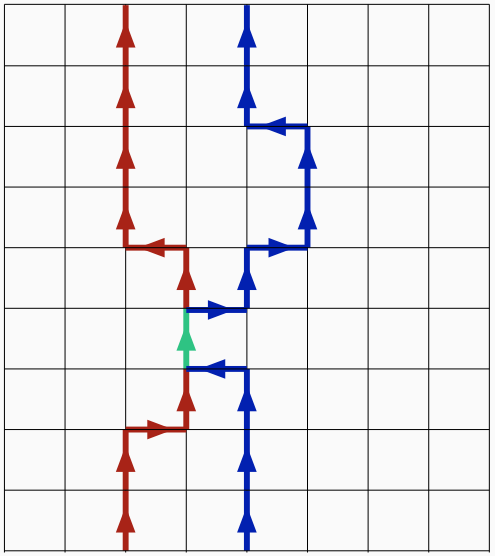


- Bond 2-flips:



- Bond 4-flips:



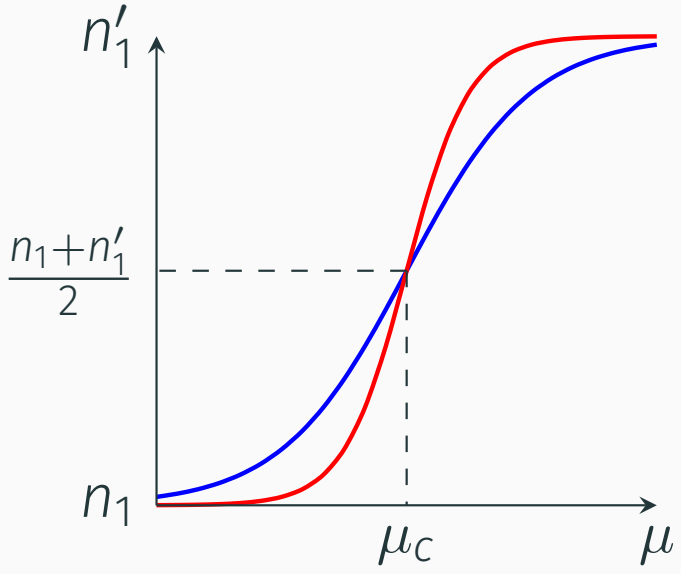


Worm Algorithm: Method 1

- At critical μ_c, for $\beta \to \infty$, the particle number jumps: $(n_1, n_2) \to (n_1', n_2')$. Here, we have

$$E_{(n_1,n_2)} - \mu_1 n_1 - \mu_2 n_2 = E_{(n_1',n_2')} - \mu_1 n_1 - \mu_2 n_2 \tag{10}$$

$$\implies E_{(n_1,n_2)} - E_{(n_1',n_2')} = \mu_1 \Delta n_1 + \mu_2 \Delta n_2 \tag{11}$$

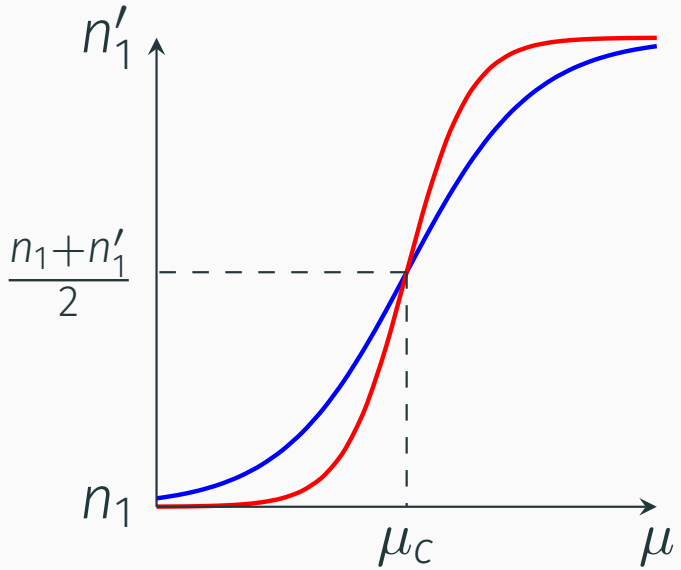


Worm Algorithm: Method 1

- We can fit a ***single*** parameter $\mu_c = \Delta E / \Delta n$ to the average particle number close to critical μ_c:

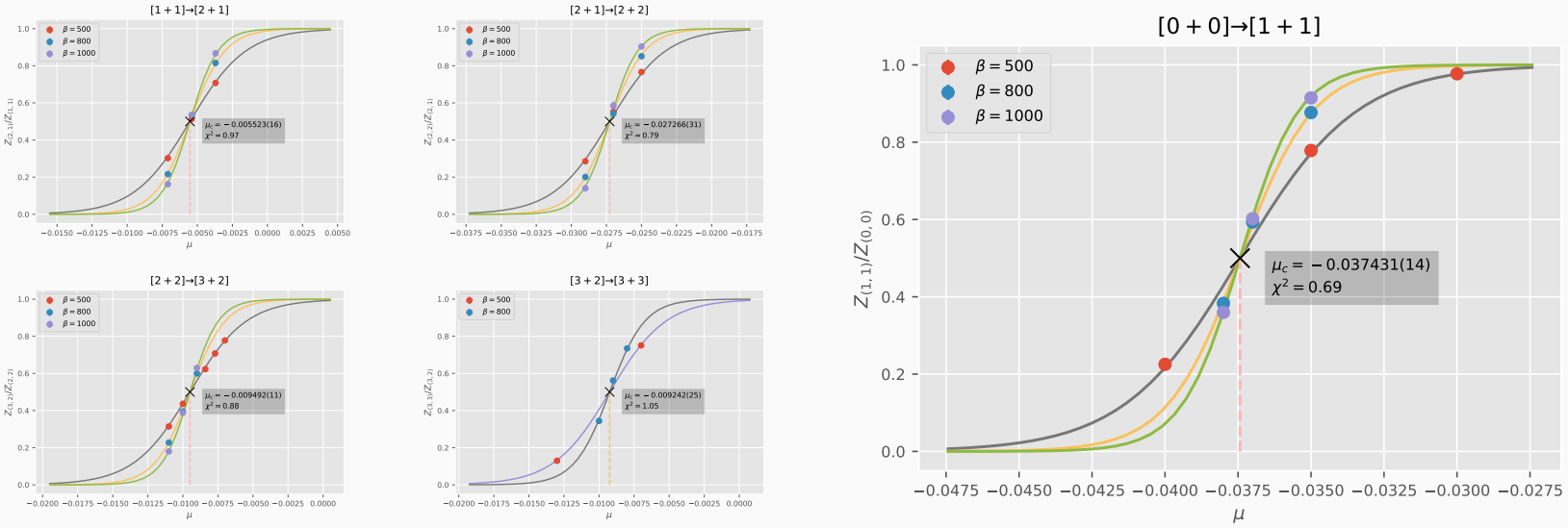
$$\langle n \rangle = \frac{n_1 Z_1 + n_2 Z_2}{Z_1 + Z_2} = \frac{g_1 n_1 + g_2 n_2 e^{-\beta(\Delta E - \mu \Delta n)}}{g_1 + g_2 e^{-\beta(\Delta E - \mu_c \Delta n)}}. \tag{12}$$

  (Note that g_1, g_2 are integers, so we can often fix them.)
- This can be used to get very precise results for the energy difference between $\Delta E = E_{n_1+1,n2} - E_{n_1,n_2}$.



Worm Algorithm: Method 1 Example

Attractive interaction, $N = N_\uparrow + N_\downarrow = 3 + 3$, $L_x = 40$, $\gamma = -3.0$



- Adding all the energy differences up, we get

$$E_{(3,3)} = -0.08895(5) \tag{13}$$

Worm Algorithm: Method 2

- Restrict the particle numbers to a fixed values, and simply measure the average energy.

$$\langle E \rangle = \frac{1}{Z} \operatorname{Tr} \hat{H} e^{-\beta \hat{H}} \tag{14}$$

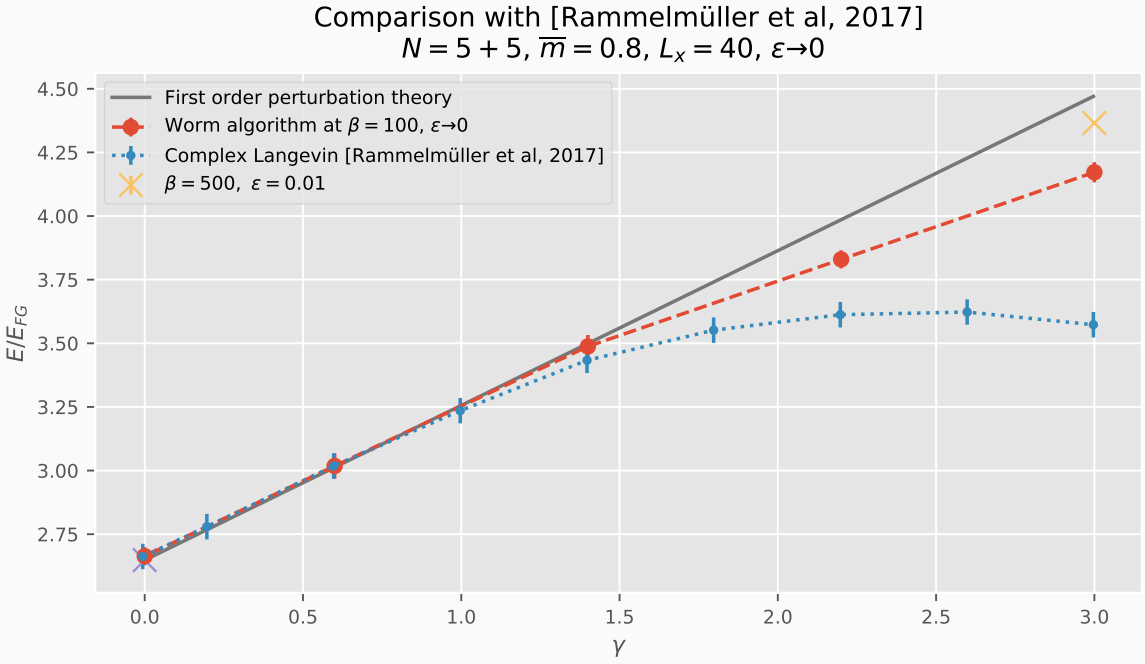
$$= \frac{1}{Z} \sum_{\mathcal{C}} E[\mathcal{C}] W[\mathcal{C}] \tag{15}$$

$$E[\mathcal{C}] = -\sum_{\alpha=\uparrow,\downarrow} \frac{N_H^\alpha}{\beta} - 2t^{(\alpha)} N_P^\alpha - U \frac{N_I}{2L_T} \tag{16}$$

where $N_H =$ number of hops, $N_P =$ number of particles, $N_I =$ number of interactions in each layer.

Results: Comparison with Complex Langevin [Preliminary!]

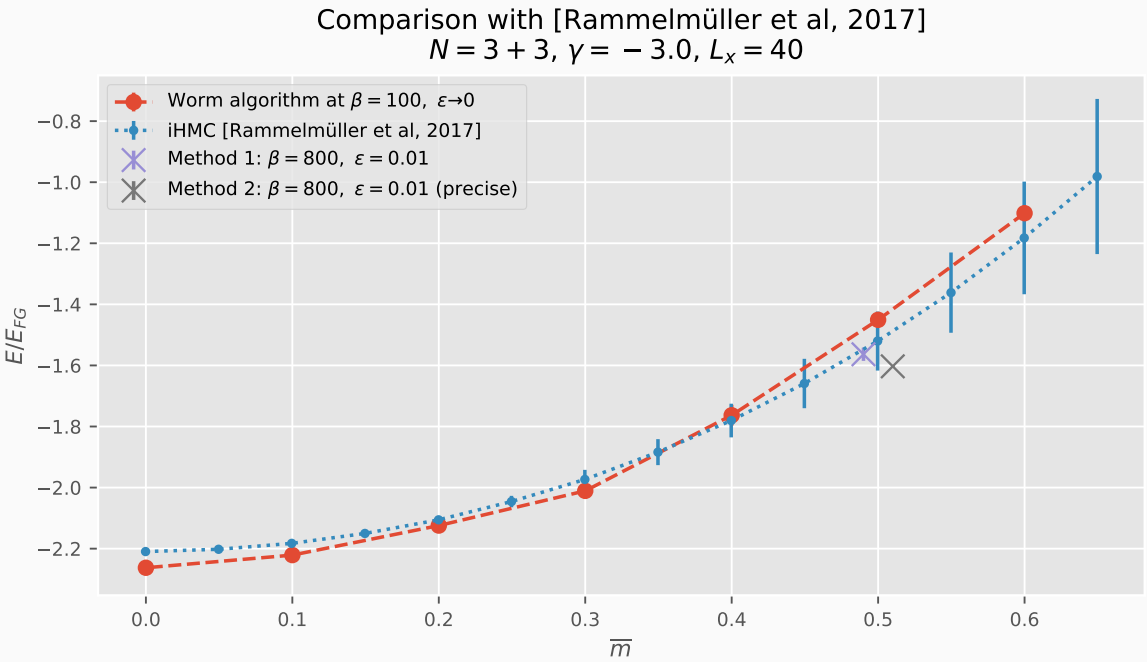
Repulsive interaction, 5+5 Particles



- Disagreement with Complex Langevin for large γ!

Results: Comparison with iHMC [Preliminary!]

Attractive interaction, 3+3 particles



- iHMC has a sign problem for repulsive interactions.

Outlook and Conclusions

- We have a new method to investigate few body physics of contact interactions in any dimension
- In 1D, the sign problem is under control – relevant for physics of ultracold gases and trapped atoms
- Exploring ways to solve the sign problems with this method in higher dimensions – relevant for nuclear physics
- There seems to be a disagreement with Complex Langevin results – ongoing investigation

Thank You!