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**
  \[ \bar{m} = \frac{m_\uparrow - m_\downarrow}{m_\uparrow + m_\downarrow}, \quad m = \frac{m_\uparrow + m_\downarrow}{2} \]  \quad (2)

- **Coupling**:
  \[ \gamma = g/n \]  \quad (3)

where \( n = N/L \) is the number density.

- **\( E_{\text{FG}} \)**: Fermi-gas energy (mass-balanced).
The Hamiltonian: Lattice

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

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

(4)

where $\alpha = \{\uparrow, \downarrow\}$ is the species label, $i$ is the position index, and $t_\alpha = \frac{1}{2m_\alpha a^2}$, $U = \frac{g}{a}$.

- 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:

$$Z = \text{Tr} \, e^{-\beta \hat{H}}$$  \hspace{1cm} (5)

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

$$= \sum_C W[C]$$  \hspace{1cm} (7)

where $C$ are world-line configurations of the particles on a space-time lattice.
Wordline Formulation : Sign Problem in 1D

- Only nearest neighbor hops $\rightarrow$ fermions effectively become \textit{hardcore bosons}, up to a sign from cyclic permutations.

- With periodic boundary conditions (both space and time),

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

- 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.

\[
\hat{H}_\mu = \hat{H} - \mu_1 \hat{N}_1 - \mu_2 \hat{N}_2
\]  

(9)

• Extension to higher dimensions is trivial
Worm Algorithm: Generating Configurations
Worm Algorithm: Generating Configurations

- **Begin/End Updates:**

- **Bond 2-flips:**

- **Bond 4-flips:**
At critical $\mu_c$, for $\beta \to \infty$, the particle number jumps: $(n_1, n_2) \to (n'_1, n'_2)$. Here, we have

\[ E(n_1, n_2) - \mu_1 n_1 - \mu_2 n_2 = E(n'_1, n'_2) - \mu_1 n_1 - \mu_2 n_2 \quad (10) \]

\[ \implies E(n_1, n_2) - E(n'_1, n'_2) = \mu_1 \Delta n_1 + \mu_2 \Delta n_2 \quad (11) \]
Worm Algorithm: Method 1

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

$$\langle n \rangle = \frac{n_1 Z_1 + n_2 Z_2}{Z_1 + Z_2} = \frac{g_1 n_1 + g_2 n_2 e^{-\beta(\Delta E - \mu_c \Delta n)}}{g_1 + g_2 e^{-\beta(\Delta E - \mu_c \Delta n)}}.$$  \hspace{1cm} (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 $\Delta E = E_{n_1+1,n_2} - E_{n_1,n_2}$. 

\[ n_1' \]
\[ n_1 + n_1' \]
\[ \mu_c \]
\[ \mu \]
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

\[
E_{(3,3)} = -0.08895(5)
\]  

(13)
Worm Algorithm: Method 2

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

\[ \langle E \rangle = \frac{1}{Z} \text{Tr} \hat{H} e^{-\beta \hat{H}} \]  

\[ = \frac{1}{Z} \sum_{C} E[C] W[C] \]  

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

where \( N_H = \text{number of hops} \), \( N_P = \text{number of particles} \), \( N_I = \text{number of interactions in each layer} \).
Results: Comparison with Complex Langevin [Preliminary!]

Repulsive interaction, 5+5 Particles

- Disagreement with Complex Langevin for large $\gamma$!
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!