Density of states techniques for fermion worldlines

Christof Gattringer

Austrian Science Fund FWF

& University of Graz

FWF

Der Wissenschaftsfonds.

UNI GRAZ

Introductory remarks

- Worldline representations are a powerful tool (finite density, topological terms ...).
- Useful and elegant properties. E.g.: particle number = winding number.
- Fermion worldlines have remnant signs from Grassmann nature and Dirac algebra.
- Can we take care of this sign problem and keep using fermion worldlines?

Here we explore density of states (DoS) techniques for fermion worldline simulations.

Compare also: O. Francesconi, PhD thesis Univ. Swansea & Univ. Grenoble, 2021
`https://tel.archives-ouvertes.fr/tel-03403475`

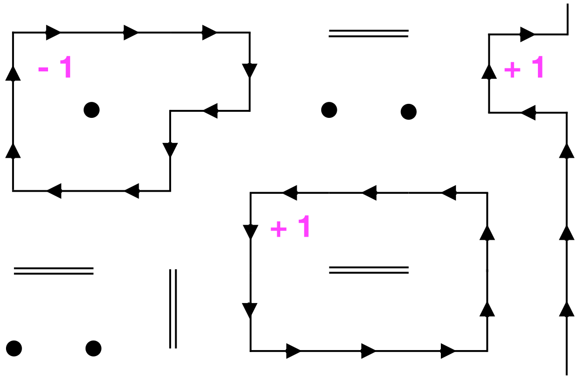
A simple model and its worldline representation

- Staggered fermions with mass term and quartic self interaction:

$$S \;=\; \sum_{x,\nu} \gamma_{x,\nu} \overline{\psi}_x \frac{\psi_{x+\hat{\nu}} - \psi_{x-\hat{\nu}}}{2} \;+\; M \sum_x \overline{\psi}_x \psi_x \;-\; \frac{J}{4} \sum_{x,\nu} \overline{\psi}_x \psi_x \overline{\psi}_{x+\hat{\nu}} \psi_{x+\hat{\nu}}$$

- Integrating out the Grassmann variables $\Rightarrow$ worldline representation:

$$Z \;=\; \sum_{\{m,d,l\}} (2M)^{\#\,m} \;\; (1+J)^{\#\,d} \;\; \prod_l \text{sign}(l)$$



Formulation as density of states problem

- Worldline representation:

$$Z \;=\; \sum_{\{m,d,l\}} (2M)^{\#\,m} \;\; (1+J)^{\#\,d} \;\; (-1)^{\mathcal{N}}$$

$$\mathcal{N} \;=\; \text{number of loops with negative sign}$$

- Introduce a density of states:

$$\rho_{n} \;=\; \sum_{\{m,d,l\}} (2M)^{\#\,m} \;\; (1+J)^{\#\,d} \;\; \delta_{n\,,\mathcal{N}}$$

- Partition function is a weighted sum of the density:

$$Z \;=\; \sum_{n=0}^{\infty} \rho_n \, (-1)^n$$

Parameterization of the density and FFA approach (Gattringer, Giuliani, Törek)

- Piecewise constant parameterization of the density in the form:

$$\rho_n \;=\; \rho_{n-1}\, e^{\,-a_n} \qquad \text{with} \qquad a_0 = 0 \;\Leftrightarrow\; \rho_0 \;=\; 1$$

- Restricted partition sum with a control parameter $\lambda \in \mathbb{R}$: (Langfeld, Lucini, Rago)

$$Z_n(\lambda) \;=\; \sum_{\{m,d,l\}} (2M)^{\#\, m}\, (1+J)^{\#\, d}\, e^{\,\lambda \mathcal{N}}\, \Theta_n(\mathcal{N})$$

$$\Theta_n(\mathcal{N}) \;=\; \begin{cases} 1 & \text{for } \mathcal{N} \in \{n, n+1\} \\ 0 & \text{otherwise} \end{cases}$$

- Restricted expectation value for the determination of the a_n:

$$\langle \mathcal{N} \rangle_n(\lambda) \;=\; \frac{\partial \ln\, Z_n(\lambda)}{\partial \lambda} \;=\; n \,+\, \frac{1}{2}\left[1 \,+\, \tanh\!\left(\frac{\lambda - a_{n+1}}{2}\right)\right]$$

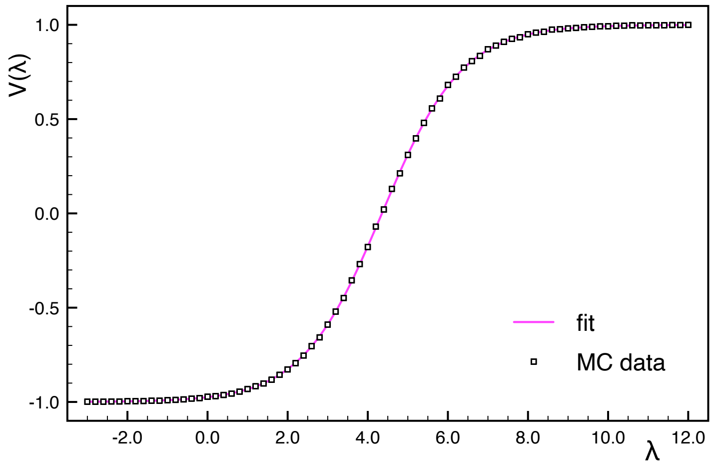
FFA determination of the parameters a_n

- Compute $\langle \mathcal{N} \rangle_n(\lambda)$ in a numerical simulation:

$$\langle \mathcal{N} \rangle_n(\lambda) \; = \; \frac{1}{Z_n(\lambda)} \sum_{\{m,d,l\}} (2M)^{\# m} \; (1+J)^{\# d} \; \Theta_n(\mathcal{N}) \, e^{\lambda \mathcal{N}}$$

- Determine the parameters a_n from a fit and from those compute ρ_n.

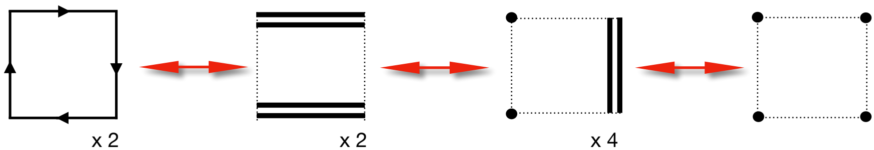
$$V(\lambda) \; = \; 2\langle \mathcal{N} \rangle_n(\lambda) - 2n - 1 \; = \; \tanh([\lambda - a_{n+1}]/2)$$



Update strategies - 1

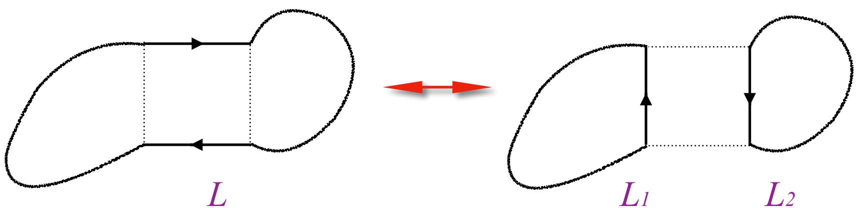
- Inserting, splitting and joining loops:

Exchanging elements on a plaquette (heat bath)



Joining/splitting loops (50/50)

sign L $=$ sign L_1 sign L_2

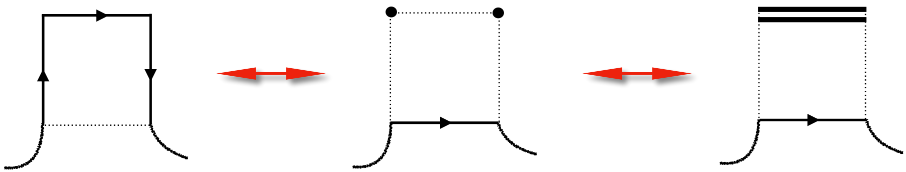


- Splitting of loops is the only update with a non-local operation for determining the sign.

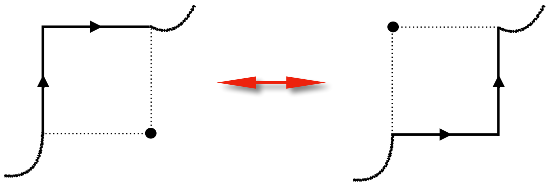
Update strategies - 2

- Deforming loops:

Shrinking/expanding loops (heat bath)



Flipping a loop corner (50/50)



sign L → - sign L

Comments

- We work with a canonical setting. $\Rightarrow$ Fixed particle number W.
  $\Rightarrow$ We use an initial configurations with net winding number W.

- Our update moves do not change the total net winding number.
  $\Rightarrow$ Update remains in the desired particle number sector.

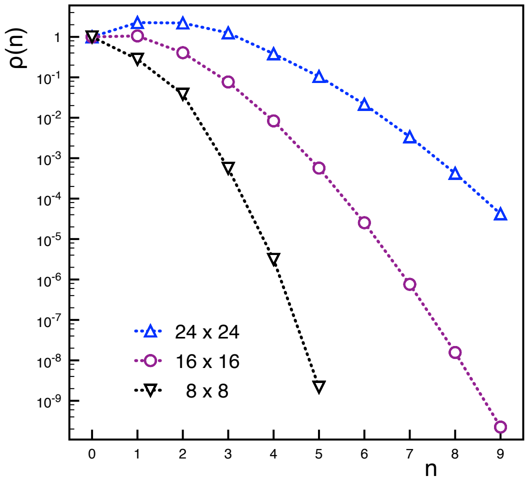
- Additional update step: Flip the orientation of non-winding loops.

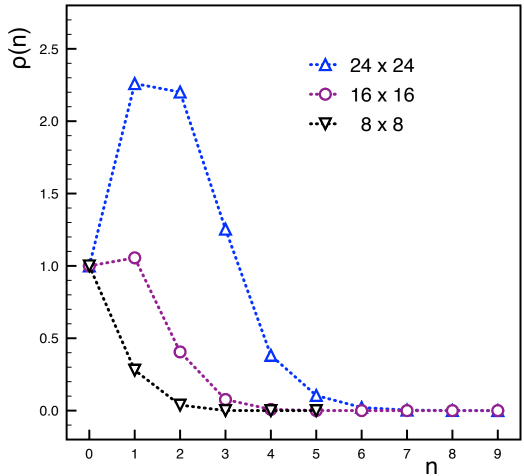
- The update moves are ergodic, and may be generalized to 4 dimensions and to fermions coupled to abelian gauge fields.

- The only move that is not strictly local is the determination of the loop sign when splitting loops.

A first look at the density - 1

- The density $\rho(n)$ for different volumes: $(M = 0.5, J = 0.0, W = 0)$

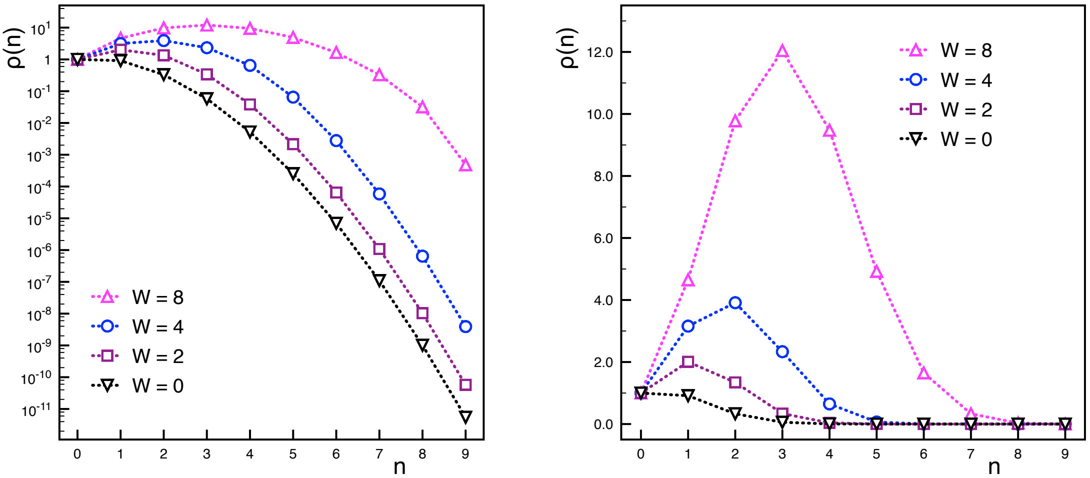




- For large n the density $\rho(n)$ decays exponentially!

A first look at the density - 2

- The density $\rho(n)$ for different particle numbers W: $(M = 0.5, J = 0.0, 24 \times 8)$



- For large n the density $\rho(n)$ decays exponentially!

Summary and outlook

- Worldline representations are a powerful tool, but for fermions the worldlines usually come with signs.
- Here we show that a DoS formulation can be set up where the density is considered as a function of the number of negative loops.
- Canonical formulation $\Rightarrow$ work at a fixed winding number.
- Suitable ergodic updates can be found for the highly constrained system of monomers, dimers and closed fermion worldlines.
- We test the approach for 2-d staggered fermions with mass and quartic self-interaction.
- The density can be determined reliably and shows exponential decrease.
- Next steps: Implementation of observables and verification in the free case.