



# Entanglement Entropy for Many-Fermion Systems



Peter Bröcker and Simon Trebst  
Institut für Theoretische Physik, Universität zu Köln

Bonn-Cologne Graduate School of Physics and Astronomy

## Entanglement in Many-Body Systems

Consider a **many-body system** described by  $\rho = |\psi\rangle\langle\psi|$

Is it possible to write  $\rho = \rho_A \otimes \rho_B$  ?

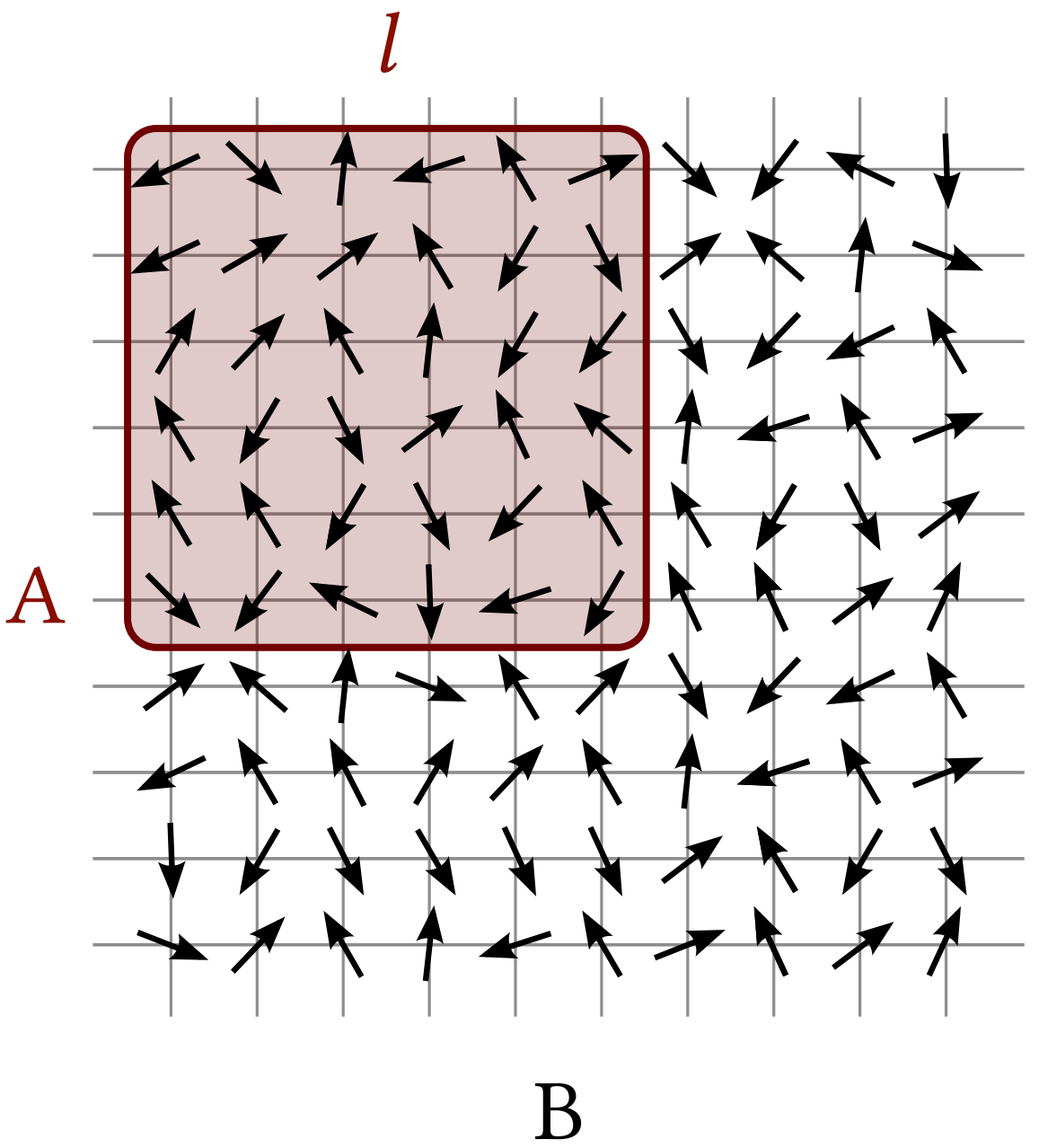
Only if there is no entanglement

How entangled is a system?

Look at the **reduced density matrices**  $\rho_A = \text{Tr}_B \rho$

And calculate the **von Neumann entropy** of subsystem A

$$S(A) = -\text{Tr}(\rho_A \log(\rho_A))$$



## Entanglement as a Resource

The entanglement entropy depends on the form of the cut and often scales as some function of the length of its boundary  $l$ . Listed below are a few prominent examples for **two dimensional systems**:

- area law e.g. valence bond crystal  $S(l) = al$
- gapless spin liquid  $S(l) = c \cdot \log(l) + \dots$
- topological spin liquid  $S(l) = al - \gamma$
- and many more ...

In **one dimensional systems**, there is an intimate connection to conformal field theories through the central charge<sup>[1]</sup>

- gapped  $S(l) = \text{const}$
- gapless  $S(l) \propto \frac{c}{3} \log\left(\frac{L}{\pi} \sin\left(\frac{\pi l}{L}\right)\right)$

The **entanglement entropy** can thus be viewed as a **resource**, namely a **diagnostic tool** to classify quantum matter

## Measuring Entanglement

Having established that the entanglement entropy is a useful quantity, we need to figure out how to measure it in our simulation. We do not have direct access to the von Neumann-Entropy itself, but we can calculate a generalized version of it, the **Renyi Entropy**.

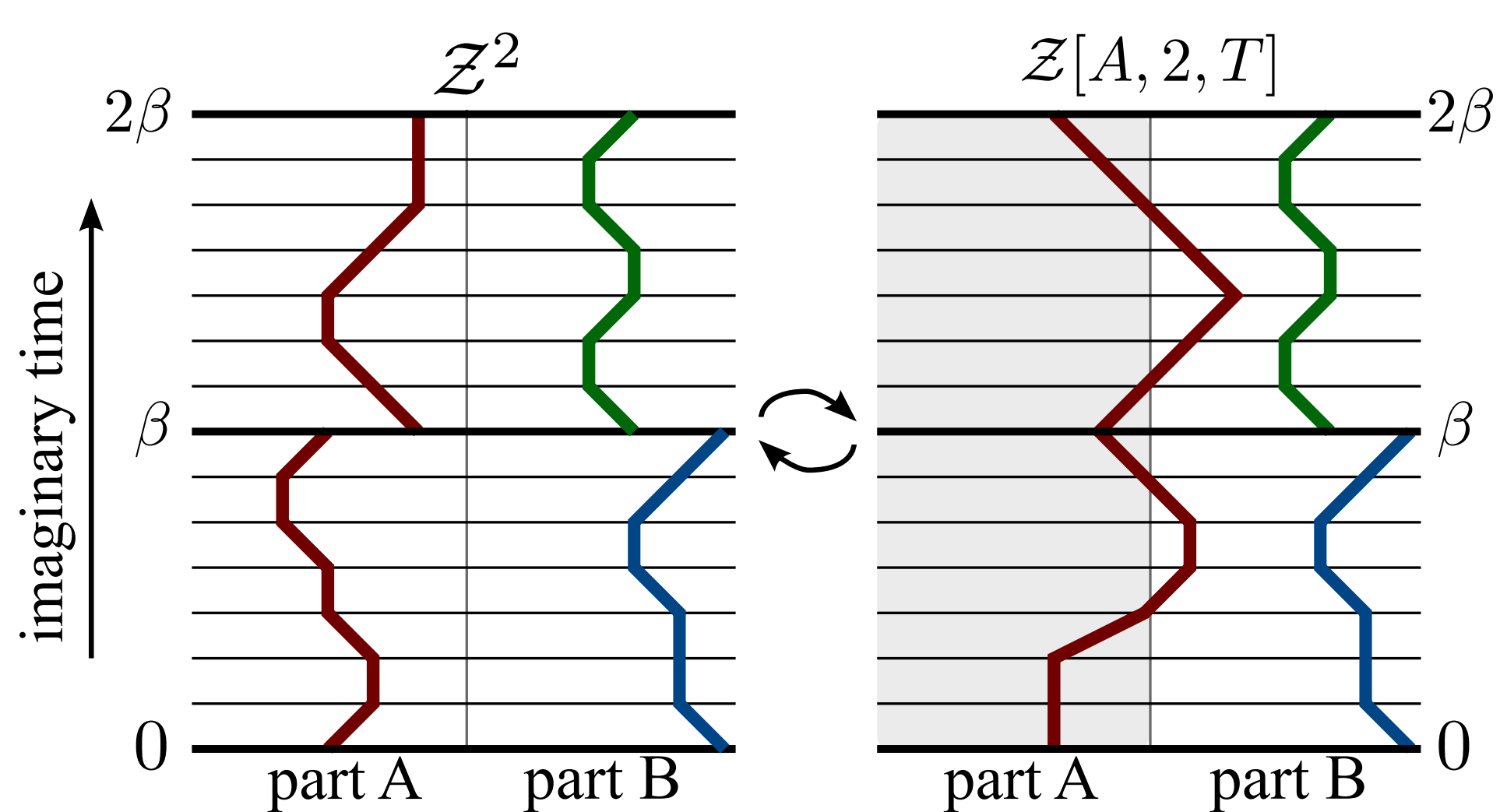
$$S_n = \frac{1}{1-n} \log(\text{Tr} \rho_A^n) \xrightarrow{n \rightarrow 1} S(A) = -\text{Tr}(\rho_A \log(\rho_A))$$

Most notably, the second Renyi entropy is the fastest to calculate in QMC. To do so, we employ a calculational scheme called **Replica Trick**<sup>[2]</sup>. For finite temperature simulations, the entropy takes the form

$$S_2(A) = -\ln\left(\frac{\mathcal{Z}[A, 2, T]}{\mathcal{Z}^2}\right) = -\ln\left(\frac{N[A, 2, T]}{N^{(2)}}\right)$$

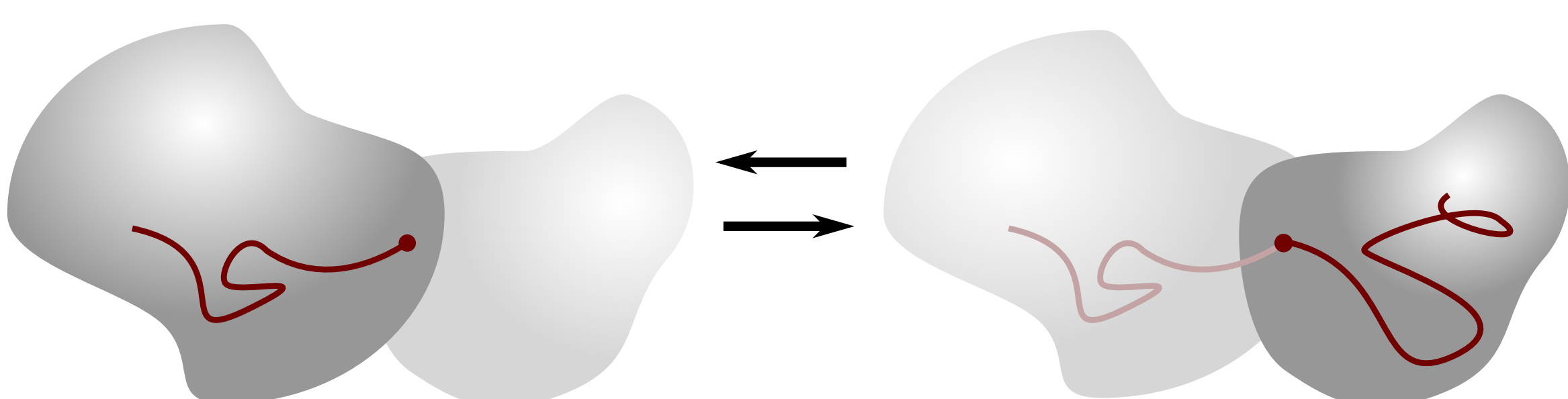
$$\mathcal{Z}[A, 2, T] = \sum_{A, A', B, B'} \langle AB' | \exp(-\beta\mathcal{H}) | A'B' \rangle \langle A'B | \exp(-\beta\mathcal{H}) | AB \rangle$$

The first identity is the statement of the replica trick, while the second one provides concrete instructions on how to evaluate the expression. We need two systems with rather peculiar boundary conditions in imaginary time. One is completely replicated in the direction of imaginary time but remains  $\beta$  periodic, while in the other system only part B is  $\beta$  periodic and part A is  $2\beta$  periodic.



The fraction appearing in the entanglement entropy can be evaluated by switching back and forth between the configuration spaces of the numerator and denominator, respectively. We then only count the number of configurations visited in each of the spaces.

$$C(\mathcal{Z}[A, 2, T]) \quad C(\mathcal{Z}^2) \quad C(\mathcal{Z}[A, 2, T]) \quad C(\mathcal{Z}^2)$$



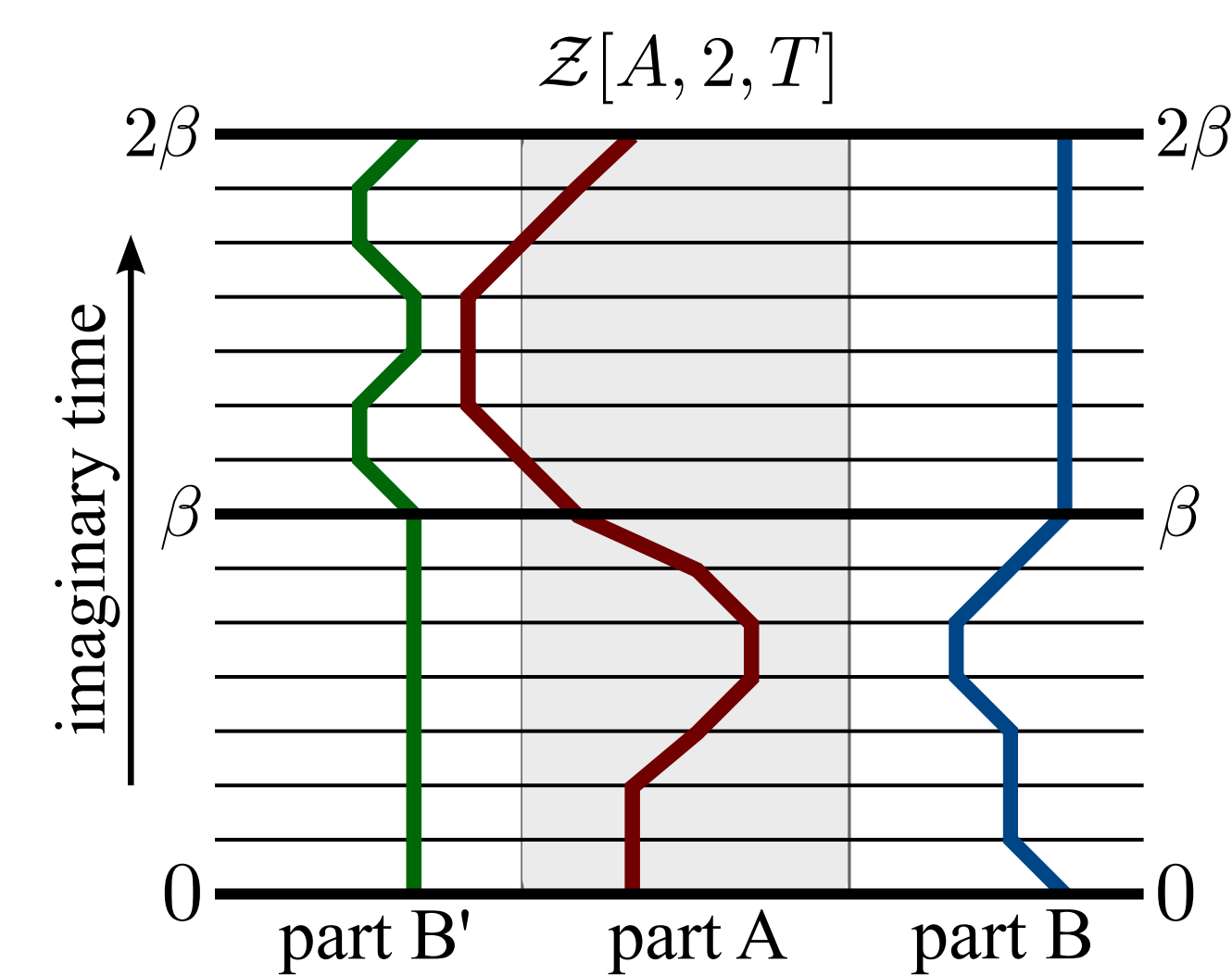
## Entangled Fermions

For fermions in more than one dimension, the method of choice is **Determinantal Quantum Monte Carlo (DQMC)**, a powerful technique applicable to a wide range of problems. However, a direct implementation of the modified partition sum would result in a factorial scaling.

One can show that the partition sum can be rewritten in such a way that the boundary conditions are taken care of by an **imaginary time dependence** of the Hamiltonian which is again efficiently tractable using the full machinery of DQMC:

$$\mathcal{H}(\tau) = \mathcal{H}_{AB} \Theta(\tau) \Theta(\beta - \tau) + \mathcal{H}_{AB'} \Theta(\tau - \beta) \Theta(2\beta - \tau)$$

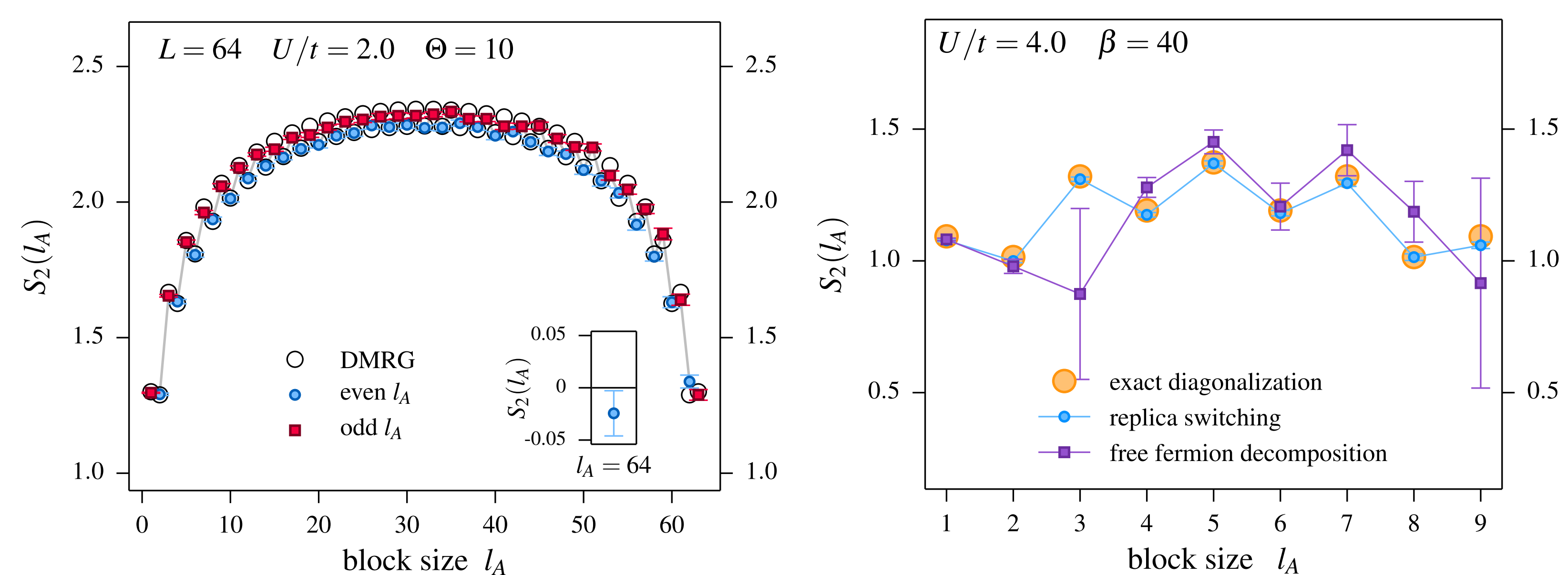
The corresponding worldline picture is the same as before but **unfolded**:



To benchmark our algorithm, we study the **one dimensional Hubbard chain**:

$$\mathcal{H} = -t \left( \sum_{\langle i, j \rangle, \sigma} c_{i, \sigma}^\dagger c_{j, \sigma} + h.c. \right) + U \sum_i n_{i, \uparrow} n_{i, \downarrow} - \mu \sum_i (n_{i, \uparrow} + n_{i, \downarrow})$$

We compare with reference data obtained using DMRG calculations and with an alternative approach based on an expansion in free fermion Green's functions.<sup>[3]</sup>



We observe good agreement with DMRG. Also, in the strongly interacting regime our approach gives superior results compared to the alternative algorithm that deviates significantly from the exact diagonalization result.

## References

- [1] P. Calabrese and J. Cardy, J. Stat. Mech.: Theor. Exp. P06002 (2004)  
[2] R. G. Melko, A. B. Kallin, and M. B. Hastings, Phys. Rev. B 82, 100409 (2010)

- [3] T. Grover, Phys. Rev. Lett. 111, 130402 (2013)

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