Real-time dynamics without Hamiltonians

Debasish Banerjee

with F.-J. Jiang, M. Kon, U.-J. Wiese

Albert Einstein Center for Fundamental Physics
Institute for Theoretical Physics
University of Bern

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Outline

The Schwinger-Keldysh (closed-time) contour

- Quantum many-body system governed by $\hat{H}(t)$
- At some point in time $t = 0$, the initial state of the system is specified by a density-matrix $\hat{\rho}(0)$.
- Evolution of the density matrix: $\frac{d\hat{\rho}(t)}{dt} = -i[\hat{H}(t), \hat{\rho}(t)]$
- Formally solved as: $\hat{\rho}(t) = \hat{U}(t,0)\hat{\rho}(0)[\hat{U}(t,0)]^\dagger$

$$\begin{aligned}\hat{U}(t,t') &= \mathcal{T}\exp\left[-i\int_t^{t'}\hat{H}(\tau)d\tau\right] \\ &= \lim_{N\to\infty} e^{-i\hat{H}(t'-\delta_t)\delta_t}\cdots e^{-i\hat{H}(t+\delta_t)\delta_t}e^{-i\hat{H}(t)\delta_t}\end{aligned}$$

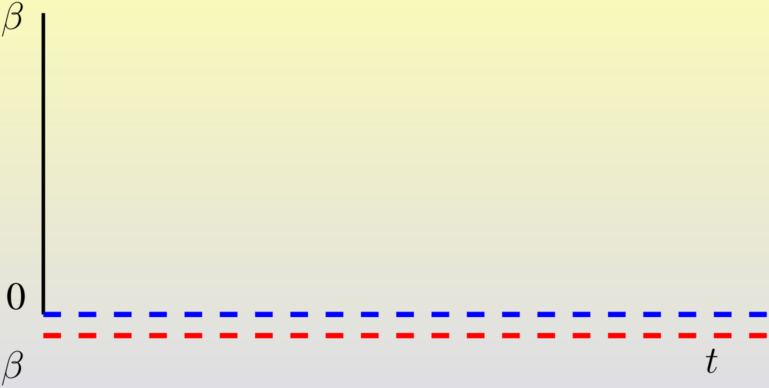
with $\delta_t = (t' - t)/N$.

- Expectation value of an observable:

$$\langle\hat{\mathcal{O}}(t)\rangle = \mathrm{Tr}\left\{\hat{\mathcal{O}}\hat{\rho}(t)\right\} = \mathrm{Tr}\left\{\hat{U}(0,t)\hat{\mathcal{O}}\hat{U}(t,0)\hat{\rho}(0)\right\}$$

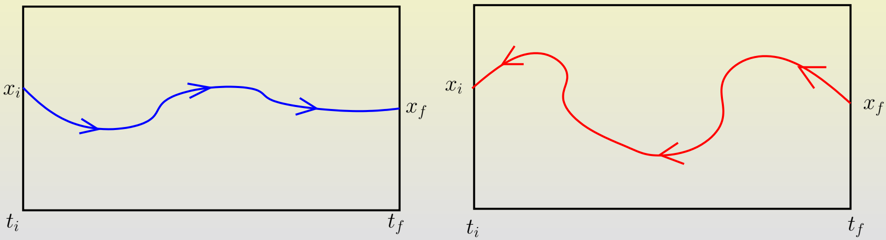
where the density matrix is normalized.

The Schwinger-Keldysh (closed-time) contour



- “forward-backward” evolution along the real-time contour.
- Entanglement in quantum systems presents a major obstacle for numerical methods
- Idea: make repeated measurements on the system to reduce entanglement

Measurements to help us out



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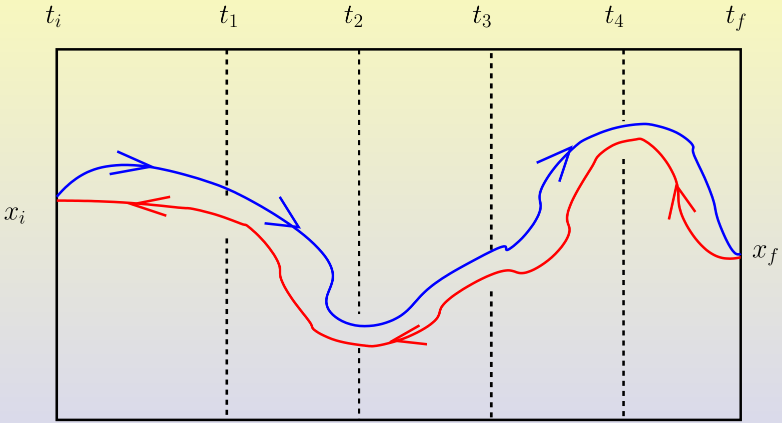
Measurements to help us out



- Idea: make repeated measurements on the system to reduce entanglement

Path-Integral with measurements

- General quantum system with (possibly) time-dependent Hamiltonian.
- Time-evolution $t_k \to t_{k+1}$ described by $U(t_{k+1}, t_k) = U(t_k, t_{k+1})^\dagger$.
- At time t_k $(k \in \{1, 2, \cdots, N\})$ observable O_k measured with eigenvalue o_k.
- Represented by the Hermitian operator P_{o_k}: projects on to the sub-space of the Hilbert space spanned by eigenvectors of O_k with eigenvalue o_k.
- Consider an initial state, specified by a normalized density matrix $\rho = \sum_i p_i |i\rangle\langle i|$; with $0 \leq p_i \leq 1$ and $\sum_i p_i = 1$.
- Probability of making a single measurement of O_k at time t_k while evolving from t_i to t_f is:
  $p_{\rho f}(o_k) = \sum_i \langle i|U(t_i, t_k) P_{o_k} U(t_k, t_f)|f\rangle \langle f|U(t_f, t_k) P_{o_k} U(t_k, t_i)|i\rangle \, p_i$
- With many measurements,
  $$p_{\rho f}(o_1, o_2, \cdots, o_N) = \sum_i \langle i|U(t_i, t_1) P_{o_1} U(t_1, t_2) P_{o_2} \cdots P_{o_N} U(t_N, t_f)|f\rangle \langle f|U(t_f, t_N) P_{o_N} \cdots P_{o_2} U(t_2, t_1) P_{o_1} U(t_1, t_i)|i\rangle \, p_i$$

Away with the Hamiltonian!

- Matrix elements of both $U(t_{k+1}, t_k)$ and P_{o_k} are in general complex, leading to a severe complex weight and/or sign problem.
- Measurements disentangle the quantum system, and are expected to alleviate the sign-problem.
- Take an extreme case: switch off the Hamiltonian completely for the real-time evolution. $U(t_{k+1}, t_k) = \mathbb{I}$
- Time-evolution is driven entirely by (non-commuting) measurements!
- With only the measurements:
  $$p_{\rho f}(o_1, o_2, \cdots, o_N) = \sum_i \langle i|P_{o_1} P_{o_2} \cdots P_{o_N}|f\rangle\langle f|P_{o_N} \cdots P_{o_2} P_{o_1}|i\rangle \, p_i$$
  $$= \sum_i p_i \langle ii|(P_{o_1} \otimes P_{o_1}^T)(P_{o_2} \otimes P_{o_2}^T) \cdots (P_{o_N} \otimes P_{o_N}^T)|ff\rangle$$
- Insert complete sets of states: $\sum_{n_k} |n_k\rangle\langle n_k| = \mathbb{I}$; $\sum_{n'_k} |n'_k\rangle\langle n'_k| = \mathbb{I}$
- In the doubled Hilbert space of states $|n_k n'_k\rangle$, for both pieces of the Keldysh contour (using $\langle n_0 n'_0| = \langle ii|$ & $|n_{N+1} n'_{N+1}\rangle = |ff\rangle$):

$$p_{\rho f}(o_1, o_2, \cdots, o_N) = \sum_i p_i \sum_{n_1 n'_1} \cdots \sum_{n_N n'_N} \prod_{k=0}^{N} \langle n_k n'_k|P_{o_k} \otimes P_{o_k}^T|n_{k+1} n'_{k+1}\rangle$$

A concrete example

- Don't pay attention to the "intermediate" measurement results!
- The probability $p_{\rho f}$ to reach the final state $|f\rangle$:

$$p_{\rho f} = \sum_{o_1}\sum_{o_2}\cdots\sum_{o_N} p_{\rho f}(o_1, o_2, \cdots, o_N) = \sum_i p_i \sum_{n_1, n_1'} \cdots \sum_{n_N, n_N'} \prod_{k=0}^{N} \langle n_k n_k' | \tilde{P}_k | n_{k+1} n_{k+1}' \rangle$$

$\widetilde{P_k} = \sum_{o_k} P_{o_k} \otimes P_{o_k}^T$, summing over all possible measurement results.

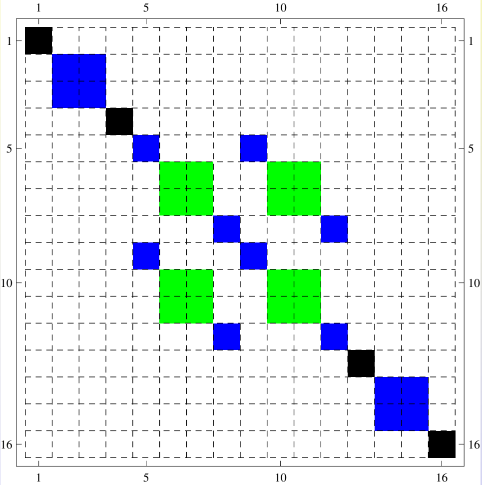
- Example: Two spins $\vec{S}_x$ and $\vec{S}_y$ forming total spin eigenstates:
  $|11\rangle = \uparrow\uparrow,\ |10\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow),\ |1-1\rangle = \downarrow\downarrow;\ |00\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$
- Projection operator on spin-1:
  $P_1 = |11\rangle\langle 11| + |10\rangle\langle 10| + |1-1\rangle\langle 1-1|$
- Projection operator on spin-0: $P_0 = |00\rangle\langle 00|$

$$P_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & & 1 \end{pmatrix} \qquad P_0 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & & 0 \end{pmatrix}$$

- Negative entries in P_0 give rise to a sign problem.

The sign-problem and it's solution

In the doubled Hilbert space, $P_1 \otimes P_1^T$ is a 16×16 matrix with entries:



Legend: black $\rightarrow$ 1; blue $\rightarrow \frac{1}{2}$; green $\rightarrow \frac{1}{4}$; red $\rightarrow -\frac{1}{4}$

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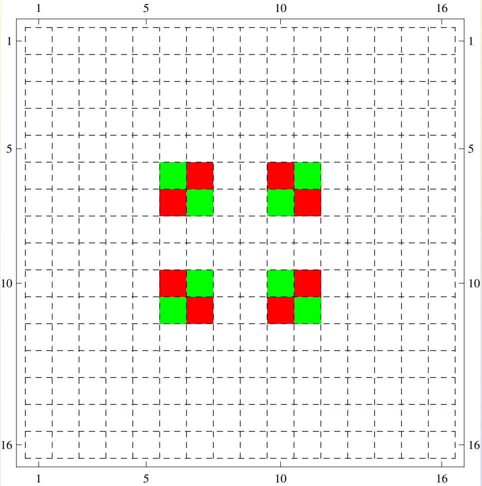

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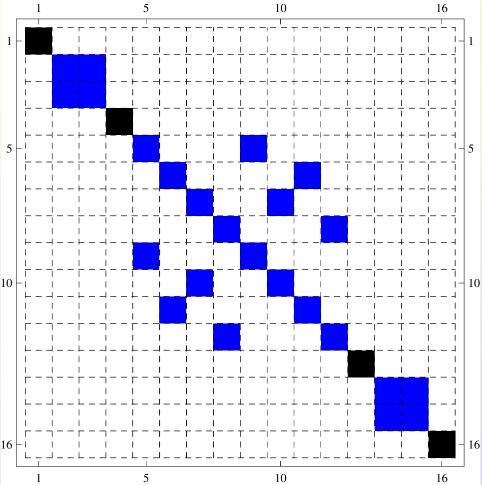
The sign-problem and it's solution

$\widetilde{P} = P_0 \otimes P_0^T + P_1 \otimes P_1^T$ is a 16×16 matrix with entries:



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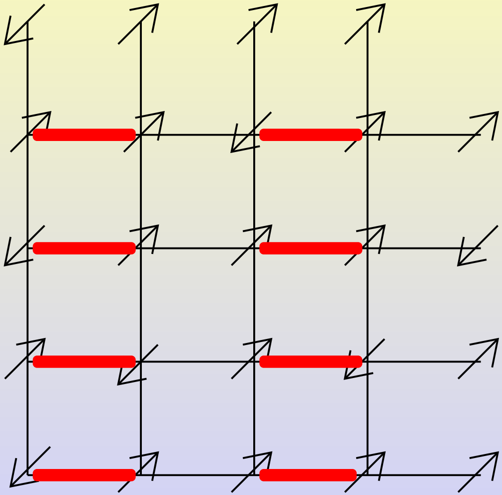
Extension to large systems

- Example of two-spin system easily extendable to large systems.
- System of quantum spins $\frac{1}{2}$ on a square lattice $L \times L$ with periodic boundary conditions.
- To define the initial density matrix $\hat{\rho} = \exp(-\beta \hat{H})$, use the Heisenberg anti-ferromagnet: $\hat{H} = J \sum_{<xy>} \vec{S}_x \cdot \vec{S}_y; \quad J > 0$.
- Real-time evolution is driven via measurements of the total spin $(\vec{S}_x + \vec{S}_y)^2$ of the nearest-neighbor spins $\vec{S}_x$ and $\vec{S}_y$.

Non-commuting measurements



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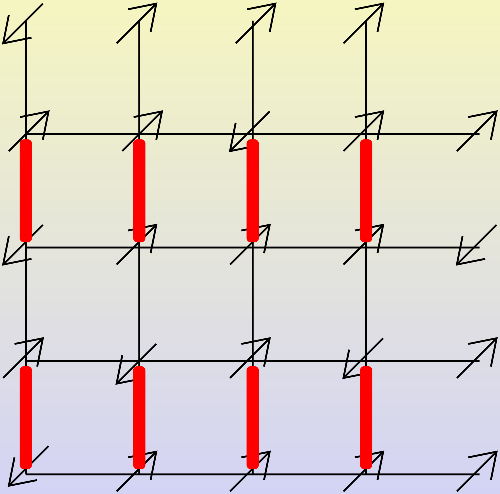

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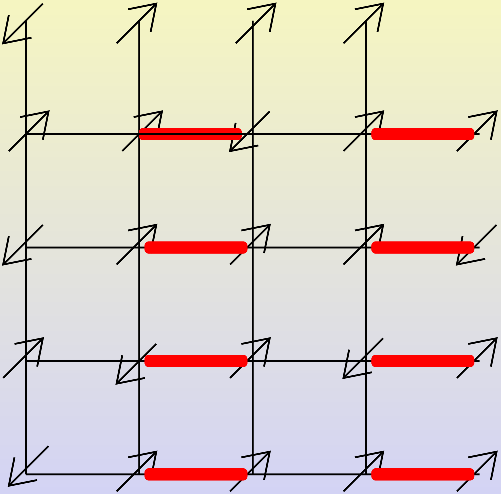

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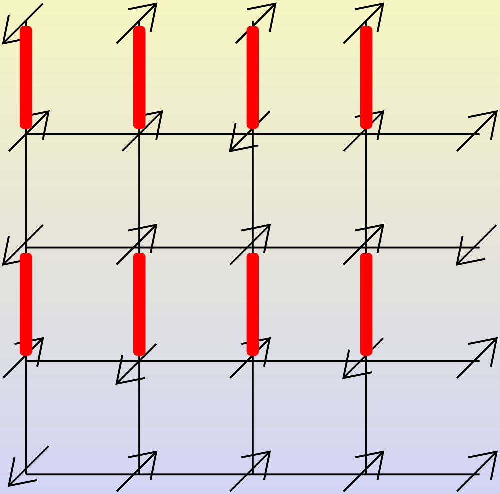

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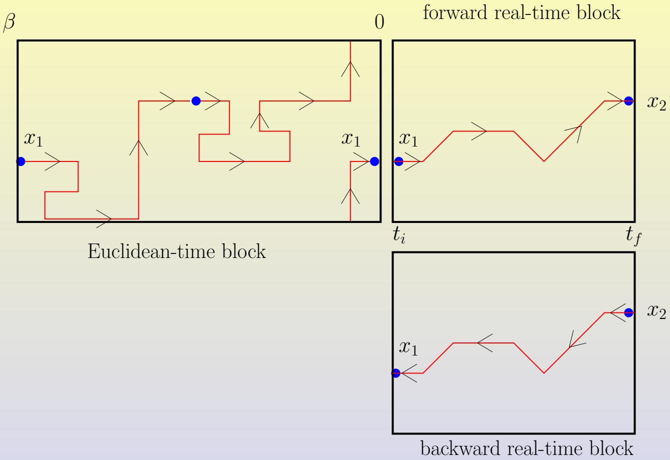
- Real-time evolution is driven via measurements of the total spin $(\vec{S}_x + \vec{S}_y)^2$ of the nearest-neighbor spins $\vec{S}_x$ and $\vec{S}_y$.
- The particular measurement sequence is arbitrary; but well defined and corresponds to a definite "real-time physics".
- The existing highly efficient loop-cluster algorithm for anti-ferromagnets can be naturally extended to this particular case of real-time evolution.
- Resulting clusters are closed loops extending in both Euclidean and real-time, which are updated together.

An example of a cluster

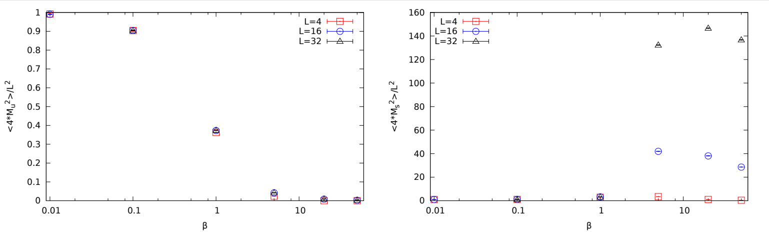


Identical clusters in the forward and backward real-time evolution is due to the condition that we have summed over “all intermediate measurements” $\rightarrow$ cluster bonds are decided with the matrix elements in the matrix $\widetilde{P} = P_1 \otimes P_1^T + P_0 \otimes P_0^T$.

Properties of the initial state

- Initial state is the ground state (or thermal ensemble depending on inverse temperature β) of the Heisenberg anti-ferromagnet in (2+1)-d.
- At low-T (large β), there is a strong Néel order which disappears for higher temperature.
- Diagnostics for measuring the ferromagnet and the Néel orders are the uniform and staggered magnetization:

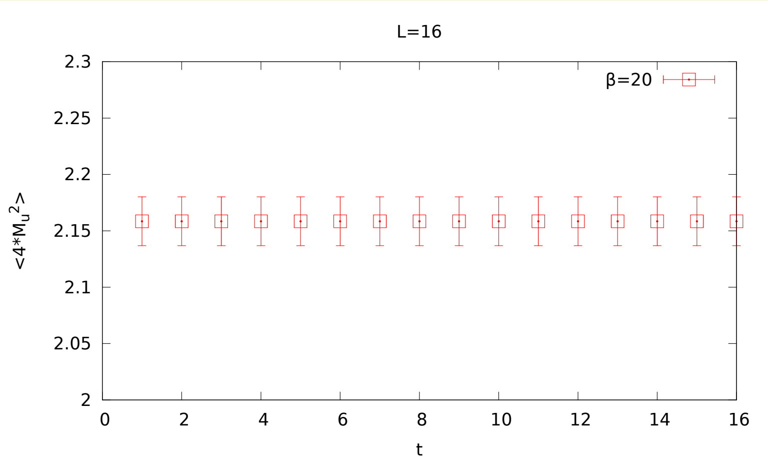
$$M_u = \frac{1}{2}\sum_x S_x^3; \quad M_{stag} = \frac{1}{2}\sum_x (-1)^{x_1+x_2} S_i^3$$



Uniform (left) and staggered (right) magnetization for a 2-d Heisenberg model

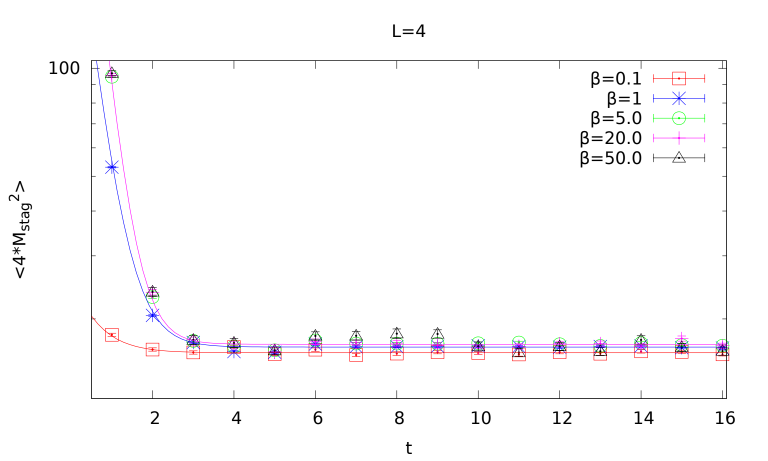
Uniform magnetization

The uniform magnetization $M_u = \frac{1}{2}\sum_x S_x^3$ should be constant since it commutes both with the Hamiltonian and the measurement.



Staggered magnetization

The staggered magnetization is destroyed by the measurements, and a new state is established.



Lines are fit to $A \exp(-N/\tau) + B$

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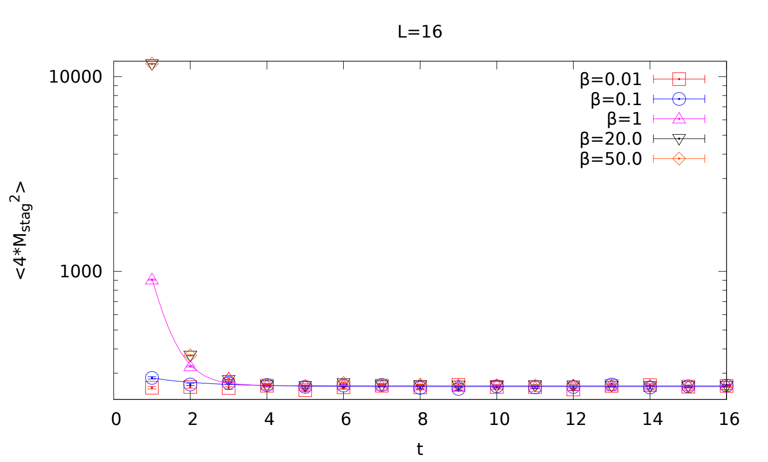

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In progress

- Larger lattices (obvious!)
- Keep track of measurements $\rightarrow$ brings back the sign problem due to measurement of a singlet
- ”Tunable” sign problem. More measurements make the sign problem more severe.
- Can we solve it? $\rightarrow$ adapt the nested-cluster algorithm
- Immediate generalizations to different models.
- Reverse engineering: think of a Hamiltonian which will allow for positive matrix elements and/or a case where a sign problem, can be solved by meron (and fermion-bag) methods.

Thank you for your attention!