Alternating-basis quantum Monte Carlo method for correlated electrons on a lattice

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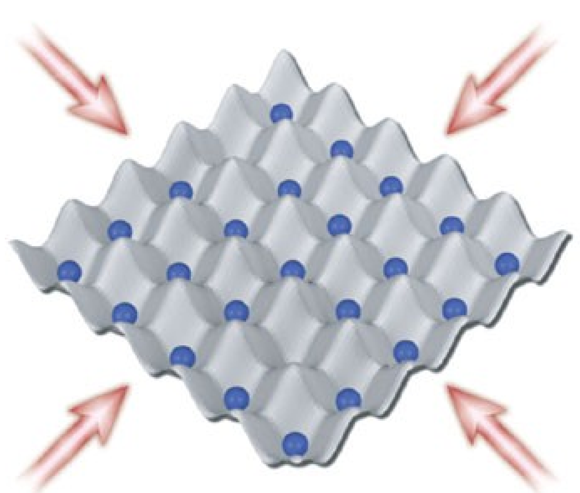
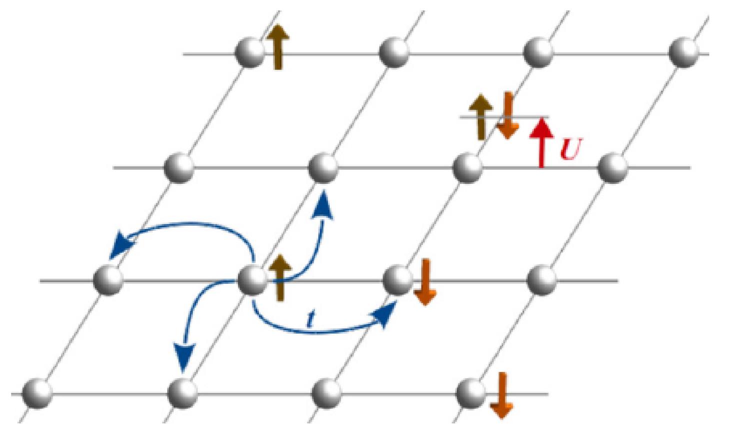
Optical lattices [1]



- quantum gas microscopes
- single-site resolution
- mass, charge, and spin transport
- equilibrium and time-dependent multipoint correlation functions
- existing numerical methods can't easily reproduce raw exptl. data

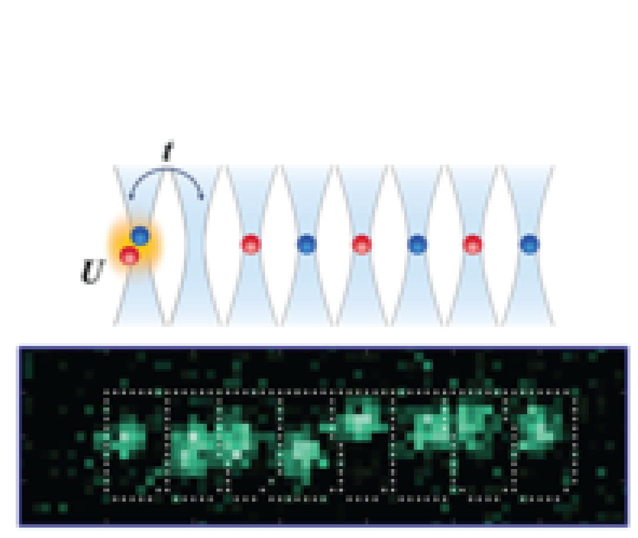
Hubbard model



$$H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}$$

$$\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) \underbrace{[-\mu]}_{\text{GCE}}$$

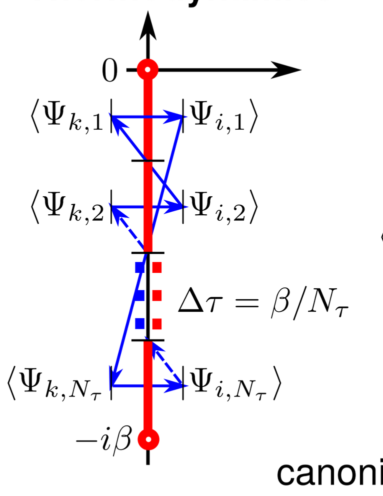
Optical-tweezers arrays [2]



- low-entropy (almost pure) many-body states
- various lattice geometries
- charge-density and spin-density waves

ABQMC Formalism [3]

Thermodynamics



$$\mathcal{C} = \{|\Psi_{k,l}\rangle, |\Psi_{i,l}\rangle | l = 1, \ldots, N_\tau\}$$

$$\mathcal{D}(\mathcal{C}) = \prod_{l=1}^{N_\tau} \langle\Psi_{k,l}|\Psi_{i,l}\rangle\langle\Psi_{i,l}|\Psi_{k,l\ominus 1}\rangle$$

$$Z_{N_\tau} = \sum_{\mathcal{C}} \mathrm{Re}\{\mathcal{D}(\mathcal{C})\} e^{-\Delta\tau\varepsilon(\mathcal{C})}$$

$$\varepsilon(\mathcal{C}) = \varepsilon_k(\mathcal{C}) + \varepsilon_i(\mathcal{C})$$

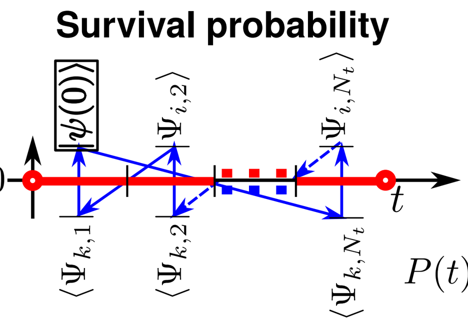
$$\langle A_a\rangle = \frac{\left\langle \mathrm{sgn}(\mathcal{C}) \frac{1}{N_\tau} \sum_{l=1}^{N_\tau} \mathcal{A}_a(\Psi_{a,l}) \right\rangle_w}{\langle \mathrm{sgn}(\mathcal{C})\rangle_w}$$

$$w(\mathcal{C}) = |\mathrm{Re}\{\mathcal{D}(\mathcal{C})\}|\, e^{-\Delta\tau\varepsilon(\mathcal{C})}$$

$$\mathrm{sgn}(\mathcal{C}) = \frac{\mathrm{Re}\{\mathcal{D}(\mathcal{C})\}}{|\mathrm{Re}\{\mathcal{D}(\mathcal{C})\}|}$$

canonical & grand-canonical ensemble

Survival probability



$$\Delta t = t/N_t$$

$$P(t) = |\langle\psi(0)|e^{-iHt}|\psi(0)\rangle|^2$$

$$|\Psi_{i,1}\rangle \equiv |\psi(0)\rangle$$

$$TB|\psi(0)\rangle = e^{i\chi}|\psi(0)\rangle$$

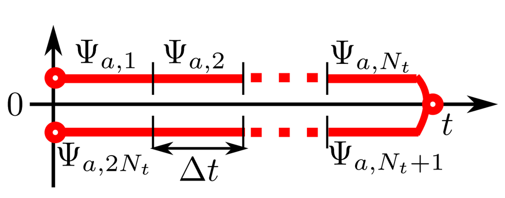
time-reversal symmetry
bipartite lattice symmetry

$$P(t) = \left| \frac{\langle \mathrm{sgn}(\mathcal{C}) \cos[\varepsilon_k(\mathcal{C})\Delta t]\, e^{-i\varepsilon_i(\mathcal{C})\Delta t}\rangle_w}{\langle \mathrm{sgn}(\mathcal{C})\rangle_w} \right|^2$$

$$w(\mathcal{C}) = |\mathrm{Re}\{\mathcal{D}(\mathcal{C})\}|$$

manifestly invariant under $\begin{cases} \varepsilon_i(\mathcal{C}) \to -\varepsilon_i(\mathcal{C}) \\ \Delta t \to -\Delta t \\ \varepsilon_k(\mathcal{C}) \to -\varepsilon_k(\mathcal{C}) \end{cases}$

Keldysh contour



$$TB|\psi(0)\rangle = e^{i\chi}|\psi(0)\rangle$$

$$TBA_aBT = A_a$$

$$|\Psi_{i,1}\rangle \equiv |\psi(0)\rangle$$

$$w(\mathcal{C}) = |\mathrm{Re}\{\mathcal{D}(\mathcal{C})\}|$$

$$\langle A_a(t)\rangle = \frac{\langle \mathrm{sgn}(\mathcal{C}) \mathcal{A}_a(\Psi_{a,l_a}) \cos[\Delta\varepsilon_i(\mathcal{C})\Delta t] \cos[\Delta\varepsilon_k(\mathcal{C})\Delta t]\rangle_w}{\langle \mathrm{sgn}(\mathcal{C})\rangle_w}$$

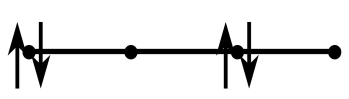
manifestly invariant under $\begin{cases} \varepsilon_i(\mathcal{C}) \to -\varepsilon_i(\mathcal{C}) \\ \Delta t \to -\Delta t \\ \varepsilon_k(\mathcal{C}) \to -\varepsilon_k(\mathcal{C}) \end{cases}$

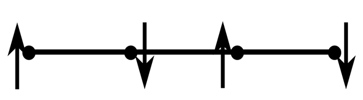
a single Markov chain for all interactions and times
(the same holds for the survival probability)

Dynamical symmetries of the Hubbard model [3, 4]

$$P(t)_{+U} = P(t)_{-U} \qquad \langle A_a(t)\rangle_{+U} = \langle A_a(t)\rangle_{-U}$$

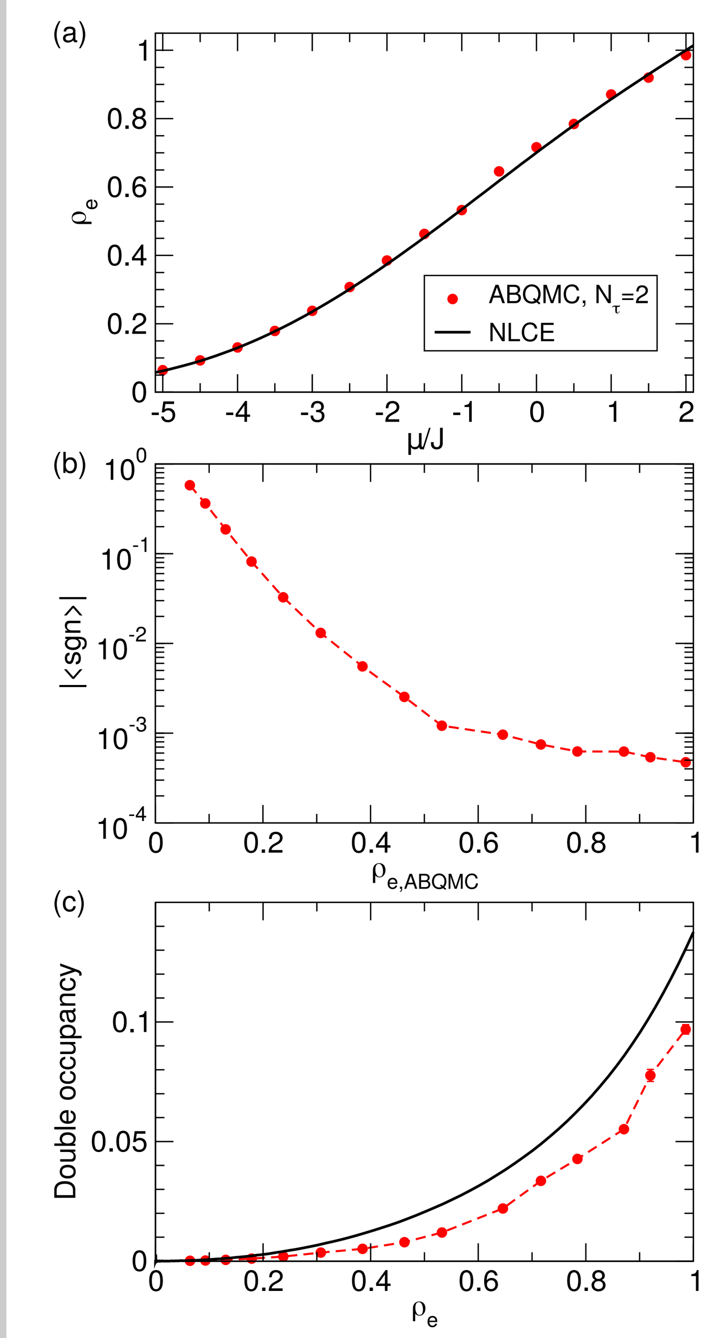
$$P(t)_{\mathrm{CDW}} = P(t)_{\mathrm{SDW}} \qquad \langle A_a(t)\rangle_{\mathrm{CDW}} = \langle A_a(t)\rangle_{\mathrm{SDW}}$$

an exemplary CDW state 

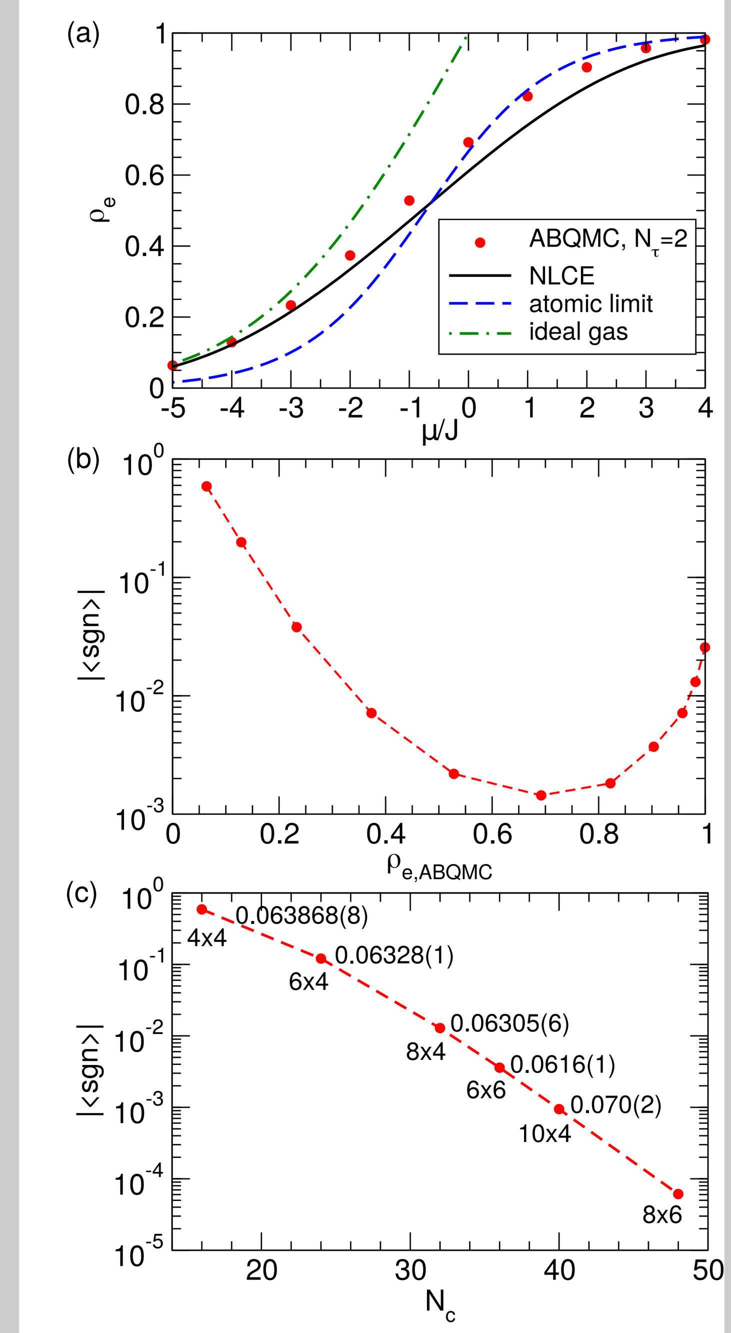
an exemplary SDW state 

partial particle-hole transformation (only on spin-dn electrons)
we combine Markov chains for CDW and SDW

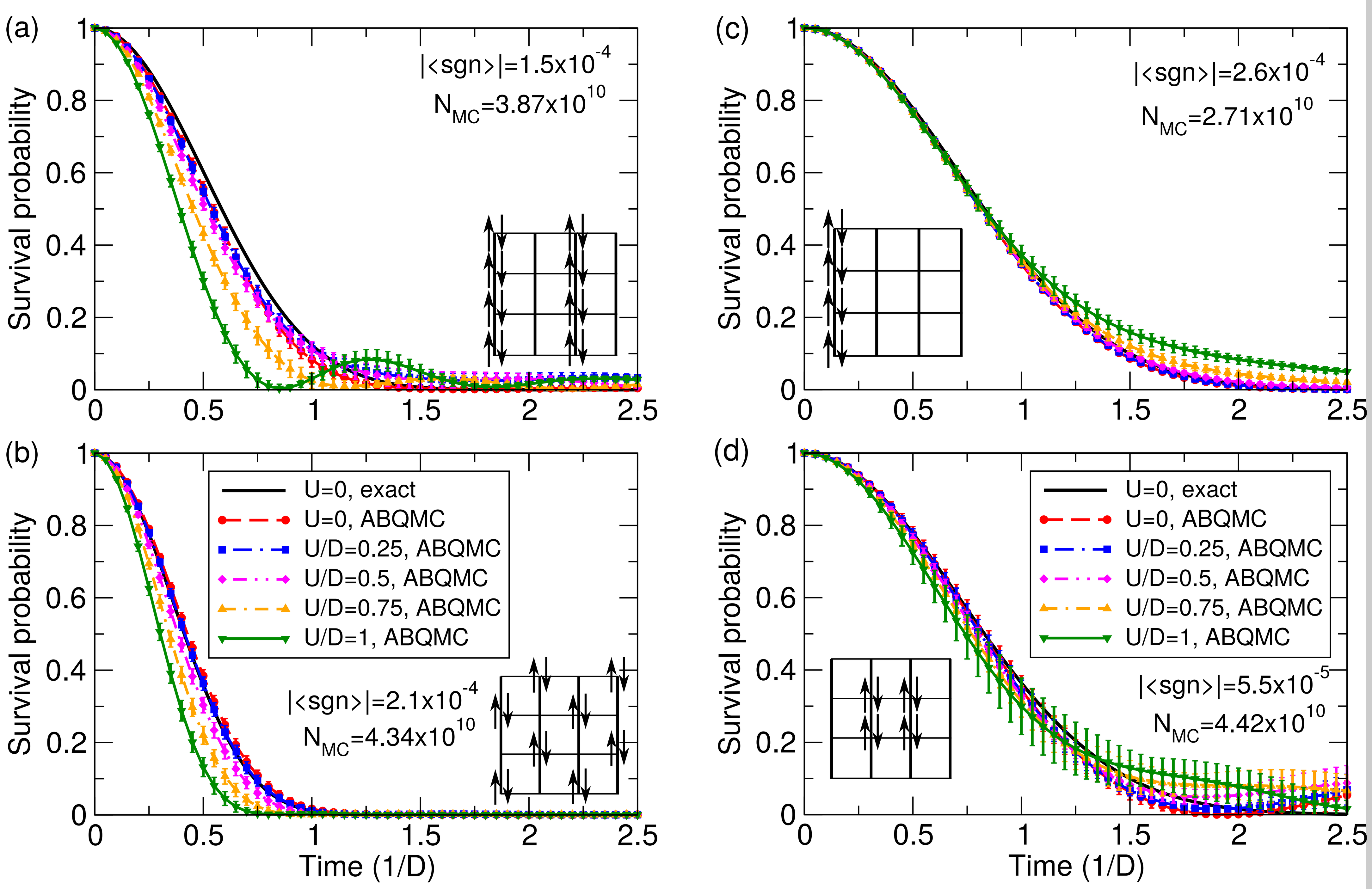
$U/t=4$, $T/t=1$, 4×4



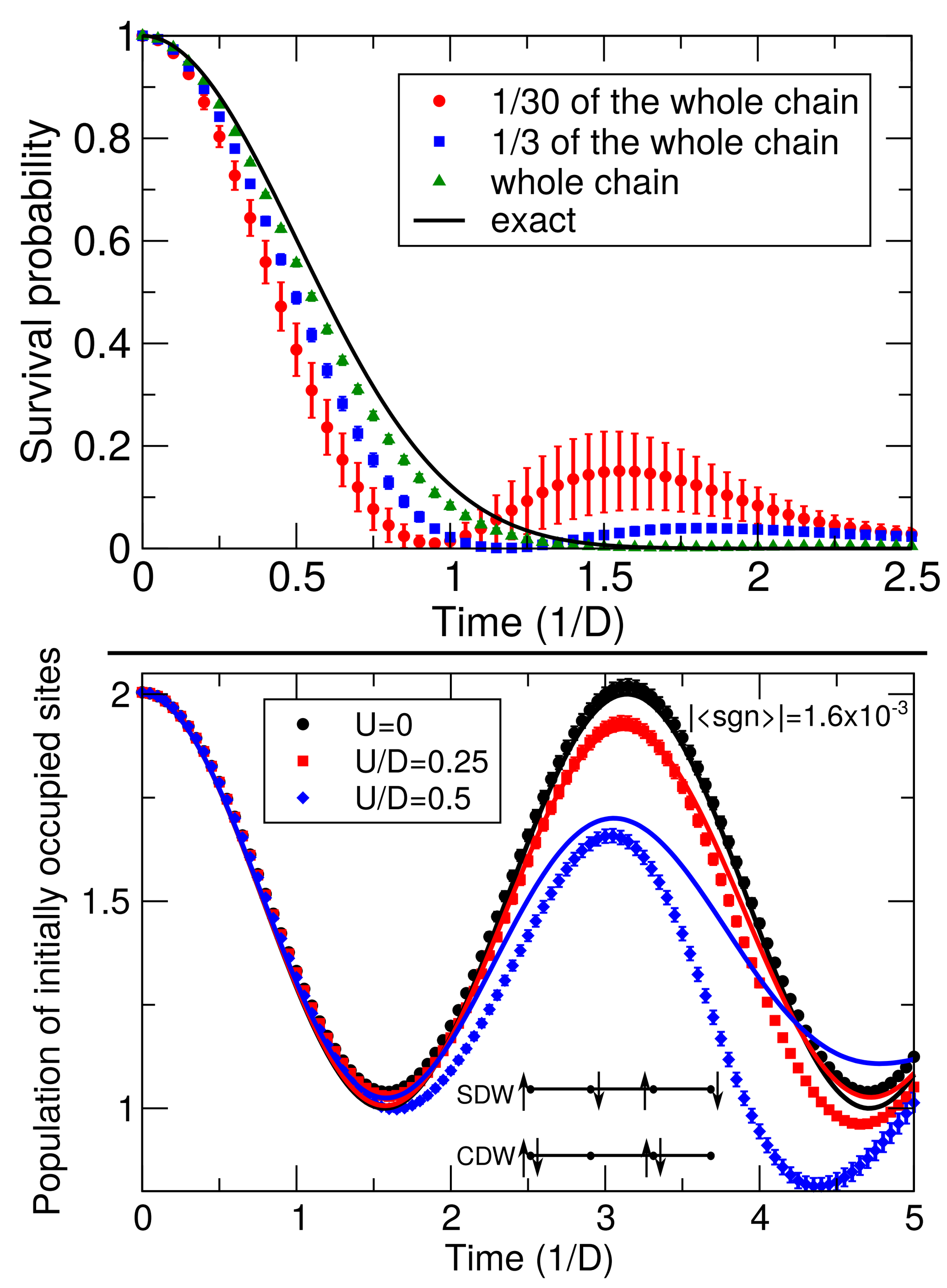
$U/t=24$, $T/t=1$, 4×4



Survival probabilities, 4×4 cluster, $N_t=2$



Sign problem / Keldysh contour



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References

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[2] B. M. Spar et al., Phys. Rev. Lett. **128**, 223202 ('22).
[3] V. Janković and J. Vučičević, arXiv:2206.08844 ('22).
[4] H. Zhai et al., New J. Phys. **21**, 015003 ('19).