Directed-loop quantum Monte Carlo method for retarded interactions

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1D Holstein model:

$$\hat{H} = -t \sum_i \left(\hat{c}_i^\dagger \hat{c}_{i+1} + \text{H.c.} \right) + \omega_0 \sum_i \hat{a}_i^\dagger \hat{a}_i + \gamma \sum_i \hat{\rho}_i \left(\hat{a}_i^\dagger + \hat{a}_i \right)$$

Simulation of fermion-boson models is challenging because:

- unbound bosonic Hilbert space (ED, DMRG)
- long autocorrelation times (QMC)

Our solution to the autocorrelation problem:

- integrate out the phonons in action-based formulation

$$\mathcal{S}_{\text{ret}} = -2\lambda t \iint d\tau_1 d\tau_2 \sum_i \rho_i(\tau_1) P(\tau_1 - \tau_2) \rho_i(\tau_2)$$

- generalize the directed-loop algorithm (SSE) to the case of retarded interactions

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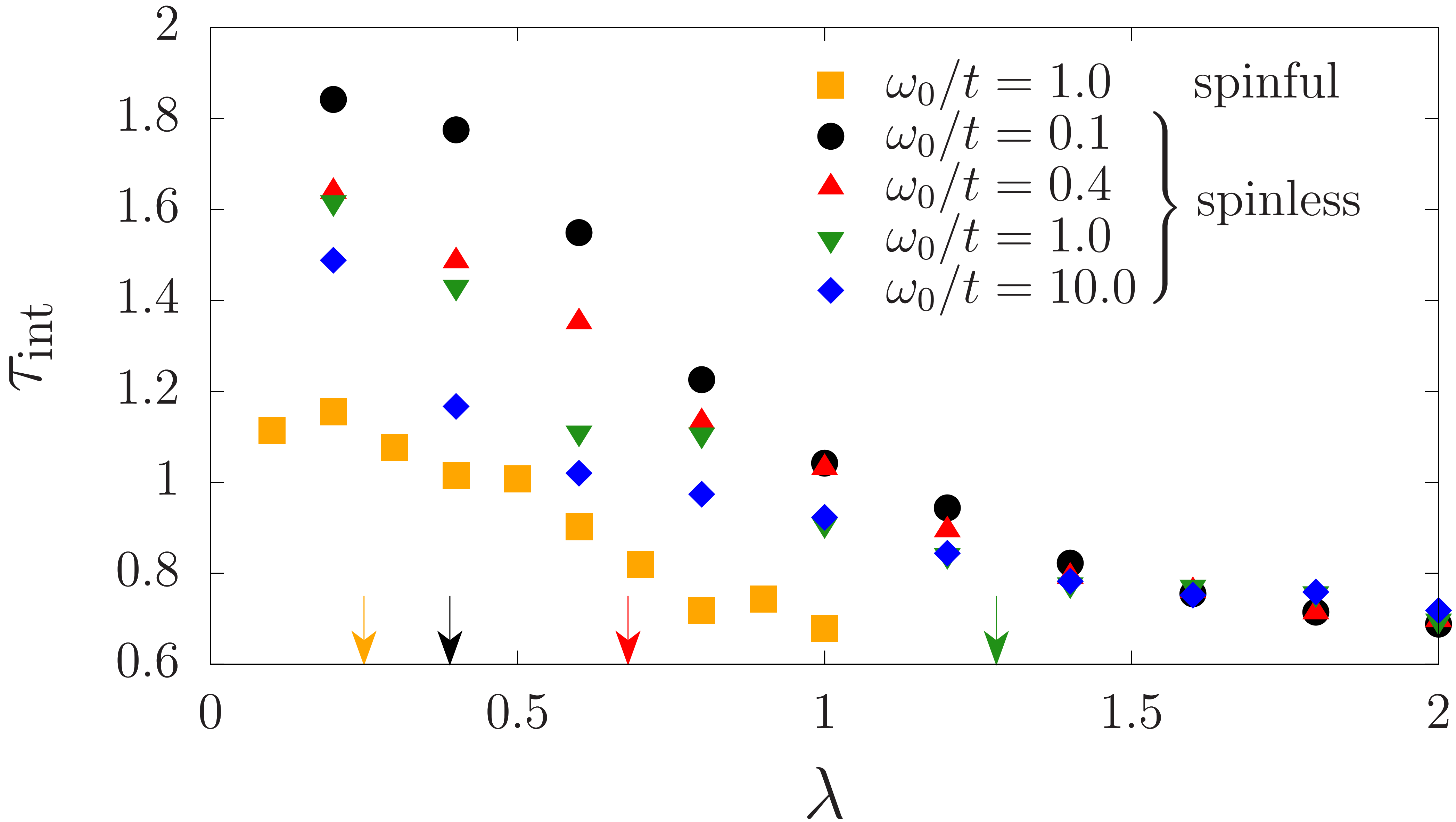
Autocorrelation times are always small!

$L = 18, \beta t = 36$



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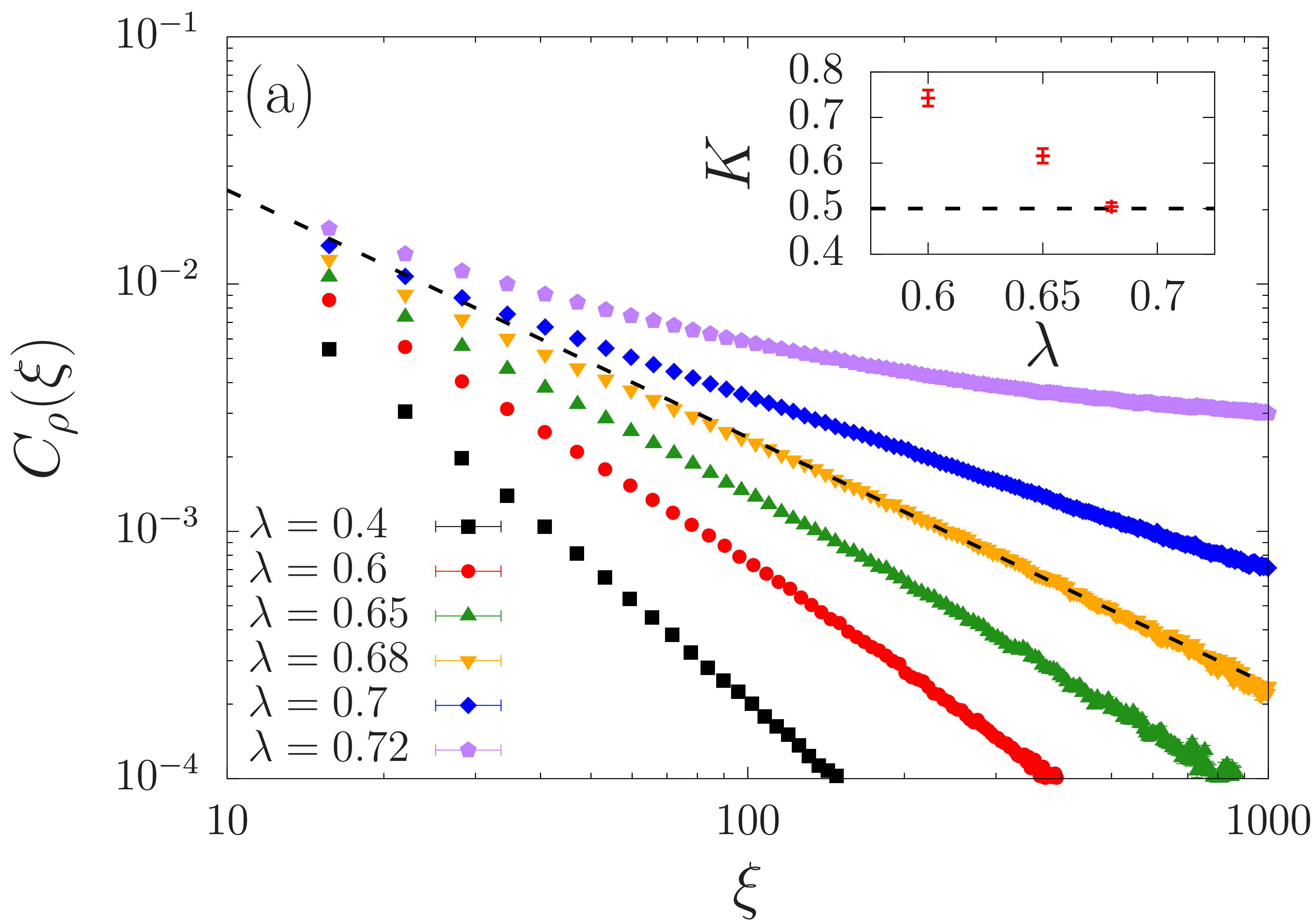
We reach system sizes up to: $L = 1282, \beta t = 2L$



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Motivation

Numerical simulation of fermion-boson models is very challenging:

- **DMRG** and **ED** are limited by the unbound bosonic Hilbert space that needs a truncation;
- **QMC** suffers from long autocorrelation times as only local boson updates are available [1].

We solve the **autocorrelation problem** by

- integrating out the bosons in the path integral to obtain a retarded fermionic interaction [2];
- generalizing the directed-loop algorithm [3] to the case of retarded interactions.

Retarded interactions

Consider the 1D spinless Holstein model

$$\hat{H} = -t \sum_i \hat{B}_{i,i+1} + \omega_0 \sum_i \hat{a}_i^\dagger \hat{a}_i + \gamma \sum_i \hat{\rho}_i \, (\hat{a}_i^\dagger + \hat{a}_i)$$

where $\hat{B}_{i,i+1} = (\hat{c}_i^\dagger \hat{c}_{i+1} + \text{H.c.})$ and $\hat{\rho}_i = (\hat{c}_i^\dagger \hat{c}_i - 1/2)$. Integrating out the bosons in

$$Z = \int \mathcal{D}(\bar{c},c)\, e^{-\mathcal{S}_{\text{f}}[\bar{c},c]} \underbrace{\int \mathcal{D}(\bar{a},a)\, e^{-\mathcal{S}_{\text{b}}[\bar{a},a] - \mathcal{S}_{\text{fb}}[\bar{a},a,\bar{c},c]}}_{=\mathcal{N}\, e^{-\mathcal{S}_{\text{ret}}[\bar{c},c]}}$$

leads to the retarded interaction

$$\mathcal{S}_{\text{ret}} = -2\lambda t \iint d\tau_1 d\tau_2 \sum_i \rho_i(\tau_1) P(\tau_1 - \tau_2) \rho_i(\tau_2)$$

mediated by the free boson propagator $P(\tau)$.

Application

- Bosonic observables are obtained from the vertex distribution via generating functionals [4].
- With the directed-loop updates, autocorrelation times are of order 1 (see Fig. 3).

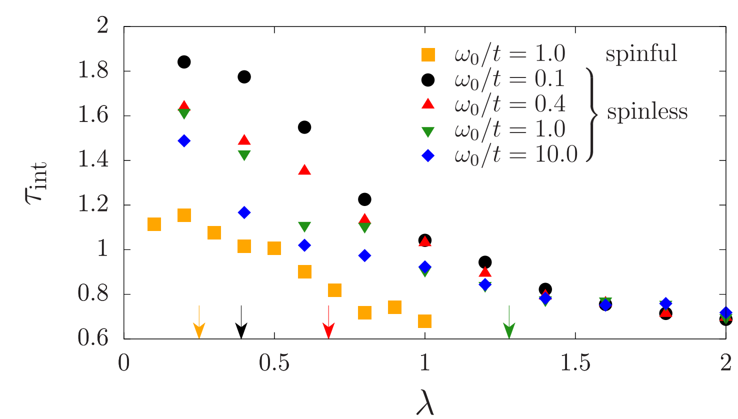
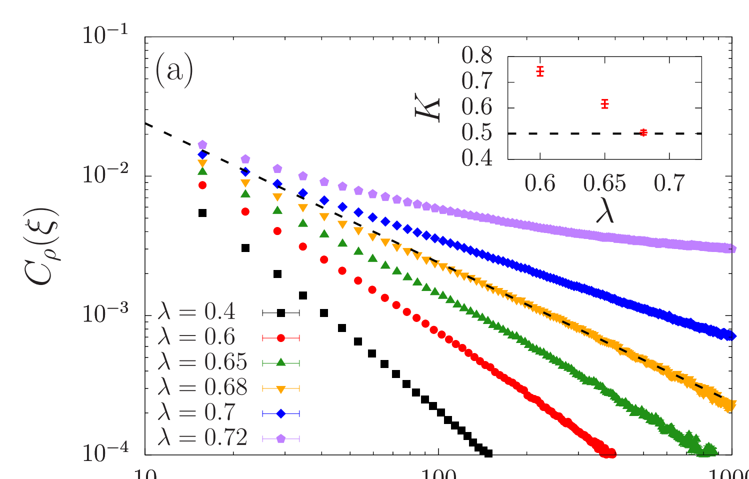


FIG. 3. Autocorrelation time τ_{int} for the total energy, as determined from a rebinning analysis, for the spinless and the spinful Holstein model. Here, $L = 18$, $\beta t = 2L$. Arrows indicate Peierls critical values $\lambda_c(\omega_0)$.

- Our algorithm reaches system sizes of $L = \beta t/2 = 1282$, as demonstrated in Fig. 4.



Formulation of the directed-loop algorithm

Stochastic series expansion from the path integral

The SSE representation corresponds to an expansion of $Z = \int \mathcal{D}(\bar{c},c)\, e^{-\mathcal{S}_0 - \mathcal{S}_1}$ around $\mathcal{S}_0 = \int d\tau \sum_i \bar{c}_i(\tau)\, \partial_\tau\, c_i(\tau)$. We write $\mathcal{S}_1$ as a sum over vertices,

$$\mathcal{S}_1 = -\sum_\nu w_\nu h_\nu \, . \qquad (1)$$

A **vertex** is specified by a superindex ν, a weight w_ν, and the Grassmann representation h_ν of an operator. Z becomes

$$Z = \sum^{\infty} \sum \frac{Z_0}{n!} w_{\nu_1} \dots w_{\nu_n} \langle h_{\nu_1} \dots h_{\nu_n} \rangle_0 \, ,$$

i.e., $\nu = \{a, b, \tau\}$ with operator type a, bond variable b, and time τ, $w_\nu = d\tau$, and $h_\nu = H_{a,b}(\tau)$. We can map to an operator string

$$\sum_{S_n} Z_0 \langle h_{\nu_1} \dots h_{\nu_n} \rangle_0 = \sum_{S_n} \sum_\alpha \langle \alpha | \prod_p \hat{H}_{a_p, b_p} | \alpha \rangle \, ,$$

where time labels become obsolete. Updates are based on the diagonal and directed-loop updates depicted in Fig 1.