Monte Carlo simulations of quantum systems with global updates

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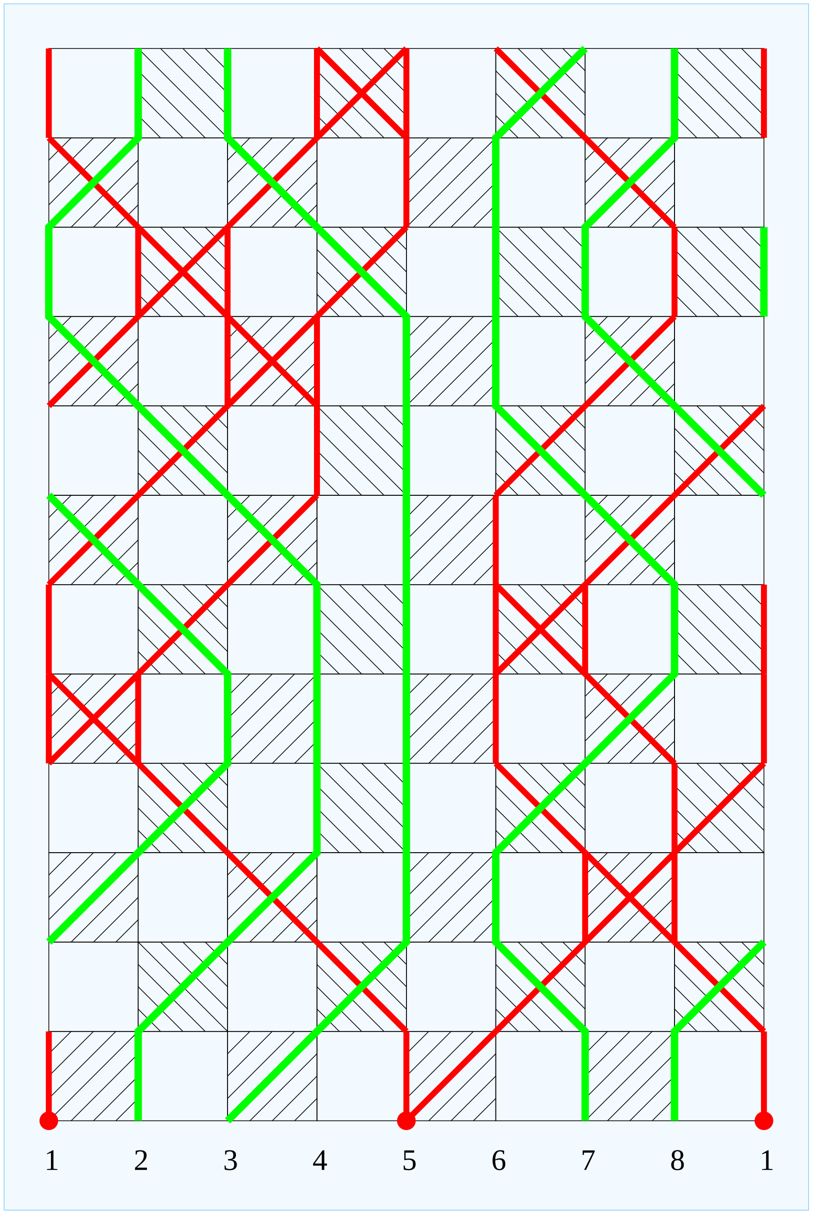
The hybrid-loop algorithm



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$$< \mathcal{O} >= \lim_{\theta\to\infty} \frac{\sum_{\{s_0\}} < s_0|\otimes < \Psi_T|\mathcal{P}\exp\left(-\theta H/2\right)\mathcal{O}\exp\left(-\theta H/2\right)\mathcal{P}|\Psi_T > \otimes|s_0 >}{\sum_{\{s_0\}} < s_0|\otimes < \Psi_T|\mathcal{P}\exp\left(-\theta H\right)\mathcal{P}|\Psi_T > \otimes|s_0 >},$$

where $\{|s_0>\}$ **is a complete set of spin states**
$|\Psi_T>$ **is a trial wavefunction for spinless fermions**
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As long as the overlap with the ground-state is finite

$$\lim_{\theta\to\infty} \mathrm{e}^{-\frac{\theta}{2}H}\mathcal{P}|\Psi_T > \otimes|s_0 >= \lim_{\theta\to\infty} \mathrm{e}^{-\frac{\theta}{2}E_G}|\Psi_G > ,$$

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Then

$$< \mathcal{O} > = \lim_{\theta\to\infty} \frac{\mathcal{N}\mathrm{e}^{-\theta E_G} < \Psi_G|\mathcal{O}|\Psi_G >}{\mathcal{N}\mathrm{e}^{-\theta E_G} < \Psi_G|\Psi_G >} = \frac{< \Psi_G|\mathcal{O}|\Psi_G >}{< \Psi_G|\Psi_G >} ,$$

Trotter splitting and introduction of complete sets of spin states

$$
\begin{aligned}
< \mathcal{O} > \;=\; & \lim_{\theta \to \infty} \Big[\sum_{\{s_i\}} < \Psi_T | \otimes < s_0 | \mathcal{P} \mathrm{e}^{-\Delta\tau H} | s_{L-1} > \cdots < s_{\frac{L}{2}+1} | \mathrm{e}^{-\Delta\tau H} | s_{\frac{L}{2}+1} > \\
& \times < s_{\frac{L}{2}+1} | \mathcal{O} | s_{\frac{L}{2}} >< s_{\frac{L}{2}} | \mathrm{e}^{-\Delta\tau H} | s_{\frac{L}{2}-1} > \\
& \times \cdots < s_1 | \mathrm{e}^{-\Delta\tau H} \mathcal{P} | s_0 > \otimes | \Psi_T > \Big] \\
& \times \Big[\sum_{\{s_i\}} < \Psi_T | \otimes < s_0 | \mathcal{P} \mathrm{e}^{-\Delta\tau H} | s_{L-1} > \cdots \\
& \times < s_1 | \mathrm{e}^{-\Delta\tau H} \mathcal{P} | s_0 > \otimes | \Psi_T > \Big]^{-1}
\end{aligned}
$$

where $\Delta\tau = \theta / L$**.**

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The Hamiltonian has only nearest neighbor terms
$\longrightarrow$ **checkerboard decomposition**

4.2 Matrix elements with spin states

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Bond Hamiltonian for the t-J model

$$H_{<i,j>} = \hat{\mathcal{A}} \left(1 + \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j\right) + \left[\frac{J}{4} - \hat{\mathcal{B}}\right] \left(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j - 1\right) \ ,$$

where $\hat{\mathcal{A}} \equiv \frac{t}{2}\left(f_i^\dagger f_j + f_j^\dagger f_i\right) \ ,$ **and** $\hat{\mathcal{B}} \equiv \frac{J}{4}\left(f_i^\dagger f_i + f_j^\dagger f_j\right) \ .$

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It holds $[\mathcal{A},\mathcal{B}] = 0$**.**

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Bond Hamiltonian for the Heisenberg model

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$$H^H_{<i,j>} = \frac{J}{4}\,(\boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j - 1)\ .$$

Canonical transformation for the spin part

$$\sigma_i^x \to (-1)^i\,\sigma_i^x\ , \qquad \sigma_i^y \to (-1)^i\,\sigma_i^y\ , \qquad \sigma_i^z \to \sigma_i^z\ ,$$

$$\hookrightarrow \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \quad \to \quad -2\left(\sigma_i^+\sigma_j^- + \sigma_i^-\sigma_j^+\right) + \sigma_i^z\sigma_j^z$$

Matrix elements

i**)** $<\uparrow\uparrow|\,\mathrm{e}^{-\Delta\tau H_{<i,j>}}\,|\uparrow\uparrow>=\exp\left(-\Delta\tau 2\hat{\mathcal{A}}\right)\,.$

ii**)** $<\downarrow\downarrow|\,\mathrm{e}^{-\Delta\tau H_{<i,j>}}\,|\downarrow\downarrow>=\exp\left(-\Delta\tau 2\hat{\mathcal{A}}\right)\,.$

iii**)** $<\uparrow\downarrow|\,\mathrm{e}^{-\Delta\tau H_{<i,j>}}\,|\uparrow\downarrow>=\frac{1}{2}\left\{\exp\left(-\Delta\tau 2\hat{\mathcal{A}}\right)+\exp\left[\Delta\tau\left(2\hat{\mathcal{A}}+J-4\hat{\mathcal{B}}\right)\right]\right\}\,.$

iv**)** $<\uparrow\downarrow|\,\mathrm{e}^{-\Delta\tau H_{<i,j>}}\,|\downarrow\uparrow>=\frac{1}{2}\left\{-\exp\left(-\Delta\tau 2\hat{\mathcal{A}}\right)+\exp\left[\Delta\tau\left(2\hat{\mathcal{A}}+J-4\hat{\mathcal{B}}\right)\right]\right\}\,.$

v**)** $<\downarrow\uparrow|\,\mathrm{e}^{-\Delta\tau H_{<i,j>}}\,|\uparrow\downarrow>=$ iv**).**

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4.3 Partition function

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Although we are at $T = 0$, we have formally a partition function (or generating functional)

$$
\begin{aligned}
Z &\equiv \sum_{\{s_i\}} < \Psi_T| \otimes < s_0|\mathcal{P}\mathrm{e}^{-\Delta\tau H}|s_{L-1} > \cdots < s_1|\mathrm{e}^{-\Delta\tau H}\mathcal{P}|s_0 > \otimes |\Psi_T > \\
&\equiv \sum_{\{s_i\}} W_S\left[\{s_i\}\right] W_F\left[\{s_i\}\right] \ ,
\end{aligned}
$$

where $W_S\left[\{s_i\}\right]$ is the weight of a pure Heisenberg model for a spin-configuration $\{s_i\}$, and

$$
W_F\left[\{s_i\}\right] \equiv < \Psi_T| \otimes \overline{< s_0|\mathrm{e}^{-\Delta\tau H}|s_{L-1} >} \cdots \overline{< s_1|\mathrm{e}^{-\Delta\tau H}|s_0 >} \otimes |\Psi_T > ,
$$

with the definition

$$
\overline{< s_\ell|\mathrm{e}^{-\Delta\tau H}|s_{\ell-1} >} = \frac{< s_\ell|\mathrm{e}^{-\Delta\tau H}|s_{\ell-1} >}{< s_\ell|\mathrm{e}^{-\Delta\tau H^H}|s_{\ell-1} >}
$$

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For the trial wavefunction, take a Slater determinant, i.e. an antisymmetrized product of one-particle states

$$| \Psi_T > \ = \ \prod_{j=1}^{N_p} \sum_{i=1}^{N} P_{ij} \, f_i^\dagger \, | \, 0 > ,$$

where N is the number of sites, and N_p is the number of holes.

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Orthonormalized states $\longrightarrow \sum_i P_{ij} P_{ik} = \delta_{jk}$

$\hookrightarrow$ **normalized trial wavefunction**

$$< \Psi_T \,|\, \Psi_T > \;=\; \sum_{\substack{i_1 \cdots i_{N_p} \\ j_1 \cdots j_{N_p}}} P_{i_1 1} \cdots P_{i_{N_p} N_p} P_{j_1 1} \cdots P_{j_{N_p} N_p} \times < 0 \,|\, f_{i_{N_p}} \cdots f_{i_1} f_{j_1}^\dagger \cdots f_{j_{N_p}}^\dagger \,|\, 0 > ,$$

where

$$< 0 \,|\, f_{i_{N_p}} \cdots f_{i_1} f_{j_1}^\dagger \cdots f_{j_{N_p}}^\dagger \,|\, 0 > \;=\; \varepsilon^{k_1 \cdots k_{N_p}} \delta_{i_i j_{k_1}} \cdots \delta_{i_{N_p} j_{k_{N_p}}} .$$

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$$\mathrm{e}^{-\Delta\tau 2\hat{\mathcal{A}}} = \mathrm{e}^{-\Delta\tau t(f_i^\dagger f_{i+1} + h.c.)} \tag{1}$$

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Introduce new operators

$$\begin{aligned} \tilde{f}_i &= \frac{1}{\sqrt{2}}(f_i + f_{i+1}) \\ \tilde{f}_{i+1} &= \frac{1}{\sqrt{2}}(f_i - f_{i+1}) \end{aligned}$$

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$\hookrightarrow$ $f_i^\dagger f_{i+1} + f_{i+1}^\dagger f_i = \tilde{f}_i^\dagger \tilde{f}_i - \tilde{f}_{i+1}^\dagger \tilde{f}_{i+1}$ **such that**

$$(1) \quad = \quad e^{-\Delta\tau t(\tilde{f}_i^\dagger \tilde{f}_i - \tilde{f}_{i+1}^\dagger \tilde{f}_{i+1})}$$

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$$\begin{aligned} (1) &= e^{-\Delta\tau t(\tilde{f}_i^\dagger \tilde{f}_i - \tilde{f}_{i+1}^\dagger \tilde{f}_{i+1})} \\ &= e^{-\Delta\tau t \tilde{f}_i^\dagger \tilde{f}_i} e^{\Delta\tau t \tilde{f}_{i+1}^\dagger \tilde{f}_{i+1}} \end{aligned}$$

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$$\begin{aligned}(1) &= e^{-\Delta\tau t(\tilde{f}_i^\dagger \tilde{f}_i - \tilde{f}_{i+1}^\dagger \tilde{f}_{i+1})} \\ &= e^{-\Delta\tau t \tilde{f}_i^\dagger \tilde{f}_i} e^{\Delta\tau t \tilde{f}_{i+1}^\dagger \tilde{f}_{i+1}} \\ &= \left[1 + \left(e^{-\Delta\tau t} - 1\right) \tilde{f}_i^\dagger \tilde{f}_i\right] \left[1 + \left(e^{\Delta\tau t} - 1\right) \tilde{f}_{i+1}^\dagger \tilde{f}_{i+1}\right]\end{aligned}$$

Change of basis in the Slater determinant

$$\sum_{i=1}^{N} P_{i,j}[s_0]\, f_i^\dagger \quad = \quad \sum_{i\,\mathrm{odd}}^{N-1} \left(P_{i,j}\, f_i^\dagger + P_{i+1,j}\, f_{i+1}^\dagger \right)$$

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&= \sum_{i\,\mathrm{odd}}^{N-1} \left[P_{i,j}\, \frac{1}{\sqrt{2}} \left(\tilde{f}_i^\dagger + \tilde{f}_{i+1}^\dagger \right) + P_{i+1,j}\, \frac{1}{\sqrt{2}} \left(\tilde{f}_i^\dagger - \tilde{f}_{i+1}^\dagger \right) \right] \\
&= \sum_{i=1}^{N} \tilde{P}_{i,j}[s_0]\, \tilde{f}_i^\dagger
\end{aligned}$$

with $\tilde{P}_{i,j} = P_{i,j} + (-1)^{i+1} P_{i+1,j}$ **(assumed splitting with first index odd)**

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Explicit form for a Slater determinant

$$\prod_{j=1}^{N_p} \sum_{\ell=1}^{N} \tilde{P}_{\ell,j}\, \tilde{f}_\ell^\dagger \mid 0 > \;=\; \sum_{i_1,\ldots,i_{N_p}=1}^{N} \sum_{P} P \begin{pmatrix} i_1 i_2 \cdots i_{N_p} \\ j_1 j_2 \cdots j_{N_p} \end{pmatrix} (-1)^p \times \tilde{P}_{j_1,1} \tilde{P}_{j_2,2} \cdots \tilde{P}_{j_{N_p},N_p}\, \tilde{f}_{i_1}^\dagger \cdots \tilde{f}_{i_{N_p}}^\dagger \mid 0 >$$

with $i_1 < i_2 < \cdots < i_{N_p}$

Consider the product

$$
\begin{aligned}
\left[1 + \left(\mathrm{e}^{-\Delta\tau J} - 1\right) \tilde{f}_i^\dagger \tilde{f}_i\right] \mid \Psi_T > \quad &= \quad \mid \Psi_T > + \left(\mathrm{e}^{-\Delta\tau J} - 1\right) \tilde{f}_i^\dagger \tilde{f}_i \\
&\times \sum_{i_1,\ldots,i_{N_p}} \sum_P P \begin{pmatrix} i_1 i_2 \cdots i_{N_p} \\ j_1 j_2 \cdots j_{N_p} \end{pmatrix} (-1)^p \\
&\qquad \times \tilde{P}_{j_1,1} \tilde{P}_{j_2,2} \cdots \tilde{P}_{j_{N_p},N_p} \tilde{f}_{i_1}^\dagger \cdots \tilde{f}_{i_{N_p}}^\dagger \mid 0 >
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&=\; \prod_{j=1}^{N_p} \sum_{\ell=1}^{N} \tilde{P}'_{\ell,j} \tilde{f}_\ell^\dagger \mid 0 > ,
\end{aligned}
$$

where

$$
\tilde{P}'_{\ell,j} = \begin{cases} \mathrm{e}^{-\Delta\tau J} \tilde{P}_{\ell,j} & \text{for } \ell = i, \\ \tilde{P}_{\ell,j} & \text{for } \ell \neq i. \end{cases}
$$

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$$\begin{aligned}\left[1+\left(\mathrm{e}^{-\Delta\tau J}-1\right)\tilde{f}_i^\dagger\tilde{f}_i\right] \mid \Psi_T > &= \mid \Psi_T > + \left(\mathrm{e}^{-\Delta\tau J}-1\right)\tilde{f}_i^\dagger\tilde{f}_i \\ &\quad \times \sum_{i_1,\ldots,i_{N_p}}\sum_P P\begin{pmatrix} i_1 i_2\cdots i_{N_p} \\ j_1 j_2\cdots j_{N_p}\end{pmatrix}(-1)^p \\ &\quad\quad \times \tilde{P}_{j_1,1}\tilde{P}_{j_2,2}\cdots\tilde{P}_{j_{N_p},N_p}\tilde{f}_{i_1}^\dagger\cdots\tilde{f}_{i_{N_p}}^\dagger \mid 0 > \\ &= \prod_{j=1}^{N_p}\sum_{\ell=1}^{N}\tilde{P}'_{\ell,j}\,\tilde{f}_\ell^\dagger \mid 0 > ,\end{aligned}$$

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For the full operator we have

$$\tilde{P}'_{\ell,j} = \begin{cases} \mathrm{e}^{\Delta\tau t}\tilde{P}_{\ell,j} & \text{for } \ell = i+1, \\ \mathrm{e}^{-\Delta\tau t}\tilde{P}_{\ell,j} & \text{for } \ell = i, \\ \tilde{P}_{\ell,j} & \text{else.} \end{cases}$$

Back to the original representation

$$P'_{i,j} = \frac{1}{2}\left(\tilde{P}'_{i,j} + \tilde{P}'_{i+1,j}\right)$$

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&= \frac{1}{2}\left[\mathrm{e}^{-\Delta\tau t}\left(P_{i,j} + P_{i+1,j}\right) + \mathrm{e}^{\Delta\tau t}\left(P_{i,j} - P_{i+1,j}\right)\right]
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&= \frac{1}{2}\left[\mathrm{e}^{-\Delta\tau t}\left(P_{i,j} + P_{i+1,j}\right) + \mathrm{e}^{\Delta\tau t}\left(P_{i,j} - P_{i+1,j}\right)\right] \\
&= \cosh\left(\Delta\tau t\right)\, P_{i,j} - \sinh\left(\Delta\tau t\right)\, P_{i+1,j}
\end{aligned}
$$

Back to the original representation

$$
\begin{aligned}
P'_{i,j} &= \frac{1}{2}\left(\tilde{P}'_{i,j} + \tilde{P}'_{i+1,j}\right) \\
&= \frac{1}{2}\left(\mathrm{e}^{-\Delta\tau t}\tilde{P}_{i,j} + \mathrm{e}^{\Delta\tau t}\tilde{P}_{i+1,j}\right) \\
&= \frac{1}{2}\left[\mathrm{e}^{-\Delta\tau t}\left(P_{i,j} + P_{i+1,j}\right) + \mathrm{e}^{\Delta\tau t}\left(P_{i,j} - P_{i+1,j}\right)\right] \\
&= \cosh\left(\Delta\tau t\right)\, P_{i,j} - \sinh\left(\Delta\tau t\right)\, P_{i+1,j}
\end{aligned}
$$

$$P'_{i+1,j}$$

Back to the original representation

$$
\begin{aligned}
P'_{i,j} &= \frac{1}{2}\left(\tilde{P}'_{i,j} + \tilde{P}'_{i+1,j}\right) \\
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\end{aligned}
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Back to the original representation

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&= \frac{1}{2}\left(\mathrm{e}^{-\Delta\tau t}\tilde{P}_{i,j} - \mathrm{e}^{\Delta\tau t}\tilde{P}_{i+1,j}\right)
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$$

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&= \frac{1}{2}\left(\mathrm{e}^{-\Delta\tau t}\tilde{P}_{i,j} - \mathrm{e}^{\Delta\tau t}\tilde{P}_{i+1,j}\right) \\
&= \frac{1}{2}\left[\mathrm{e}^{-\Delta\tau t}\left(P_{i,j} + P_{i+1,j}\right) - \mathrm{e}^{\Delta\tau t}\left(P_{i,j} - P_{i+1,j}\right)\right]
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Back to the original representation

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&= \frac{1}{2}\left(\mathrm{e}^{-\Delta\tau t}\tilde{P}_{i,j} - \mathrm{e}^{\Delta\tau t}\tilde{P}_{i+1,j}\right) \\
&= \frac{1}{2}\left[\mathrm{e}^{-\Delta\tau t}\left(P_{i,j} + P_{i+1,j}\right) - \mathrm{e}^{\Delta\tau t}\left(P_{i,j} - P_{i+1,j}\right)\right] \\
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&= \frac{1}{2}\left[\mathrm{e}^{-\Delta\tau t}\left(P_{i,j} + P_{i+1,j}\right) - \mathrm{e}^{\Delta\tau t}\left(P_{i,j} - P_{i+1,j}\right)\right] \\
&= -\sinh\left(\Delta\tau t\right)\ P_{i,j} + \cosh\left(\Delta\tau t\right)\ P_{i+1,j}\ ,
\end{aligned}
$$

Equivalent to matrix $\times$ vector

$$
\mathrm{e}^{-\Delta\tau 2\hat{\mathcal{A}}}\ |\ \Psi_S > \longrightarrow \begin{pmatrix} \cosh\left(\Delta\tau t\right) & -\sinh\left(\Delta\tau t\right) \\ -\sinh\left(\Delta\tau t\right) & \cosh\left(\Delta\tau t\right) \end{pmatrix} \times P_{ij}\ .
$$

Exponential of a bilinear form transforms a Slater determinant into another Slater determinant .

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After the evolution we have a scalar product of two Slater determinants

$$< \Psi_T | \otimes < s_0 | \mathcal{P} \mathrm{e}^{-\Delta\tau H} | s_{L-1} > \cdots < s_1 | \mathrm{e}^{-\Delta\tau H} \mathcal{P} | s_0 > \otimes | \Psi_T > = < \Psi_T \mid \tilde{\Psi} >$$

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Recall

$$< 0 \mid f_{i_{N_p}} \cdots f_{i_1} f^{\dagger}_{j_1} \cdots f^{\dagger}_{j_{N_p}} \mid 0 > \quad = \quad \varepsilon^{k_1 \cdots k_{N_p}} \delta_{i_i j_{k_1}} \cdots \delta_{i_{N_p} j_{k_{N_p}}} \, .$$

Fermionic determinant $\longrightarrow W_F \left[\{ s_i \} \right]$

$$\begin{aligned} < \Psi_T \mid \tilde{\Psi} > \quad &= \quad \sum_{\substack{i_1 \cdots i_{N_p} \\ j_1 \cdots j_{N_p}}} P_{i_1 1} \cdots P_{i_{N_p} N_p} \tilde{P}_{j_1 1} \cdots \tilde{P}_{j_{N_p} N_p} \\ &\qquad \times < 0 \mid f_{i_{N_p}} \cdots f_{i_1} f^{\dagger}_{j_1} \cdots f^{\dagger}_{j_{N_p}} \mid 0 > \\ &= \quad \det \left(P^T \tilde{P} \right) \end{aligned}$$

4.5 Matrix elements for the evolution of fermionic states

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$$\exp\left(-\Delta\tau 2\hat{\mathcal{A}}\right) \quad \rightarrow \quad \begin{bmatrix} \cosh(\Delta\tau t) & -\sinh(\Delta\tau t) \\ -\sinh(\Delta\tau t) & \cosh(\Delta\tau t) \end{bmatrix}$$

$$\exp\left(-4\Delta\tau\hat{\mathcal{B}}\right) \quad \rightarrow \quad \mathrm{e}^{-\Delta\tau J}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

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$$\exp\left(-4\Delta\tau\hat{\mathcal{B}}\right) \quad \rightarrow \quad \mathrm{e}^{-\Delta\tau J}\left(\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array}\right)$$

For the matrix elements we have finally

$$\overline{<\uparrow\uparrow|\cdots|\uparrow\uparrow>} = \overline{<\downarrow\downarrow|\cdots|\downarrow\downarrow>} \quad = \quad \left[\begin{array}{rr} \cosh\left(\Delta\tau t\right) & -\sinh\left(\Delta\tau t\right) \\ -\sinh\left(\Delta\tau t\right) & \cosh\left(\Delta\tau t\right) \end{array}\right]$$

$$\overline{<\uparrow\downarrow|\cdots|\uparrow\downarrow>} = \overline{<\downarrow\uparrow|\cdots|\downarrow\uparrow>} \quad = \quad \frac{\mathrm{e}^{-\Delta\tau J/2}}{\cosh\left(\Delta\tau J/2\right)}\left[\begin{array}{cc} \cosh\left(\Delta\tau t\right) & 0 \\ 0 & \cosh\left(\Delta\tau t\right) \end{array}\right]$$

$$\overline{<\uparrow\downarrow|\cdots|\downarrow\uparrow>} = \overline{<\downarrow\uparrow|\cdots|\uparrow\downarrow>} \quad = \quad \frac{\mathrm{e}^{-\Delta\tau J/2}}{\sinh\left(\Delta\tau J/2\right)}\left[\begin{array}{cc} 0 & \sinh\left(\Delta\tau t\right) \\ \sinh\left(\Delta\tau t\right) & 0 \end{array}\right]$$

4.6 Updating

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Weight of a configuration of pseudospins

$$W\left[\{s_i\}\right] = W_S\left[\{s_i\}\right]\, W_F\left[\{s_i\}\right]$$

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$$r \equiv \frac{W\left[\{s_i\}_{\mathrm{new}}\right]}{W\left[\{s_i\}_{\mathrm{old}}\right]}$$

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Generate new configurations with the loop-algorithm

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Generate new configurations with the loop-algorithm

↓

hybrid-loop algorithm

4.7 Stable evolution of the fermionic trial wavefunction

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Evolution operator in imaginary time is not unitary
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Define

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Define

$$| \Psi[s_0], \tau > \equiv \exp(-\tau H) \mathcal{P} |s_0> \otimes |\Psi_T>$$

Expectation value

$$\begin{aligned}
< \mathcal{O} > &= \lim_{\theta \to \infty} \frac{\sum_{\{s_0\}} < \Psi[s_0], \theta/2 \mid \mathcal{O} \mid \Psi[s_0], \theta/2 >}{\sum_{\{s_0\}} < \Psi[s_0], \theta/2 \mid \Psi[s_0], \theta/2 >} \\
&= \lim_{\theta \to \infty} \sum_{\{s_0\}} \frac{< \Psi[s_0], \theta/2 \mid \mathcal{O} \mid \Psi[s_0], \theta/2 >}{< \Psi[s_0], \theta/2 \mid \Psi[s_0], \theta/2 >} \\
&\qquad \times \frac{< \Psi[s_0], \theta/2 \mid \Psi[s_0], \theta/2 >}{\sum_{\{s_0\}} < \Psi[s_0], \theta/2 \mid \Psi[s_0], \theta/2 >} \\
&= \lim_{\theta \to \infty} \sum_{\{s_0\}} < \bar{\Psi}[s_0], \theta/2 \mid \mathcal{O} \mid \bar{\Psi}[s_0], \theta/2 > \frac{W_S[s_0] \, W_F[s_0]}{Z}
\end{aligned}$$

Normalized wavefunction

$$| \bar{\Psi} [s_0] , \theta/2 > \equiv \frac{| \Psi [s_0] , \theta/2 >}{\sqrt{< \Psi [s_0] , \theta/2 \mid \Psi [s_0] , \theta/2 >}}$$

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Gramm-Schmidt decomposition

$$| \Psi [s_0] , \tau > \longrightarrow P_\tau = U_\tau D_\tau V_\tau \ ,$$

where $U^\dagger U = \mathbf{1}_{N_p \times N_p}$, D is a diagonal matrix with (exponentially) large and small energy scales containing the norm of the one particle states, and V is an upper triangular matrix with unity in the diagonal, and hence, with determinant one.

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Norm of the wavefunction

$$\begin{aligned} < \Psi\left[s_0\right], \tau \mid \Psi\left[s_0\right], \tau > &= \det\left(V_\tau^\dagger D_\tau U_\tau^\dagger U_\tau D_\tau V_\tau\right) \\ &= \det\left(V_\tau^\dagger D_\tau D_\tau V_\tau\right) = \left(\det D\right)^2 \end{aligned}$$

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$\hookrightarrow < \mathcal{O} >$ **is numerically stable, since we need only U.**

4.8 Measurement of physical observables

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- **Equal-time correlators for fermions and diagonal operators for spins.**

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- Equal-time correlators for fermions and diagonal operators for spins.
- Time-displaced correlators $\longrightarrow$ spectral functions
- Up to now, no improved estimators
- Minus-sign problem practically non existing in one dimension

4.9 Tests

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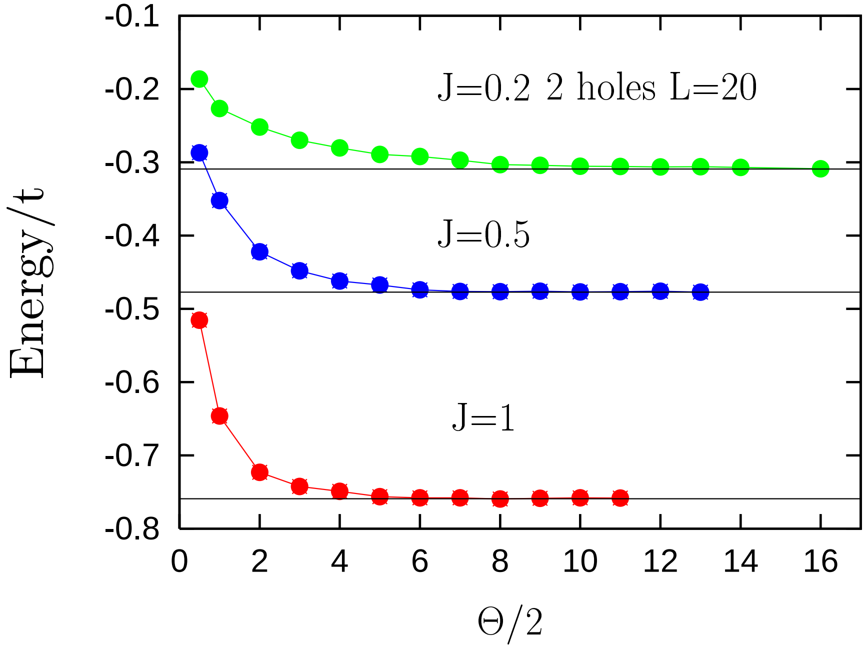
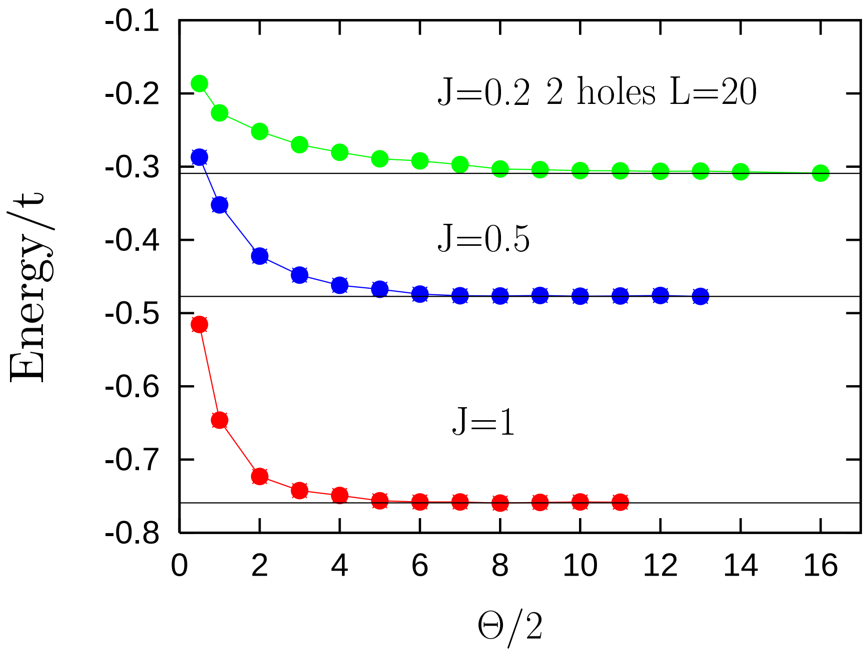
4.9.1 Comparison with exact diagonalization



4.9 Tests

4.9.1 Comparison with exact diagonalization



Convergence with $10 \leq \Theta t \leq 20$

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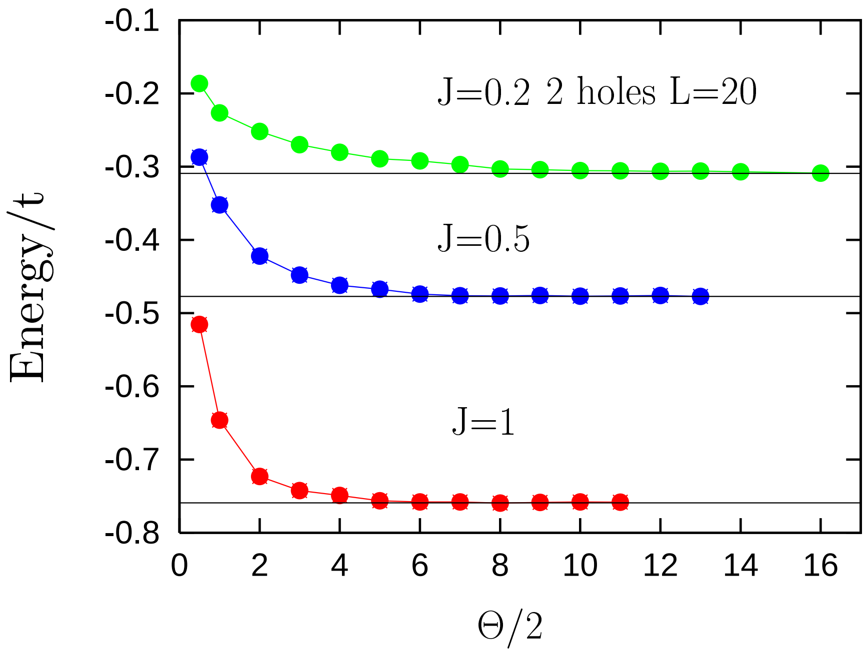

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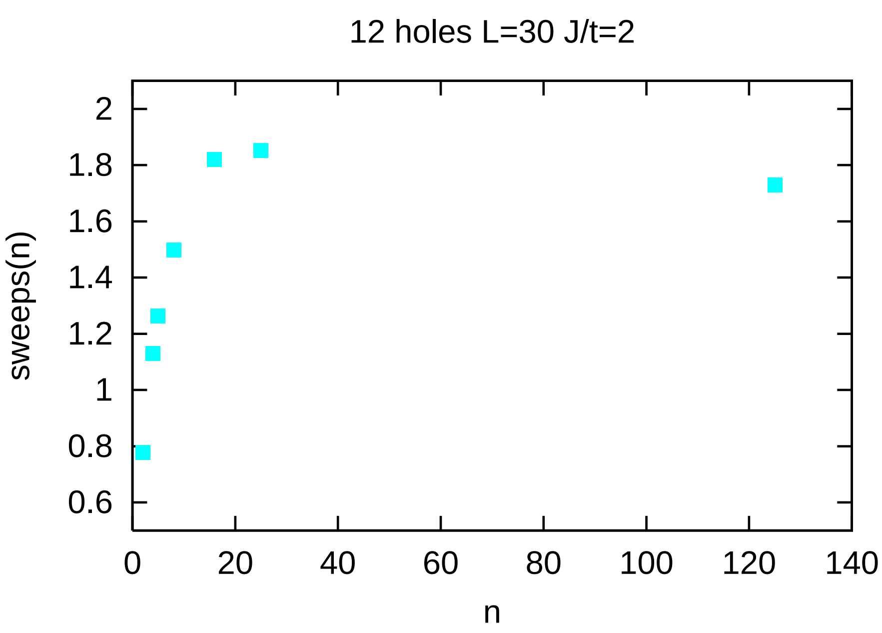
4.9.2 Autocorrelation time



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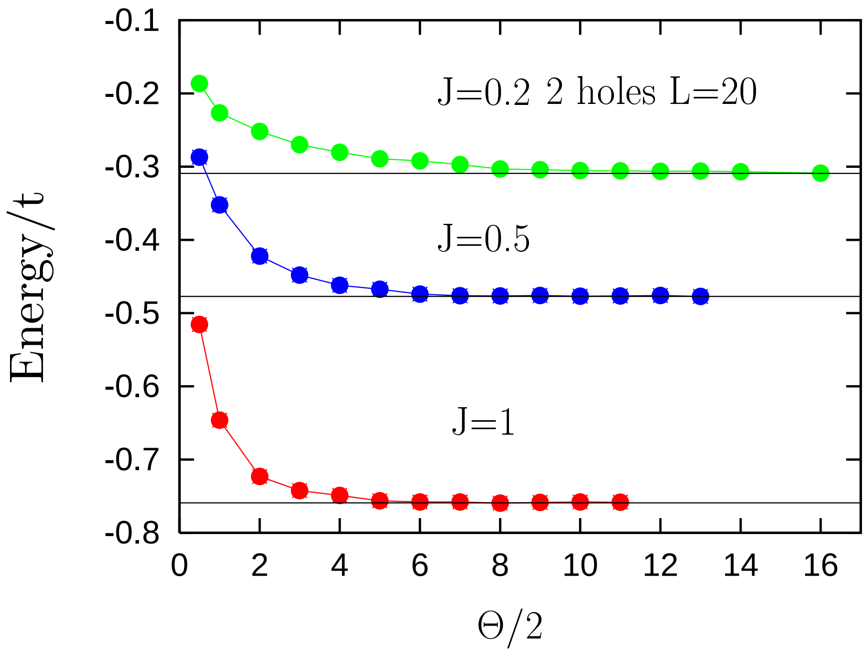

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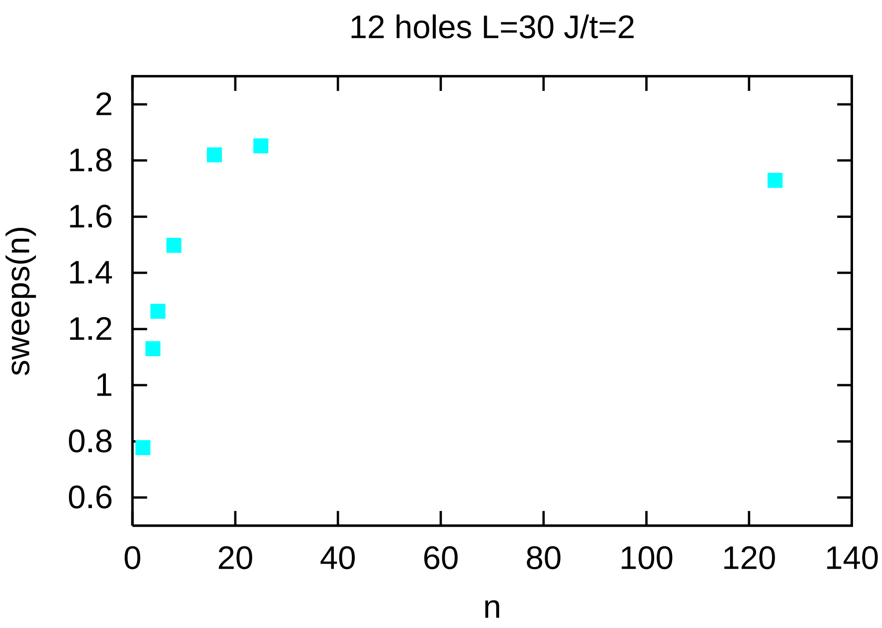

Configurations are statistically independent beyond 2 sweeps