Minimal Autocorrelation in HMC simulations using Exact Fourier Acceleration

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$$\dot{x} = \frac{\partial \mathcal{H}}{\partial p}$$
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4. Accept new x with probability $p_{\mathsf{acc}} = \min\left(1, \mathrm{e}^{-\Delta\mathcal{H}}\right)$

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2. Sample $r \sim \mathcal{N}(0{,}1)^{\dim(M)}$

3. Then $x = \mathit{\Omega} \cdot \mathrm{diag}(\omega) \cdot \mathit{\Omega}^\dagger \cdot r$ follows $x \sim \mathrm{e}^{-S(x)}$

Sampling from an *almost* normal distribution

[JO et al. *cond-mat.mtrl-sci*/**2312**.14914; Xing et al. *PRL* **126** (2021)]

Now $S(x) = \frac{1}{2}x^{\mathsf{T}}Mx + \varepsilon V(x)$

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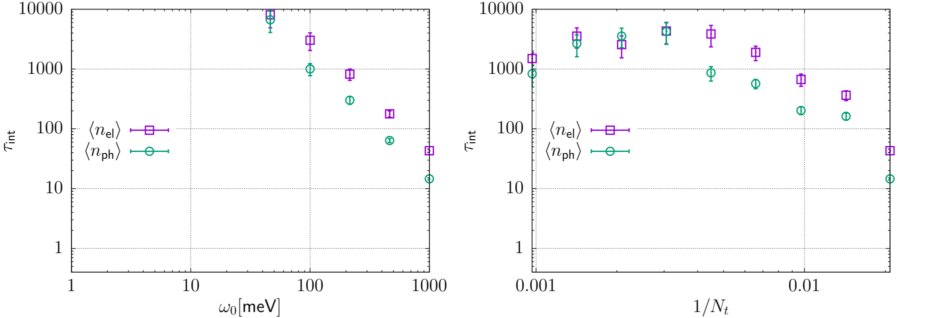

$$H_{\mathsf{SSH}} = \omega_0 \sum_{i,\alpha} \left(a^\dagger_{i,\alpha} a_{i,\alpha} + \frac{1}{2} \right) - \sum_{i,\alpha} J_\alpha \left(1 - \lambda_\alpha x_{i,\alpha}\right) \left(c^\dagger_i c_{i+\alpha} + c^\dagger_{i+\alpha} c_i \right)$$

Back to the harmonic oscillator

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- Solution

$$x_i(t) = x_i^0 \cos\left(\frac{\omega_i}{m_i} t\right) + \frac{1}{m_i \omega_i} p_i^0 \sin\left(\frac{\omega_i}{m_i} t\right)$$
$$p_i(t) = p_i^0 \cos\left(\frac{\omega_i}{m_i} t\right) - m_i \omega_i\, x_i^0 \sin\left(\frac{\omega_i}{m_i} t\right)$$

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- Choose $m_i = \omega_i$ and trajectory length $T = \frac{\pi}{2}$

“Fourier acceleration”

[Batrouni et al. *PRD* **32** (1985); Cohen-Stead et al. *PRE* **105** (2022); JO & Buividovich *hep-lat*/**2404**.09723]

Theorem (Optimal HMC trajectory length and kinetic term)

Given the harmonic action

$$S(x) = \frac{1}{2} x^\mathsf{T} M x \,,$$

then the Hamiltonian

$$\mathcal{H} = \frac{1}{2} p^\mathsf{T} M^{-1} p + S(x)$$

together with the HMC trajectory length $T = \frac{\pi}{2}$ *make HMC equivalent to uncorrelated direct sampling.*

Exact Fourier Acceleration (EFA)

[JO & Buividovich *hep-lat*/**2404**.09723; Urbach et al. *CPC* **174** (2006)]

Algorithm: Leap-Frog step for $\mathcal{H} = \frac{1}{2} p^\mathsf{T} M^{-1} p + \frac{1}{2} x^\mathsf{T} M x + V(x)$

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$(x,p) \leftarrow \text{EFA}\left(x^0, p^0, {}^h\!/_2\right)$;

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$(x(h), p(h)) \leftarrow \text{EFA}\left(x, p, {}^h\!/_2\right)$;

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$y^0 \leftarrow \Omega^\dagger \cdot x^0 ;\ q^0 \leftarrow \Omega^\dagger \cdot p^0;$

$y_i(h) \leftarrow \cos(h)\, y_i^0 + \frac{1}{\omega_i^2} \sin(h)\, q_i^0;$

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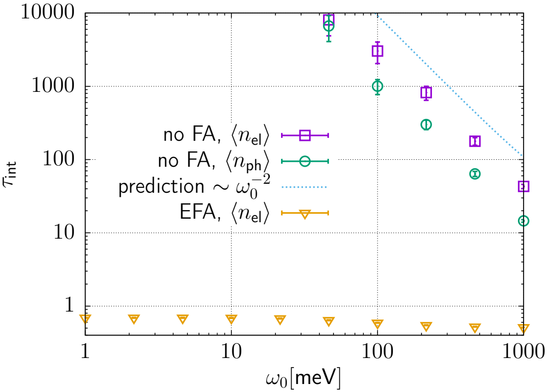
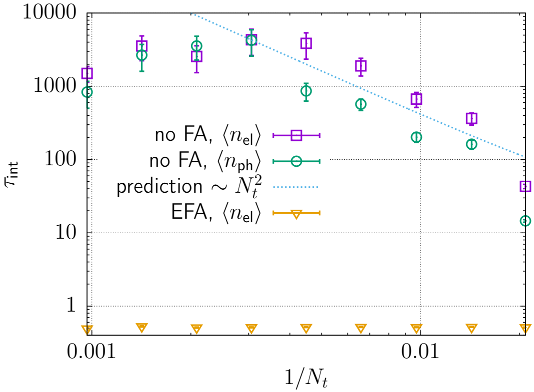
$x(h) \leftarrow \Omega \cdot y(h)$; $p(h) \leftarrow \Omega \cdot q(h)$;

Benchmarking the SSH model [JO & Buividovich *hep-lat*/**2404**.09723]

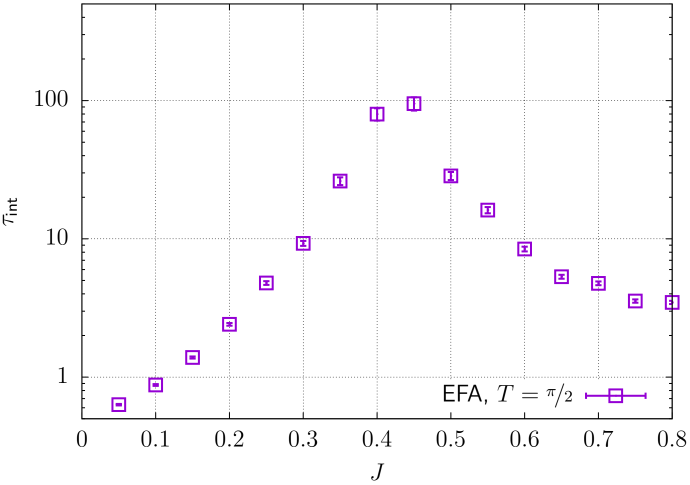
$$S_{\mathrm{SSH}} = \sum_t \left[\omega_0^2 x_t^2 + N_t^2 \left(x_{t+1} - x_t\right)^2\right] + \text{weak electron interactions}$$





Critical slowing down in the classical Ising model

[JO & Buividovich *hep-lat*/**2404**.09723]



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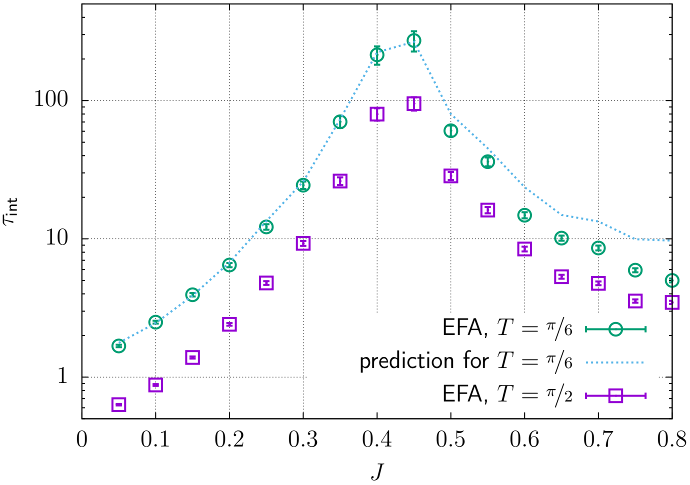
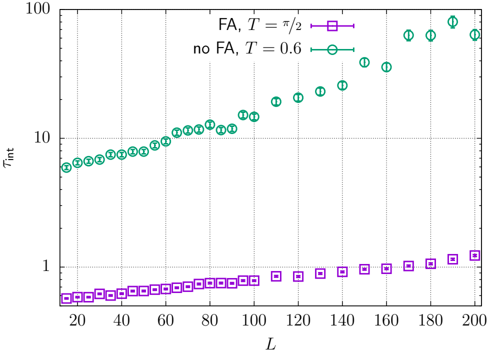


$$\tau_{\text{int}}(T) = \frac{\tau_{\text{int}}(T = \pi/2)}{1 - \cos(T)^{\pi/2T}}$$

Gauge Theories with Fourier acceleration

[Borsanyi et al. *Science* **347** (2015); Duane & Pendleton *Phys. Lett. B* **206** (1988)]

$$2D,\, U(1),\, \beta = 10$$



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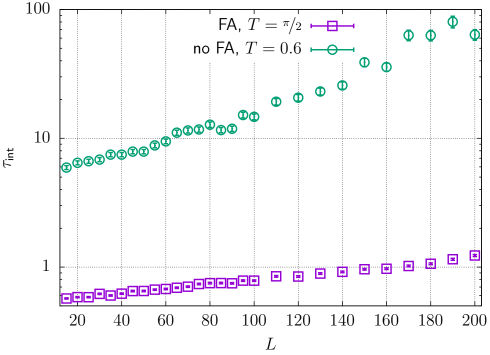
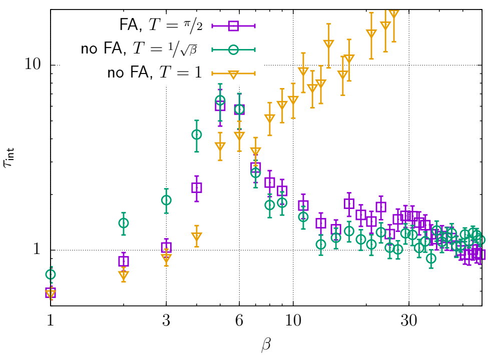


$4D,\, SU(3),\, L = 10$



Trajectory length if EFA is impossible

[Apers et al. *stat.ML*/**2209**.12771; Meyer et al. *CPC* **176** (2007)]

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$\Rightarrow$ better too long than too short

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  choose Hamiltonian
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Minimal Autocorrelation in HMC simulations using Exact Fourier Acceleration

- For action $S(x) = \frac{1}{2}x^\mathsf{T} M x + \varepsilon V(x)$ choose Hamiltonian $\mathcal{H} = \frac{1}{2}p^\mathsf{T} M^{-1} p + S(x)$
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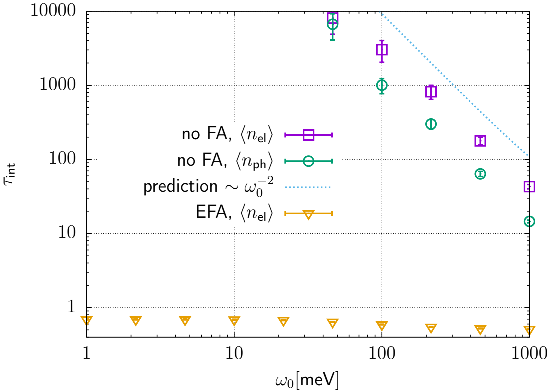

$$S_{\text{SSH}} = \sum_t \left[\omega_0^2 x_t^2 + N_t^2 \left(x_{t+1} - x_t\right)^2\right] + \dots$$

The Su-Schrieffer-Heeger (SSH) model [Su et al. *PRL* **42** (1979)] I

Without Fourier acceleration $\tau_{\text{int}} \propto 1 + \left(\frac{2N_t}{\beta\omega_0}\right)^2$.

$$
\begin{aligned}
H_{\text{SSH}} = \omega_0 \sum_{i,\alpha} \left(a^\dagger_{i,\alpha} a_{i,\alpha} + \frac{1}{2} \right) \\
- \sum_{i,\alpha} J_\alpha \left(1 - \lambda_\alpha x_{i,\alpha}\right) \left(c^\dagger_i c_{i+\alpha} + c^\dagger_{i+\alpha} c_i \right) - \mu \sum_i c^\dagger_i c_i
\end{aligned}
$$

The Su-Schrieffer-Heeger (SSH) model [Su et al. *PRL* **42** (1979)] II

$$
\begin{aligned}
S_{\mathsf{SSH}} &= \frac{1}{2} x^{\mathsf{T}} M_{\mathsf{SSH}}\, x + \text{electron interactions} \\
&= \frac{\beta}{2N_t} \sum_t \left[\omega_0^2 x_t^2 + \frac{N_t^2}{\beta^2} \left(x_{t+1} - x_t \right)^2 \right] + \text{electron interactions} \\
&= \frac{1}{2\beta N_t} \sum_\xi \left[(\beta\omega_0)^2 + 4N_t^2 \sin^2\left(\frac{\pi}{N_t}\xi \right) \right] y_\xi^2 + \text{electron interactions}\,, \\
y_\xi &= \frac{1}{\sqrt{N_t}} \sum_t \mathrm{e}^{-\,\mathrm{i}\,\frac{2\pi}{N_t}\xi t}\, x_t\,, \quad \xi = 0, \ldots, N_t - 1\,.
\end{aligned}
$$

Autocorrelation [Wolff *CPC* **156** (2004)]

Integrated autocorrelation time

$$\tau_{\text{int}} \equiv \frac{1}{2} + \sum_{t=1}^{\infty} \rho_{\mathcal{A}}(t)$$

$$\rho_{\mathcal{A}}(t) = \frac{1}{\sigma_{\mathcal{A}}^2 N} \sum_{t_0=1}^{N} \left(\mathcal{A}(t_0 + t) - \langle \mathcal{A} \rangle\right) \left(\mathcal{A}(t_0) - \langle \mathcal{A} \rangle\right)$$

No Fourier acceleration [JO & Buividovich *hep-lat*/**2404**.09723]

Corollary

If no FA is used, i.e. $\mathcal{H} = \frac{1}{2}p^2 + \frac{1}{2}x^\mathsf{T} M x$, *with fixed trajectory length, then*

$$\tau_{\mathrm{int}} \propto \left(\frac{\omega_{\mathrm{max}}}{\omega_{\mathrm{min}}}\right)^2 + \mathcal{O}\left(1\right) \ ,$$

where ω^2_{min}, ω^2_{max} *are the smallest/largest eigenvalue of* M.

Too short trajectory [JO & Buividovich *hep-lat*/**2404**.09723]

Corollary

Presuming FA is used together with short trajectory length $T < \frac{\pi}{2}$ *and observable is measured in intervals of fixed HMC time, then*

$$\tau_{\text{int}}(T) = \frac{\tau_{\text{int}}(T = {}^{\pi}/_{2})}{1 - \cos(T)^{{}^{\pi}/_{2T}}} \, .$$

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