Canonical simulations using world-line representations - an exploratory study

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Introduction

- We explore canonical world-line simulations and compare grand canonical and canonical results
- World-line formalism gives real and positive weights of finite density partition sums $\Rightarrow$ Monte Carlo simulations
- So far only grand canonical simulations with world-lines. Sometimes long autocorrelation. Canonical simulations might be interesting alternative.
- Simulations of the canonical ensemble: fixed particle number = fixed temporal winding number of world-lines
- Toy model: charged scalar field with ϕ^4 interaction in $d = 2$

$$S = \sum_{n \in \Lambda} \left((4 + m^2)|\phi_n|^2 + \lambda |\phi_n|^4 - \sum_{\nu=1}^{2} \left[e^{\mu \delta_{\nu,2}} \phi_n^* \phi_{n+\hat{\nu}} + e^{-\mu \delta_{\nu,2}} \phi_n^* \phi_{n-\hat{\nu}} \right] \right)$$

World-line representation for the charged scalar ϕ^4 field

- In the world-line approach the grand canonical partition sum is exactly rewritten in terms of dual link variables $k_{n,\nu} \in \mathbb{Z}$

$$Z_{gc} = \sum_{\{k\}} \mathrm{e}^{\mu\beta W_t[k]} \, B[k] \, \prod_n \delta(\vec{\nabla} \cdot \vec{k}_n)$$

- $W_t[k] =$ temporal winding number of the k-world-lines

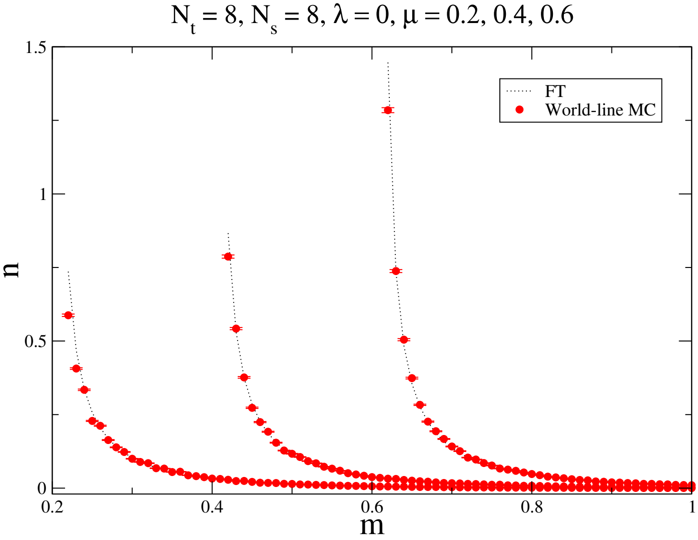
- Weight factors $B[k]$ depend on auxiliary link variables $a_{n,\nu} \in \mathbb{N}$ and radial d.o.f.

$$B[k] = \sum_{\{a\}} \prod_{n,\nu} \frac{1}{(a_{n,\nu} + |k_{n,\nu}|)! a_{n,\nu}!} \prod_n I(f_n),$$

$$I(f_n) = \int_0^\infty \mathrm{d}r \; r^{f_n+1} \mathrm{e}^{-(4+m^2)r^2 - \lambda r^4},$$

$$f_n = \sum_\nu \Big(|k_{n,\nu}| + |k_{n-\hat{\nu}}| + 2(a_{n,\nu} + a_{n-\hat{\nu}}) \Big)$$

Check of the grand canonical world-line representation



MC simulation with local Metropolis and worm algorithm

Grand canonical and canonical world-line simulations

- The complex action problem is traded for constraints $\prod_n \delta(\vec{\nabla} \cdot \vec{k}_n)$:

$$\vec{\nabla} \cdot \vec{k}_n = \sum_\nu (k_{n,\nu} - k_{n-\hat{\nu},\nu}) = 0 \;\; \forall n$$

- Allowed configuration for the k-flux are closed and oriented loops

- Net particle number N

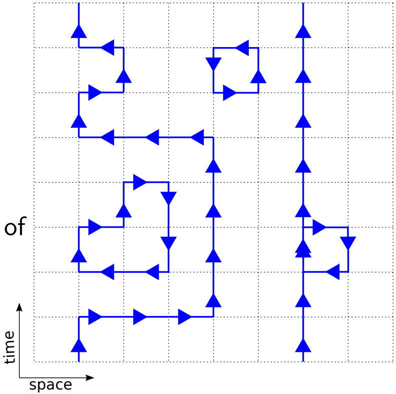
  $\Updownarrow$

  Temporal winding number $W_t[k]$

  $$e^{\mu\beta W_t[k]} \sim e^{\mu\beta N}$$

- Canonical: Simulation in fixed sectors of $N = W_t[k]$

- Grand canonical: Update also $W_t[k]$



World-line representation for the canonical ensemble

- Dualized canonical partition sum:

$$Z_c(N) = \sum_{\{k\}} \delta(W_t[k] - N)\; B[k]\; \prod_n \delta(\vec{\nabla} \cdot \vec{k}_n)$$

- Connection between ensembles: fugacity series

$$Z_{gc}(\mu) = \sum_{N \in \mathbb{Z}} \mathrm{e}^{\mu \beta N}\; Z_c(N)$$

Connecting canonical and grand canonical ensembles

- Canonical ensemble: μ is defined as the derivative of the free energy density $f_\lambda(n)$ w.r.t. the particle number density $n = N/N_s$:

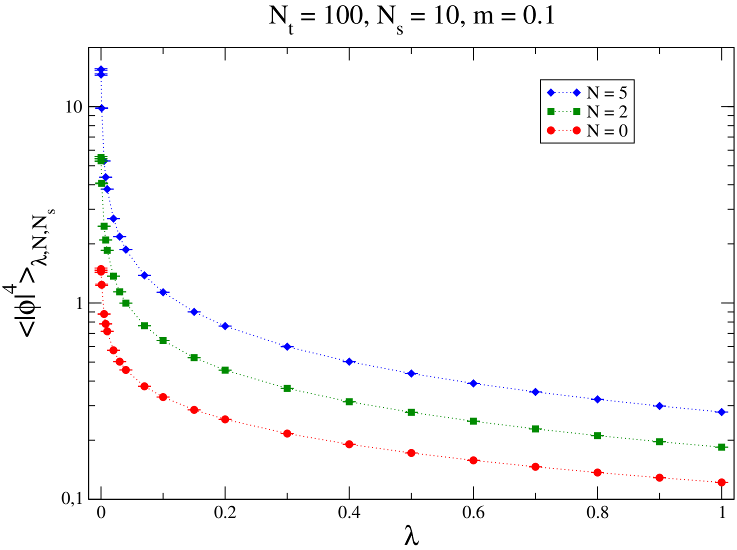
$$\mu(n) = \frac{\partial f_\lambda(n)}{\partial n} = \frac{N_s}{2}\left[f_\lambda\left(\frac{N+1}{N_s}\right) - f_\lambda\left(\frac{N-1}{N_s}\right)\right] + \mathcal{O}\left(\frac{1}{N_s^2}\right)$$

- The free energy density $f_\lambda(n)$ at a given coupling λ and number density n may be obtained from $\left\langle |\phi|^4 \right\rangle_{\lambda,N,N_s}$:

$$f_\lambda(n) \quad = \quad f_{\lambda=0}(n) + \frac{1}{N_s N_t}\int_0^\lambda \mathrm{d}\lambda' \left\langle |\phi|^4 \right\rangle_{\lambda',N,N_s}$$

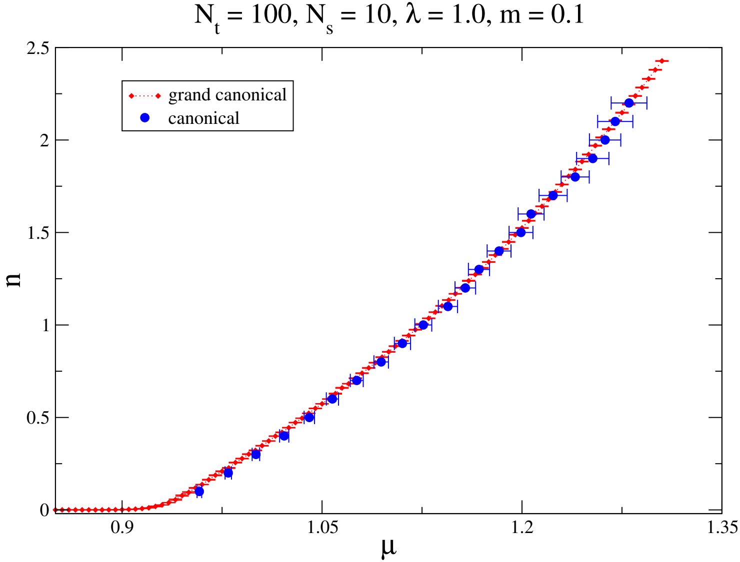
  - $f_{\lambda=0}(n)$ can be calculated in closed form with FT

Integrand for obtaining the free energy



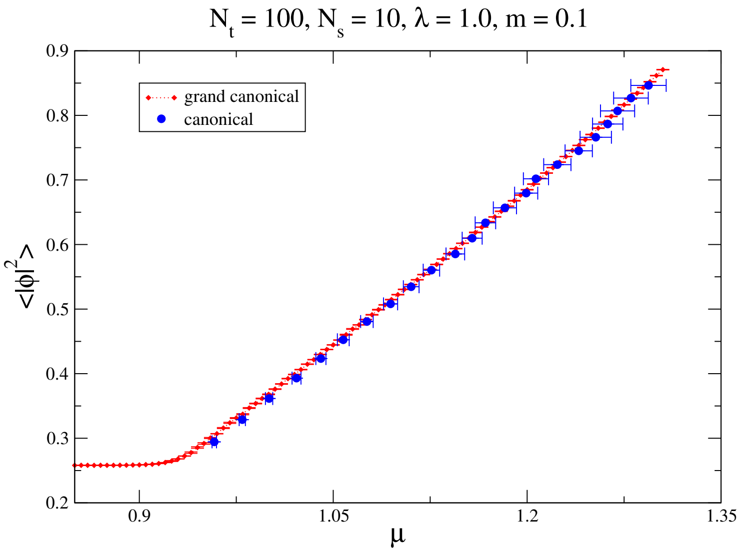
Smooth behavior ⇒ precise numerical integration with splines

Comparing grand canonical and canonical results - I



Very good agreement!

Comparing grand canonical and canonical results - II



Very good agreement!

Canonical approach to scattering on the lattice

(Work in progress)

- Canonical simulation at low temperature and net part. num. $N = 2$
- By studying the distance Δx of world-lines, we obtain the relative wave function $\psi(\Delta x)$
- For short-ranged potentials wave function is very well described by

$$\psi(\Delta x) \propto \cos\big(k\big(\Delta x - N_s/2\big)\big)$$

- Momentum k is obtained from a 1-parameter fit of the data
- Relation to scattering phase shift $\delta(k)$ with Lüscher formula

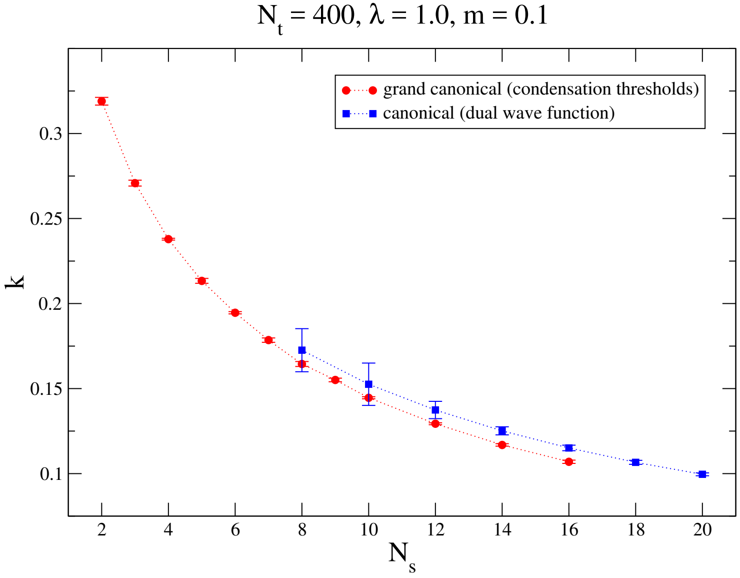
$$e^{2i\delta(k)} = e^{-ikN_s}$$

- Grand canonical ensemble: For connection between scattering data and condensation thresholds see talk by M. Giuliani

Bruckmann *et al.*, PRL 115, 231601 (2015); Lüscher, Comm. Math. Phys. 105, 153 (1986)

Comparing grand canonical and canonical results - III

Preliminary!



Summary

- Particle number is the winding number $\Rightarrow$ allows simulations of canonical ensemble
- Canonical simulations might be interesting alternative in simulations where one has long autocorrelation in updating the particle number
- We successfully implemented canonical world-line simulations
- Very good agreement of $n(\mu)$ and $\langle |\phi|^2 \rangle$ from grand canonical and canonical simulations
- Exploratory study of scattering based on a canonical 2-particle simulation (compare also PRL 115, 231601 (2015))
- Outlook: Canonical simulations for systems with fermions