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Finite-size effects in canonical and grand-canonical quantum Monte Carlo simulations for fermions

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Collaboration

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Statistical ensembles

- Grand-canonical, canonical, microcanonical ensembles
- At equilibrium, and $V \to \infty$: ensemble equivalence

  $\Rightarrow$Free choice of ensemble for thermodynamic properties

  Choice of ensemble can be dictated by the physics of the system
- In a MC simulation: finite V

  How does a finite-V observable converges to the $V \to \infty$ limit?

Goals:

- Study the finite-volume corrections in the canonical and grand-canonical ensembles
- New QMC method for fermions in the canonical ensemble

Caveat: we consider a finite mass gap (finite ξ)

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Statistical ensembles: notation

	Quantum model	Classical Ising model
Grand-canonical	$\hat{N}$ particle number operator	Map to the classical lattice gas model
	$\mathcal{H}_{\rm full} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \ldots$	$M \leftrightarrow n$
	$Z_{\rm gc} = \mathrm{Tr}_{\mathcal{H}_{\rm full}} \exp(-\beta \hat{H} + \mu \hat{N})$	$Z_{\rm gc} = \sum_{\{S_k=\pm 1\}} e^{\beta J \sum_{<ij>} S_i S_j + h \sum_i S_i}$
Canonical	$Z_{\rm can}(n) = \mathrm{Tr}_{\mathcal{H}_n} \exp(-\beta \hat{H})$	$Z_{\rm can}(m) = \sum_{\{S_k=\pm 1\}} e^{\beta J \sum_{<ij>} S_i S_j + h \sum_i S_i}$
		$\cdot \delta(m, \frac{1}{V} \sum_i S_i)$
		Fixed-magnetization ensemble

Finite-size corrections

- We consider a finite mass gap (finite ξ), periodic b.c.
- How $O(L)$ approaches $O(L=\infty)$ for $L \to \infty$?
- Grand-canonical: $O(L=\infty) - O(L) \propto \exp(-L/\xi)$
  Field theory Lüscher, 1986; Neuberger, 1989; Münster, 1985
  MC simulations
  Exact solutions: 1D Ising model
- Canonical: constraint introduces long-ranged interaction
  $\Rightarrow 1/V$ finite-size corrections Neuberger, 1989

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Finite-size corrections in the Canonical ensemble

$$F_{\rm can}(n_0, V) - F_{\rm gc}(V) = \frac{1}{2V}\ln\left(2\pi V\right) + \frac{1}{2V}\ln\left(\frac{\chi_c}{\beta}\right) + O\left(\frac{1}{V^2}\right)$$

χ_c = charge susceptibility $\sim$ particle-number fluctuations

- If $F(V=\infty) - F_{\rm gc}(V) \propto \exp(-L/\xi)$,
  $\Rightarrow 1/V$ corrections in the canonical ensemble, controlled by χ_c
- Energy:

$$E_{\rm can}(V) - E(V=\infty) = \frac{\partial\left(\chi_c/\beta\right)/\partial\beta}{2V\left(\chi_c/\beta\right)}.$$

- Generalized to other observables
- Exact solution of the 1D Ising model in the canonical ensemble

$$E_{\rm can} = -J\tanh(\beta J) + \frac{J}{L} + O\left(e^{-L/\xi}, \frac{1}{L^2}\right)$$

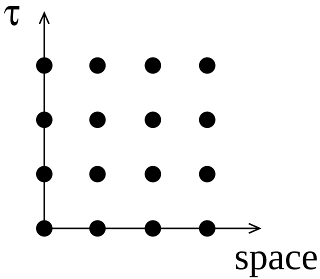
Auxiliary-field Quantum Monte Carlo

$$\hat{H} = \underbrace{\sum_{x,y} \hat{c}_x^\dagger T_{x,y} \hat{c}_y}_{\equiv \hat{T}} + \underbrace{\sum_k U_k \left(\sum_{x,y} \hat{c}_x^\dagger V_{x,y}^{(k)} \hat{c}_y + \alpha_k \right)^2}_{\equiv \hat{V}}$$

- Trotter decomposition $\exp(-\beta \hat{H}) \simeq [\exp(-\Delta\tau \hat{T}) \exp(-\Delta\tau \hat{V})]^N$
- Hubbard-Stratonovich decomposition

$$e^{\Delta\tau\lambda\hat{A}^2} \simeq \frac{1}{4} \sum_{l=\pm1,\pm2} \gamma(l) e^{\sqrt{\Delta\tau\lambda}\eta(l)\hat{A}}$$

$\Rightarrow$ Any observable computed using $G_{xy}(l) \equiv \langle \hat{c}_x^\dagger \hat{c}_y \rangle_l$

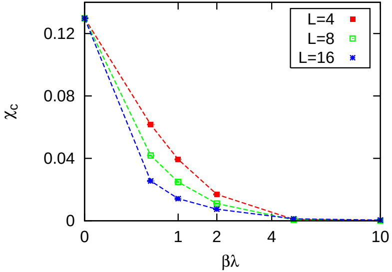


- ALF: Algorithms for Lattice Fermions
  `alf.physik.uni-wuerzburg.de`

Quantum Monte Carlo for the canonical ensemble

- We supplement the Hamiltonian

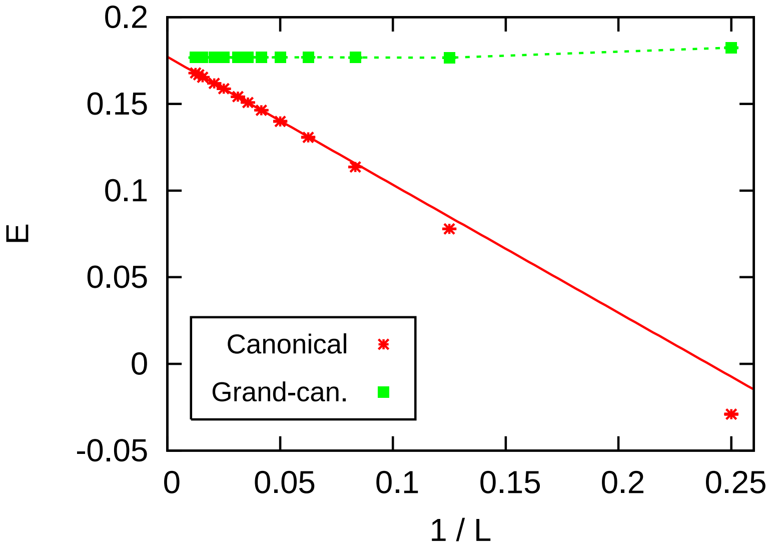
$$\hat{H}(\lambda) = \hat{H} + \hat{H}_\lambda,$$
$$\hat{H}_\lambda \equiv \lambda \left(\hat{N} - N_0\right)^2$$
$$Z_{\rm can}(N_0) = \lim_{\lambda\to\infty} \mathrm{Tr}\left[e^{-\beta\hat{H}(\lambda)}\right]$$



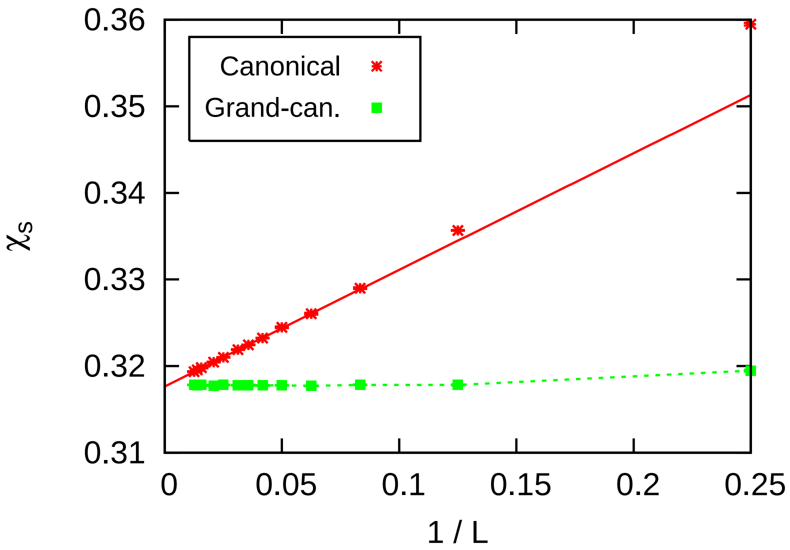
- Monitor convergence measuring charge susceptibility χ_c
- $(N - N_0)^2$ long-ranged interaction: can kill acceptance ratio
Solution:

$$e^{-\beta\hat{H}} = \prod_{\tau=1}^{N}\left[e^{-\Delta\tau\hat{T}}e^{-\Delta\tau\hat{V}}\underbrace{e^{-\frac{\Delta\tau}{n_\lambda}\hat{H}_\lambda}\cdots e^{-\frac{\Delta\tau}{n_\lambda}\hat{H}_\lambda}}_{n_\lambda\text{-times}}\right].$$

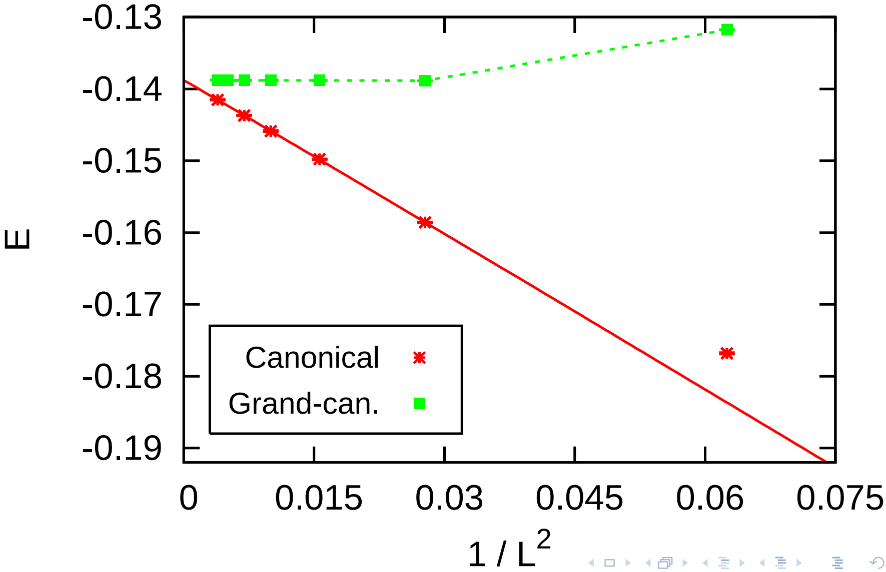
1D Hubbard Model $\beta = 0.5$



1D Hubbard Model $\beta = 0.5$



2D Hubbard Model $\beta = 0.5$



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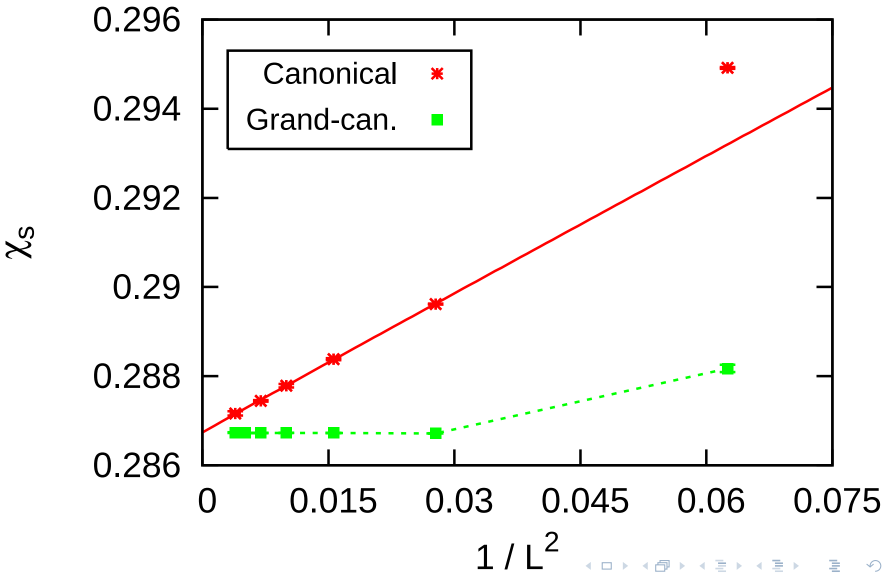
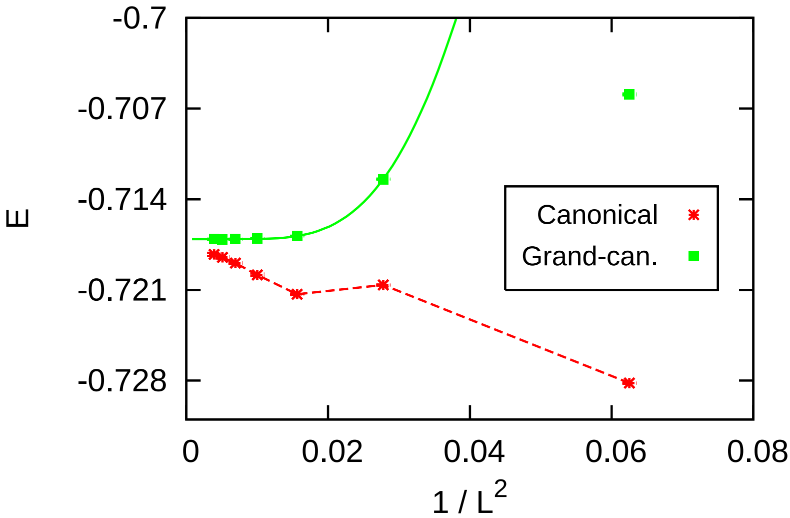
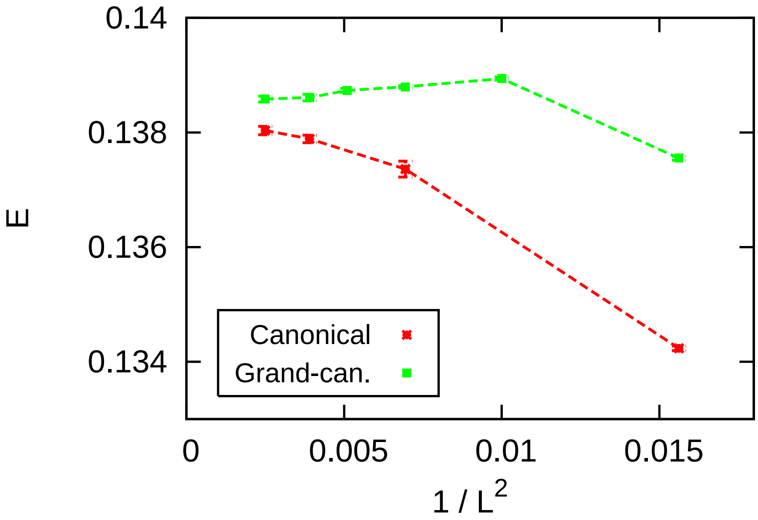


2D Hubbard Model $\beta = 2.0$



Lower temperature: increased ξ, reduced χ_c

2D Hubbard Model $\beta = 2.0$ 3/8-filling



Mild sign problem at $\beta = 2.0$

Summary

- We studied the finite-size corrections with a finite mass-gap (finite ξ), periodic b.c., in the grand-canonical and canonical ensemble

- Distinct approach to the thermodynamic limit

$$O(V=\infty) - O_{\rm gc}(V) \propto e^{-L/\xi}$$

$$O(V=\infty) - O_{\rm can}(V) \propto 1/V$$

- Exact formula for the finite-size correction in the canonical ensemble
  Exact solution for the 1D Ising model

- QMC method for fermionic systems in the canonical ensemble

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