Projection and Variational Monte Carlo simulations

A presentation for the course in *Computer Simulation*

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Code at:

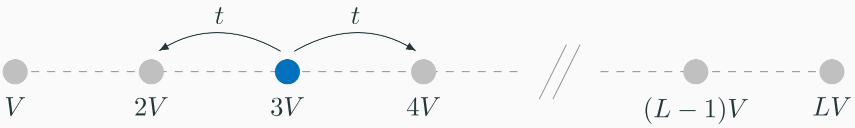
`https://github.com/matteosecli/PMC-VMC`

Projection Monte Carlo

The system

Single particle in a 1D lattice with:

- L sites
- A linear (site-dependent) potential $V(x) = V \cdot x$
- A hopping amplitude t
- Open boundary conditions



$$H = -t \sum_{\langle xx' \rangle} c^\dagger_{x'} c_x + \sum_x V(x) c^\dagger_x c_x \tag{1}$$

Simulation results

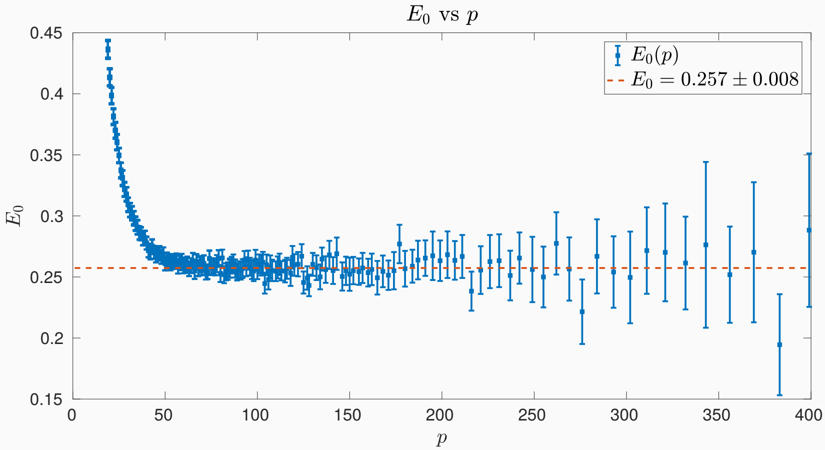


Figure 1: E_0 for $L = 20$, $t = 1$, $V = 1$ and $N = 10^7$. The mean position is $x_0 = 1.80 \pm 0.05$.

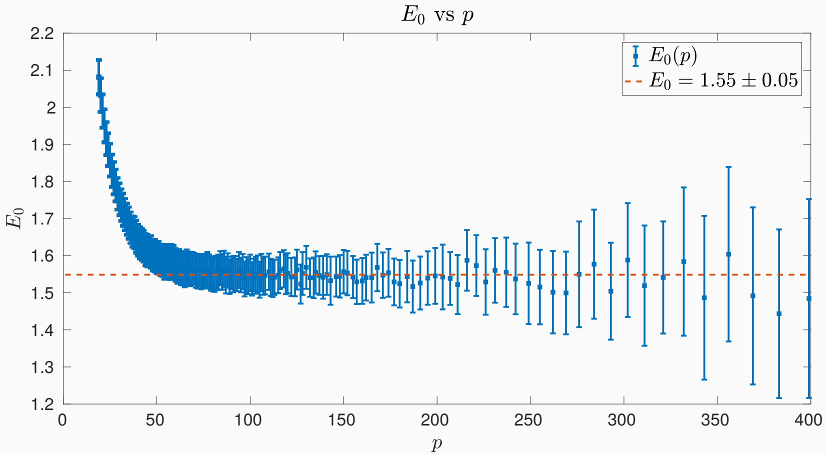


Figure 2: E_0 for $L = 20$, $t = 1$, $V = 2$ and $N = 10^7$. The mean position is $x_0 = 1.46 \pm 0.05$.

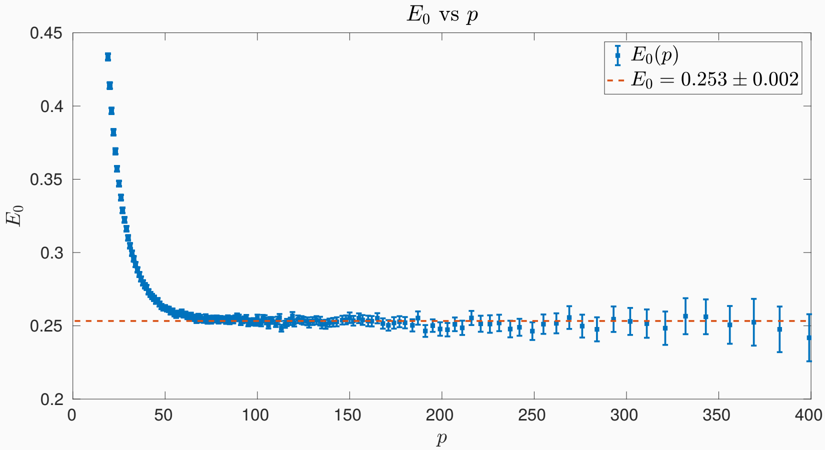


Figure 3: E_0 for $L = 20$, $t = 1$, $V = 1$ and $N = 10^8$. The mean position is $x_0 = 1.79 \pm 0.01$.

Simulation results

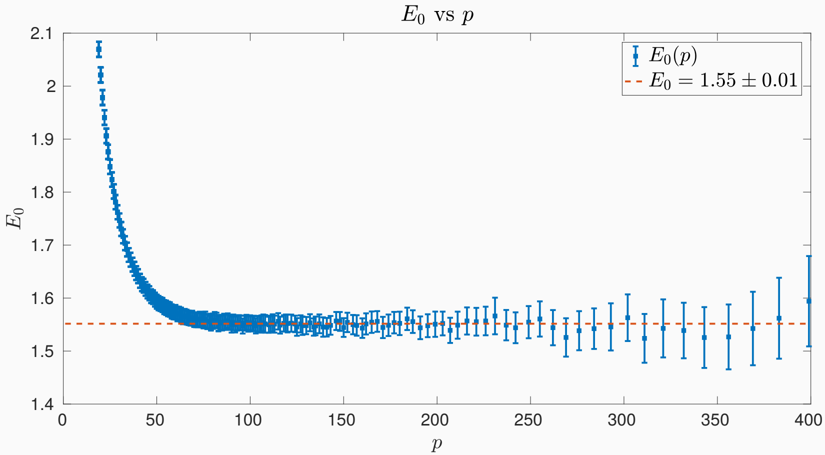
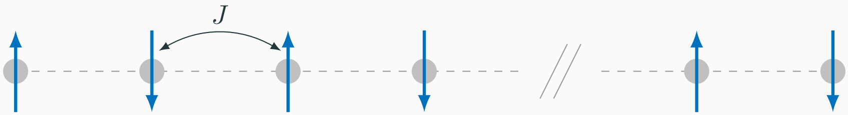


Figure 4: E_0 for $L = 20$, $t = 1$, $V = 1$ and $N = 10^8$. The mean position is $x_0 = 1.46 \pm 0.01$.

Variational Monte Carlo

Antiferromagnetic spin-$1/2$ Heisenberg model on a 1D lattice with:

- L sites
- Periodic boundary conditions
- Zero magnetization



$$H = J \sum_{i=1}^{L} \vec{S}_i \cdot \vec{S}_{i+1} = J \sum_{i=1}^{L} \left\{ S_i^z S_{i+1}^z + \frac{1}{2} \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) \right\} \quad (2)$$

with $J > 0$ in order to be antiferromagnetic.

The VMC procedure I

- Variational wavefunction on the basis of the configurations $\{|x\rangle\}$ with definite S_i^z:

$$\psi(x) = \text{Sign}_M(x) e^{\frac{\alpha}{2}\sum_{i\neq j} v_{i,j}^z (2S_i^z)(2S_{ij}^z)} \tag{3}$$

  with $\text{Sign}_M(x) = (-1)^{\sum_{i=1}^{L/2}(S_{2i}^z + 1/2)}$ and $v_{i,j}^z = 2\log(|2\sin(\pi(i-j)/L)|)$.
- Local energy:

$$E_L(x) = \frac{\langle x \,|\, H \,|\, \psi\rangle}{\langle x \,|\, \psi\rangle} = \langle x \,|\, H \,|\, x\rangle + \sum_{x' \neq x} \langle x \,|\, H \,|\, x'\rangle \frac{\langle x' \,|\, \psi\rangle}{\langle x \,|\, \psi\rangle} \tag{4}$$

- Staggered magnetization:

$$m^2 = \left\langle \left(\frac{1}{L} \sum_{i=1}^{L} (-1)^i S_i^z \right)^2 \right\rangle \tag{5}$$

- First neighbor correlation function:

$$C_1 = \left\langle \frac{1}{L} \sum_{i=1}^{L} S_i^z S_{i+1}^z \right\rangle . \tag{6}$$

Exact results from Bethe ansatz in 1D[1] ($L \to \infty$):

$$E_0 = -|J| \left(\log 2 - \frac{1}{4} \right) \simeq -0.4431471|J|$$

and

$$C_1 = \frac{1}{12} \left(1 - 4 \log 2\right) \simeq -0.14771573.$$

[1]See Minoru Takahashi, *Thermodynamics of One-Dimensional Solvable Models*. Cambridge University Press, 2005. ISBN 9780521019798.

Execution times

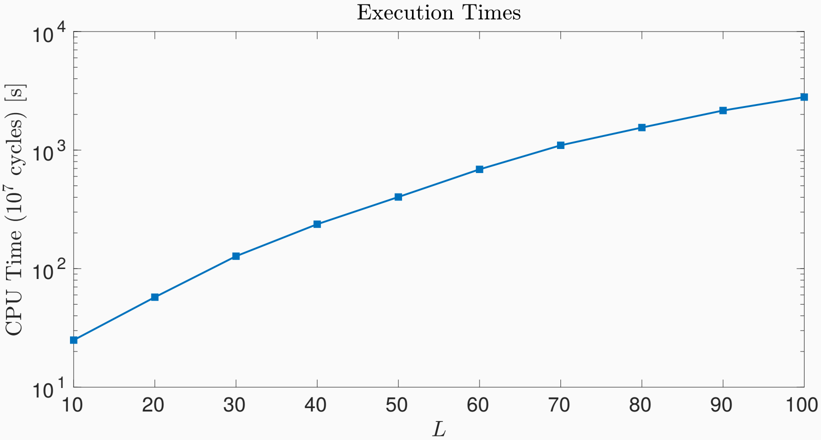


Figure 5: CPU time per variational parameter value with 10^7 MC steps.

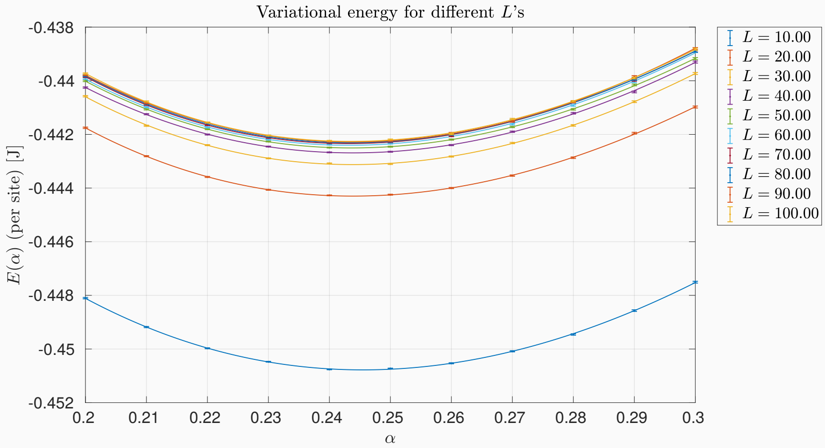


Figure 6: Variational energy. The best value for the variational parameter is estimated to be $\alpha = 0.244 \pm 0.001$.

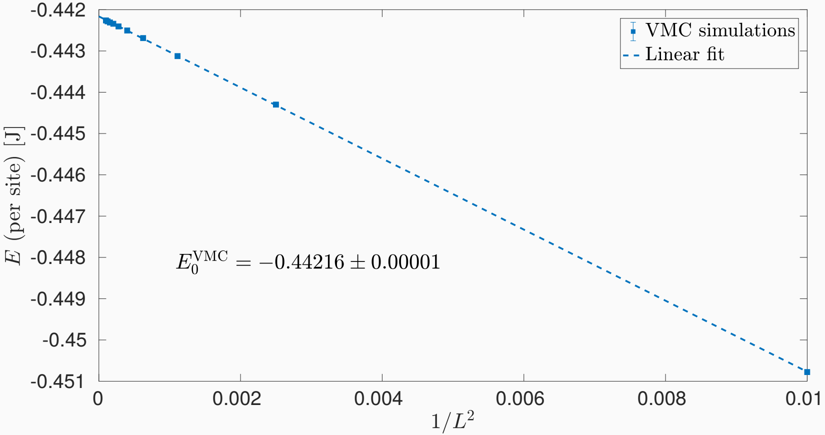


Figure 7: Extrapolation for $L \to \infty$.

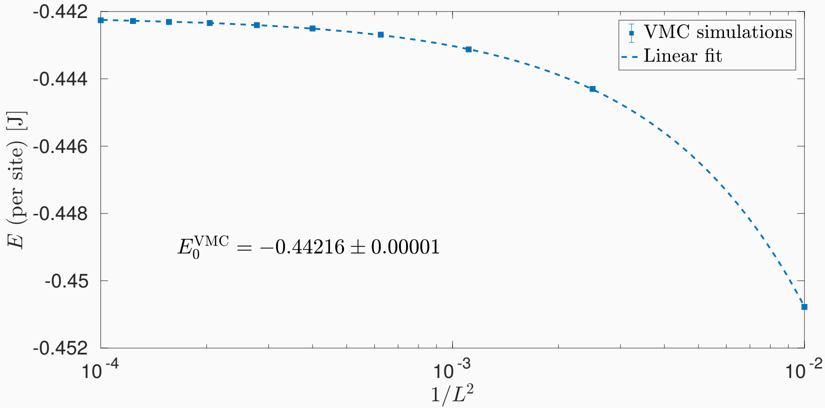


Figure 8: Extrapolation for $L \to \infty$.

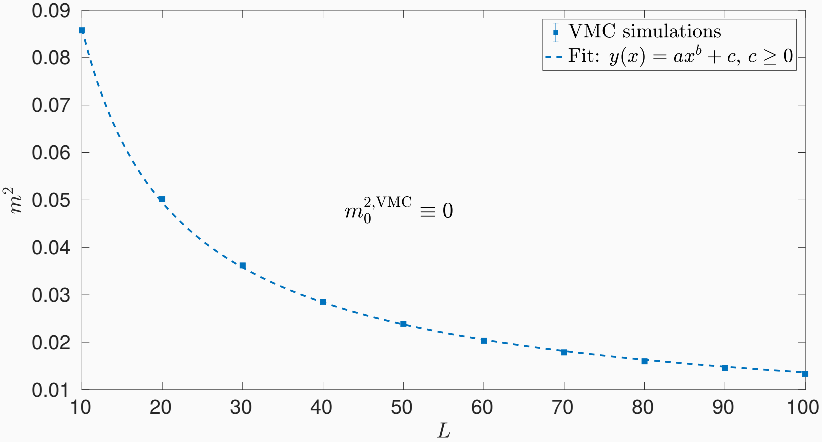


Figure 9: Extrapolation for $L \to \infty$.

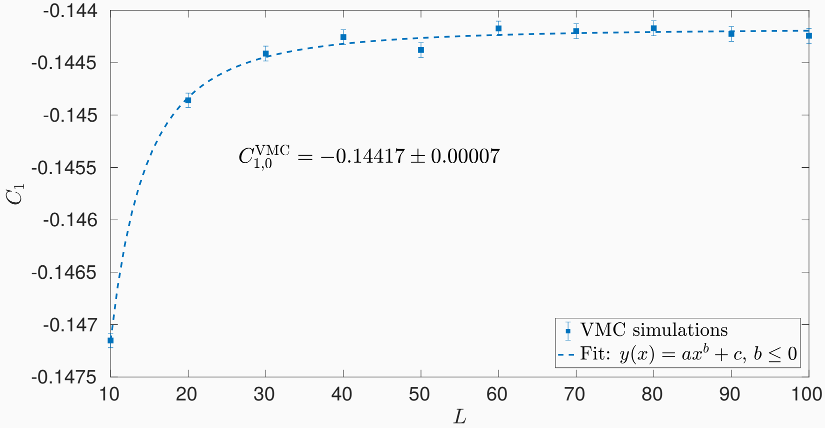


Figure 10: Extrapolation for $L \to \infty$.

Method	E_0 $[J]$	m^2	C_1
Bethe ansatz[2]	$-0.443\,147$	0	$-0.147\,716$
VMC[3]	$-0.442\,16(1)$	0	$-0.144\,17(7)$
ED/Lanczos[4]	$-0.443\,04(5)$	–	–

[2] $L \to \infty$, exact.
[3] $L \to \infty$, upper bound.
[4] Extrapolated to $L \to \infty$ from a set of calculations for $L = \{8, 10, 12, 14, 16\}$, with max 32 steps for the Lanczos. Code: `http://www.fisica.uniud.it/~giannozz/Corsi/MQ/Software/C/heisenberg_exact.c`

Conclusions

Hope this was at least a little bit interesting...

Thanks for your attention!

☺

Questions?

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