

Projection and Variational Monte Carlo simulations

A presentation for the course in *Computer Simulation*

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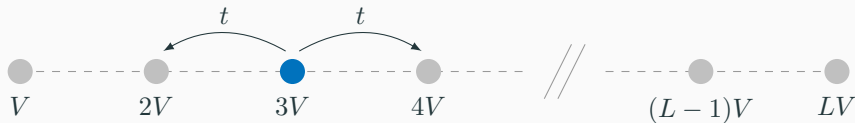
Code at:

<https://github.com/matteosecli/PMC-VMC>

Projection Monte Carlo

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



$$H = -t \sum_{\langle xx' \rangle} c_{x'}^{\dagger} c_x + \sum_x V(x) c_x^{\dagger} c_x \quad (1)$$

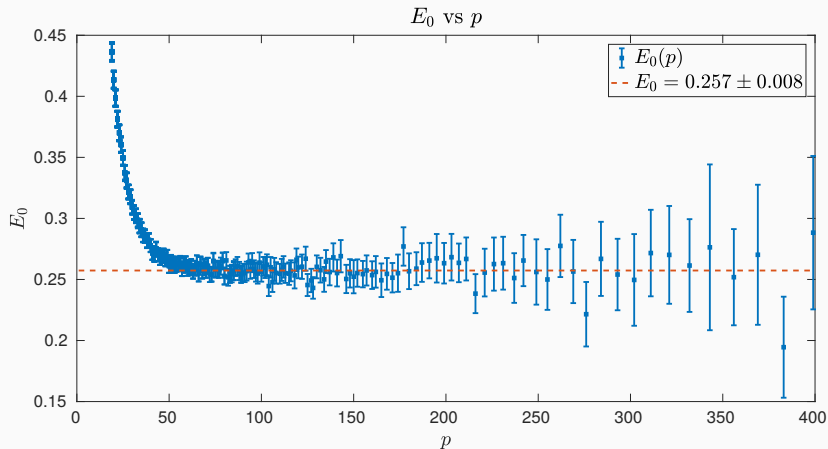


Figure 1: E_0 for $L = 20$, $t = 1$, $V = 1$ and $N = 10^7$. The mean position is $x_0 = 1.80 \pm 0.05$.

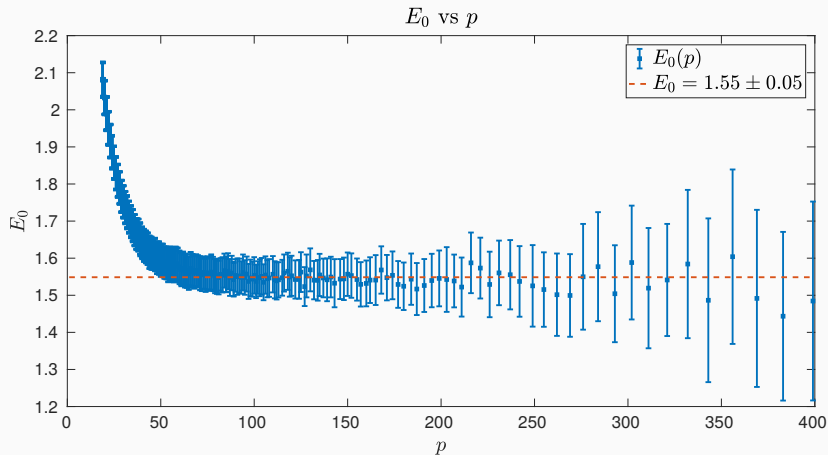


Figure 2: E_0 for $L = 20$, $t = 1$, $V = 2$ and $N = 10^7$. The mean position is $x_0 = 1.46 \pm 0.05$.

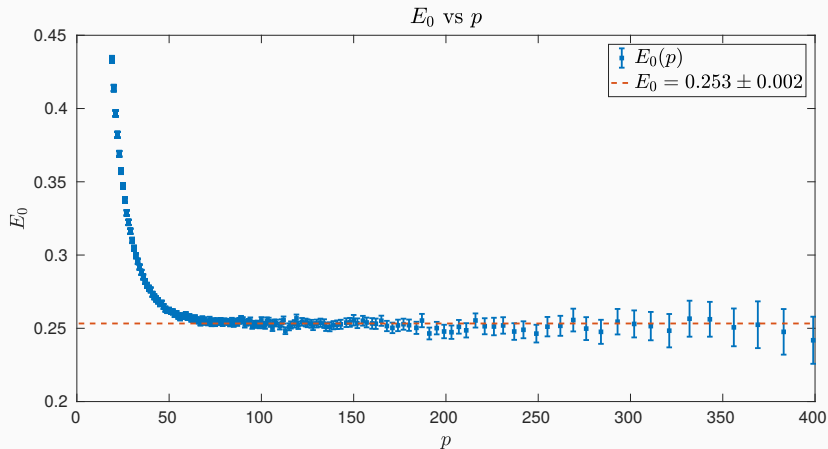


Figure 3: E_0 for $L = 20$, $t = 1$, $V = 1$ and $N = 10^8$. The mean position is $x_0 = 1.79 \pm 0.01$.

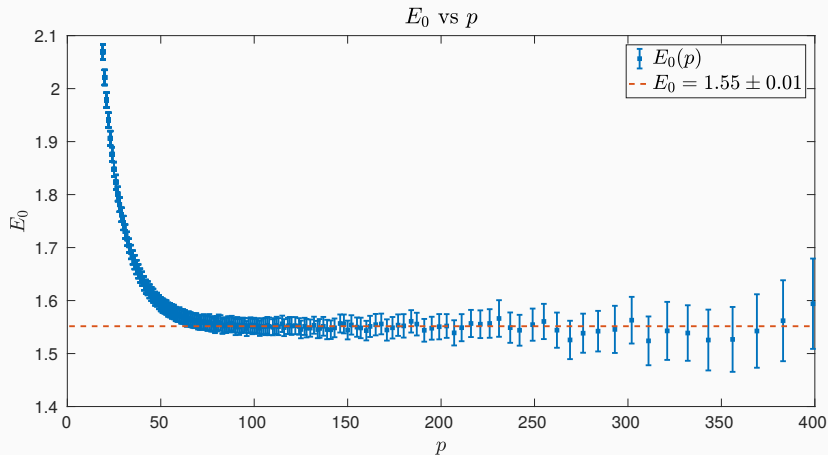
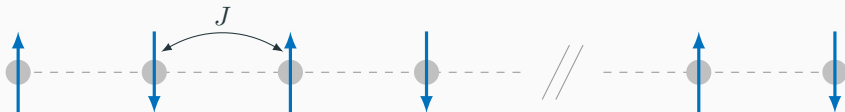


Figure 4: E_0 for $L = 20$, $t = 1$, $V = 1$ and $N = 10^8$. The mean position is $x_0 = 1.46 \pm 0.01$.

Variational Monte Carlo

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

- L sites
- Periodic boundary conditions
- Zero magnetization



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

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

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

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

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:

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

- Staggered magnetization:

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

- First neighbor correlation function:

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

Exact results from Bethe ansatz in 1D¹ ($L \rightarrow \infty$):

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

and

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

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

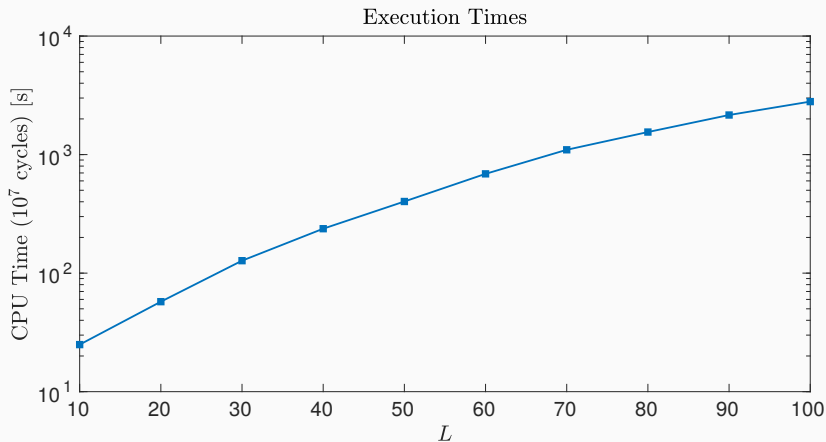


Figure 5: CPU time per variational parameter value with 10^7 MC steps.

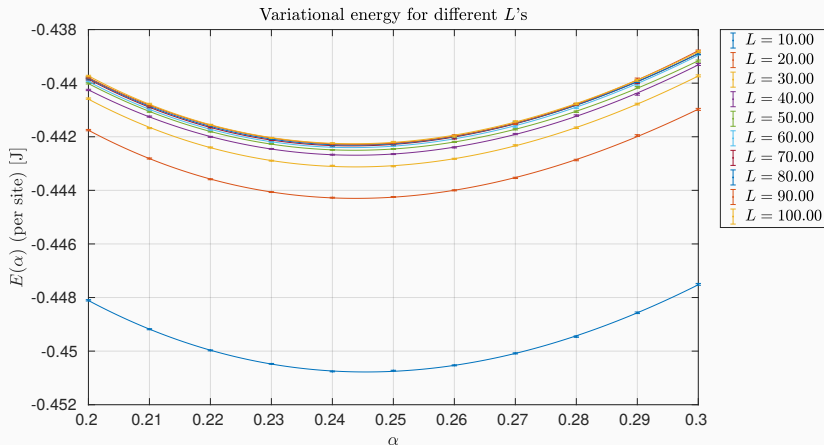


Figure 6: Variational energy. The best value for the variational parameter is estimated to be $\alpha = 0.244 \pm 0.001$.

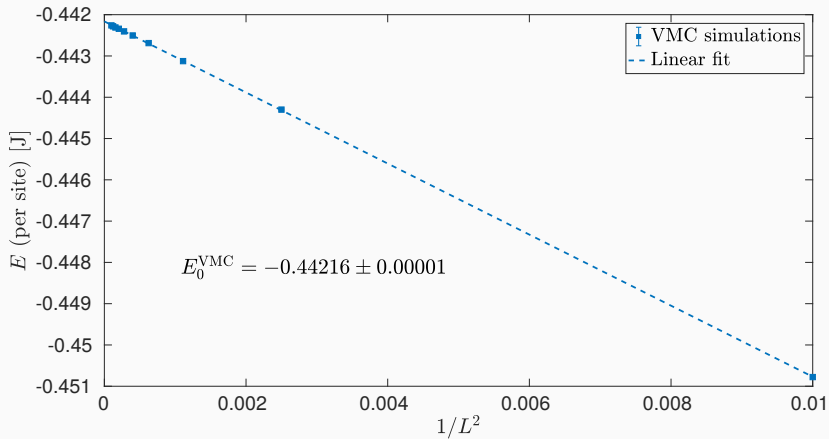


Figure 7: Extrapolation for $L \rightarrow \infty$.

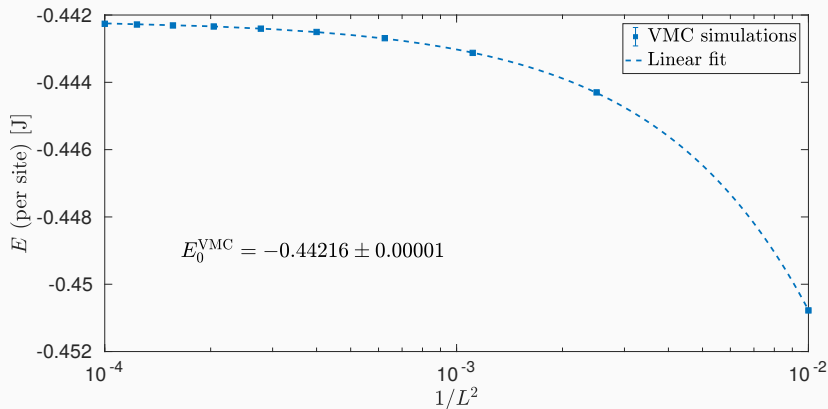


Figure 8: Extrapolation for $L \rightarrow \infty$.

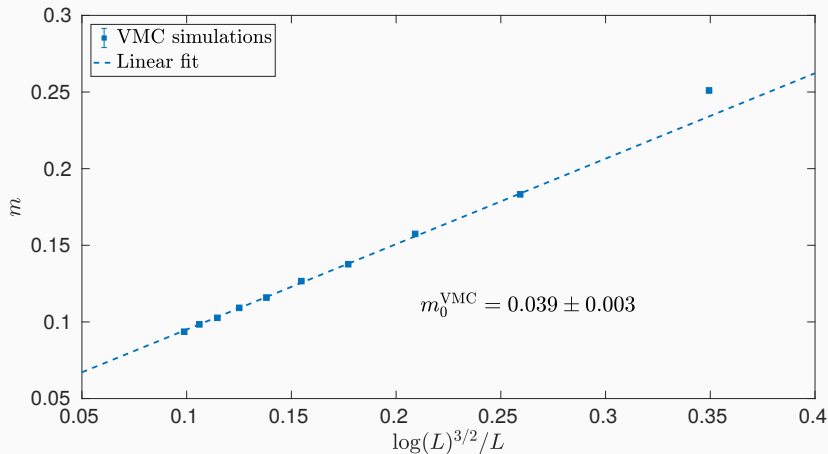


Figure 9: Extrapolation for $L \rightarrow \infty$.

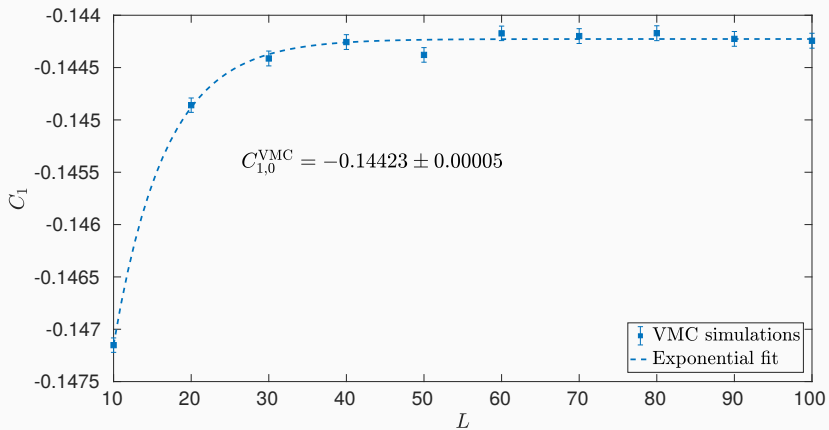


Figure 10: Extrapolation for $L \rightarrow \infty$.

Method	E_0 [J]	m	C_1
Bethe ansatz ²	-0.443 147	0	-0.147 716
VMC ³	-0.442 16(1)	0.039(3)	-0.144 23(5)
ED/Lanczos ⁴	-0.443 04(5)	–	–

² $L \rightarrow \infty$, exact.

³ $L \rightarrow \infty$, upper bound.

⁴Extrapolated to $L \rightarrow \infty$ 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

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

Thanks for your attention!



Questions?

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