# Projection and Variational Monte Carlo simulations

A presentation for the course in *Computer Simulation*

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Code at:

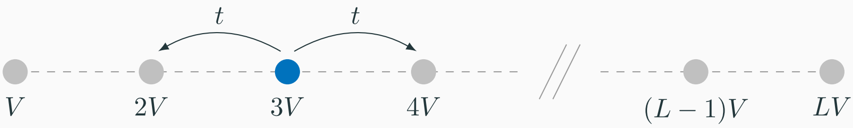
`https://github.com/matteosecli/PMC-VMC`

# 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




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

# Simulation results

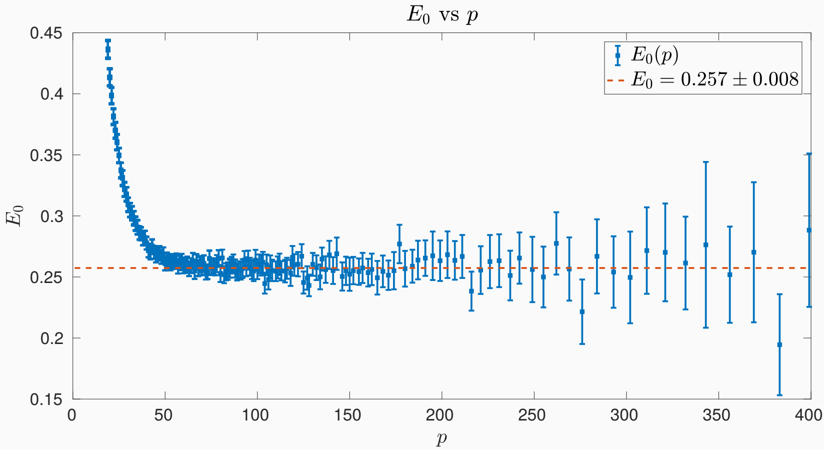



**Figure 1:** $E_0$ for $L = 20$, $t = 1$, $V = 1$ and $N = 10^7$. The mean position is $x_0 = 1.80 \pm 0.05$.

# Simulation results

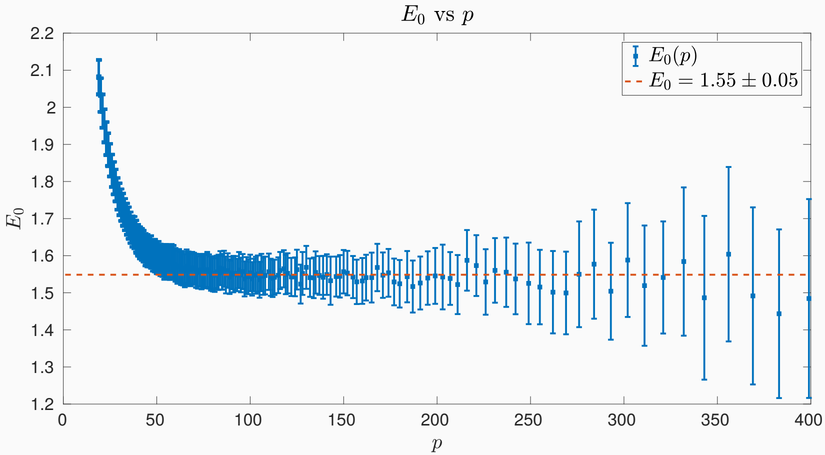



Figure 2: $E_0$ for $L = 20$, $t = 1$, $V = 2$ and $N = 10^7$. The mean position is $x_0 = 1.46 \pm 0.05$.

# Simulation results

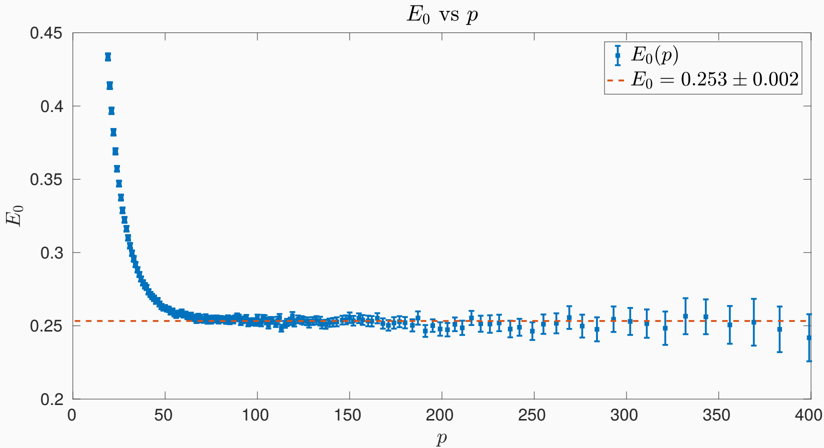



**Figure 3:** $E_0$ for $L = 20$, $t = 1$, $V = 1$ and $N = 10^8$. The mean position is $x_0 = 1.79 \pm 0.01$.

# Simulation results

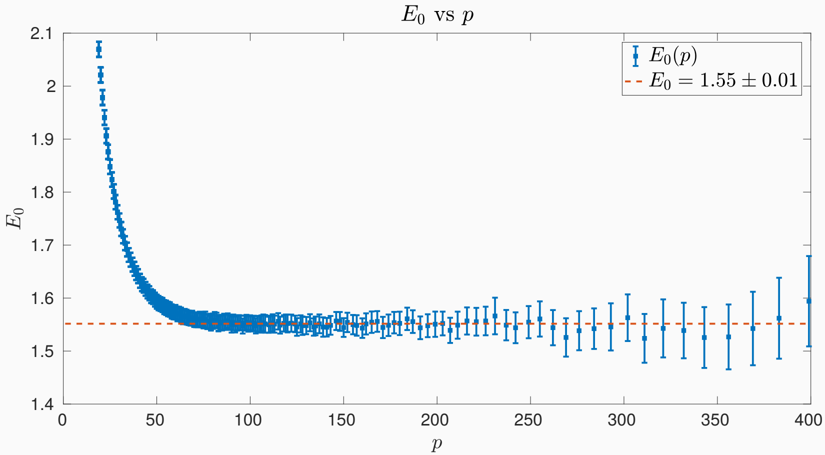
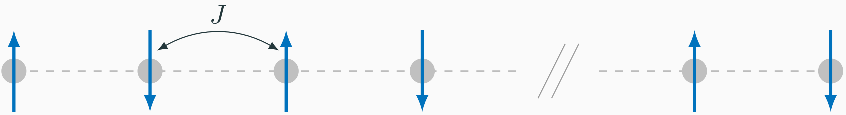



**Figure 4:** $E_0$ for $L = 20$, $t = 1$, $V = 1$ and $N = 10^8$. The mean position is $x_0 = 1.46 \pm 0.01$.

# 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:

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

- Staggered magnetization:

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

# The VMC procedure II

- 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

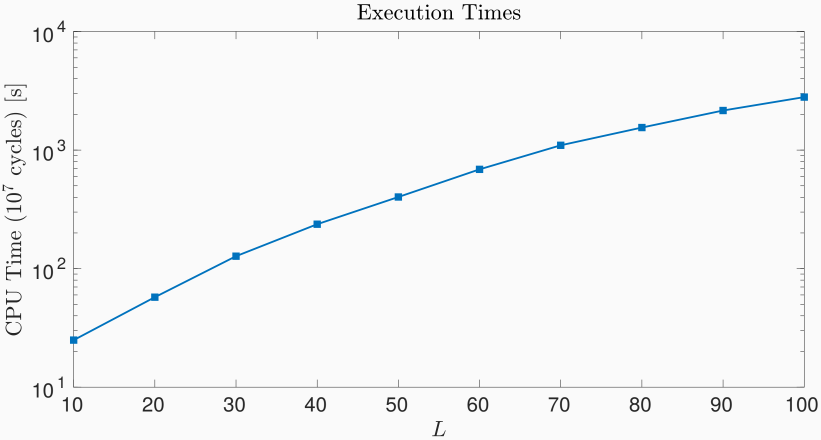



Figure 5: CPU time per variational parameter value with $10^7$ MC steps.

# Simulation results

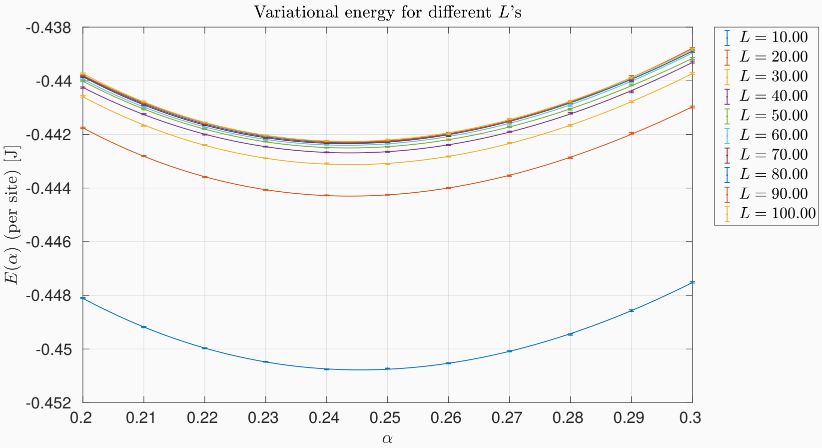



**Figure 6:** Variational energy. The best value for the variational parameter is estimated to be $\alpha = 0.244 \pm 0.001$.

# Simulation results

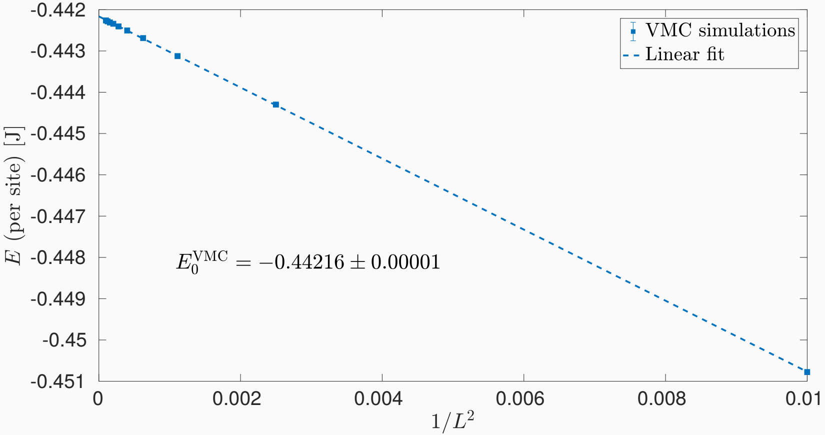



**Figure 7:** Extrapolation for $L \to \infty$.

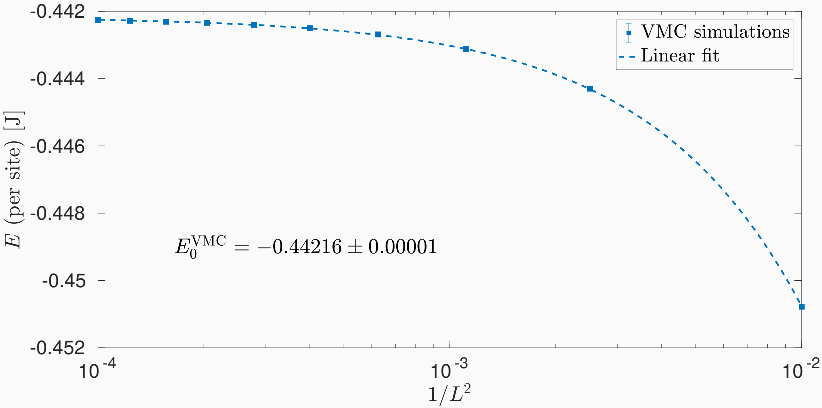



**Figure 8:** Extrapolation for $L \to \infty$.

# Simulation results

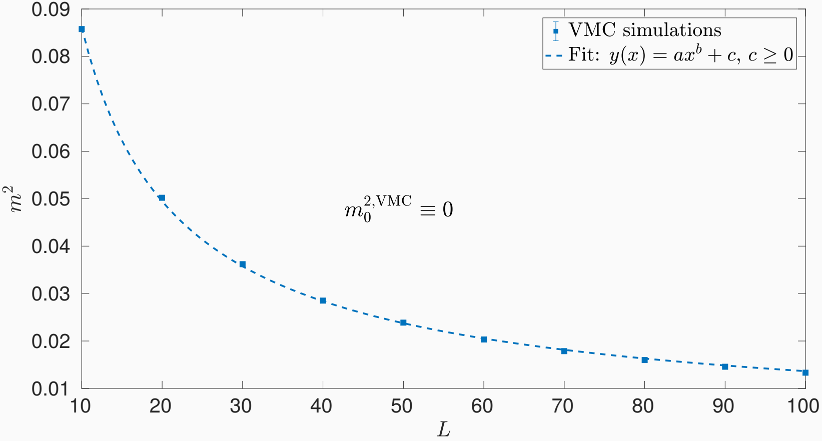



**Figure 9:** Extrapolation for $L \to \infty$.

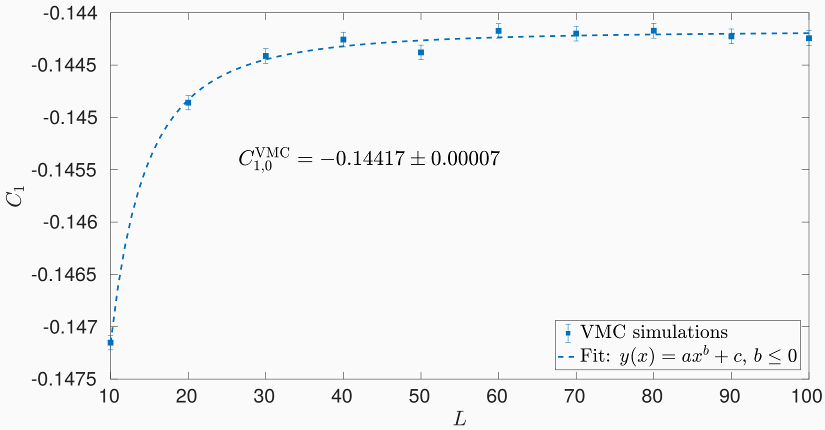



**Figure 10:** Extrapolation for $L \to \infty$.

# Summary

| 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!

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Questions?

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