TOWARDS A QUANTUM MONTE CARLO FOR LATTICE SYSTEMS

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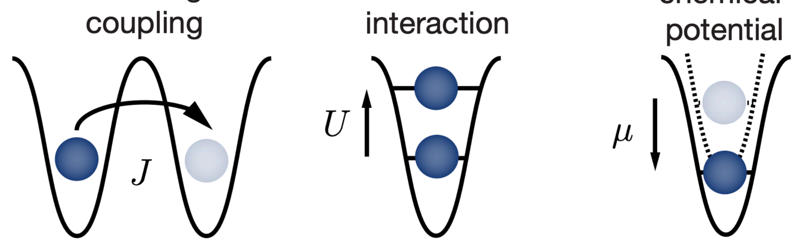
Abstract

In this work we build the foundations of a quantum Monte Carlo (QMC) as a numerical method to solve lattice many-body quantum systems with nearest-neighbor interactions. As motivation, we briefly describe a system of repulsively interacting spin-1 bosons in an optical lattice at unit filling in the Mott insulator phase with an external quadratic Zeeman field. QMC methods circumvent the difficulties that arise on these type of systems by mapping the quantum partition function into the one of an effective classical model and then, implementing a Monte Carlo sampling of the new partition function. Such a mapping is performed by the means of the Suzuki-Trotter decomposition, which transforms the original partition function into a summation of world lines. Finally, we show how the Metropolis algorithm can be implemented to sample the world lines, thus allowing us to measure certain type of observables.

Bose-Hubbard model

The Bose-Hubbard model describes interacting bosons in an optical lattice.

$$\hat{H}_{\rm BH} = \underbrace{-J\sum_{\langle i,j\rangle}\hat{b}_j^\dagger\hat{b}_i}_{\text{tunneling coupling}} + \underbrace{\frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i-1)}_{\text{on-site interaction}} \underbrace{-\mu\sum_i\hat{n}_i}_{\text{chemical potential}},$$



The model presents two phases: the Mott insulator and the superfluid.

Mott insulator: $J < U$ Superfluid: $J > U$

The interest of this work is to focus on the Mott insulator phase at unit filling and at ultralow (nK) temperatures.

Endres M., Thesis: Probing correlated quantum many-body systems at the single-particle level, Ludwig-Maximilians-Universität München, Germany, (2013).

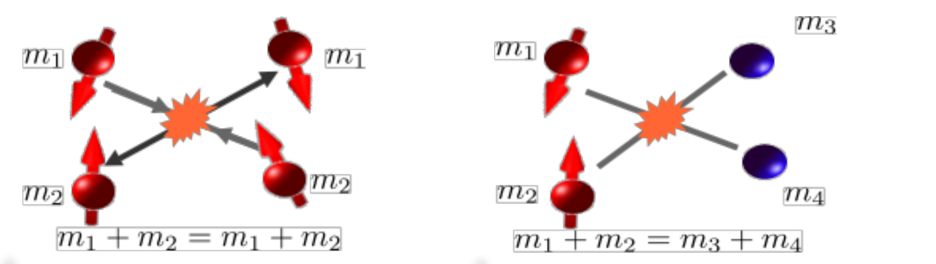
Spin-1 and external magnetic field

When the spin degree of freedom is considered and an external Zeeman field is applied, the Hamiltonian takes a more complicated form.

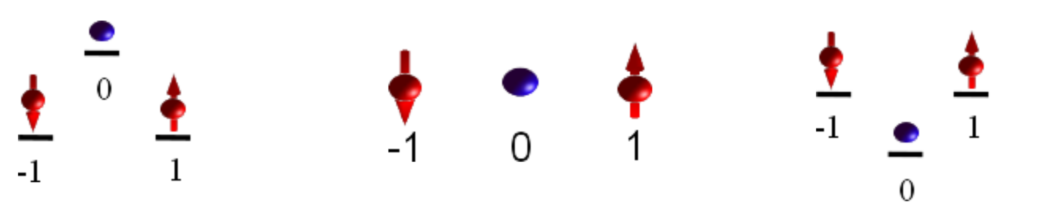
$$\hat{H} = \underbrace{-J\sum_{\langle i,j\rangle,\sigma}\left(\hat{b}_{j,\sigma}^\dagger\hat{b}_{i,\sigma}\right)}_{\text{tunneling coupling}} \underbrace{-\mu\sum_{i,\sigma}\hat{n}_{i,\sigma}}_{\text{chemical potential}} \underbrace{+q\sum_{i,\sigma}\sigma^2\hat{n}_{i,\sigma}}_{\text{quadratic Zeeman field}}$$
$$\underbrace{\begin{aligned}&+\frac{U_0+2U_2}{6}\hat{b}_0^\dagger\hat{b}_0^\dagger\hat{b}_0\hat{b}_0 + \frac{U_2}{2}\left(\hat{b}_1^\dagger\hat{b}_1^\dagger\hat{b}_1\hat{b}_1 + \hat{b}_{-1}^\dagger\hat{b}_{-1}^\dagger\hat{b}_{-1}\hat{b}_{-1}\right)\\ &+\frac{2U_0+U_2}{3}\hat{b}_1^\dagger\hat{b}_{-1}^\dagger\hat{b}_{-1}\hat{b}_1 + U_2\left(\hat{b}_0^\dagger\hat{b}_{-1}^\dagger\hat{b}_{-1}\hat{b}_0 + \hat{b}_1^\dagger\hat{b}_0^\dagger\hat{b}_0\hat{b}_1\right)\\ &+\frac{U_2+U_0}{3}\left(\hat{b}_0^\dagger\hat{b}_0^\dagger\hat{b}_{-1}\hat{b}_1 + \hat{b}_1^\dagger\hat{b}_{-1}^\dagger\hat{b}_0\hat{b}_0\right)\end{aligned}}_{\text{on-site interaction}}$$

We want to study the field induced phases in the regimen of interest [1]. The field strength is comparable with the tunneling.

Spin preserving and spin changing collisions appear with the addition of the spin.



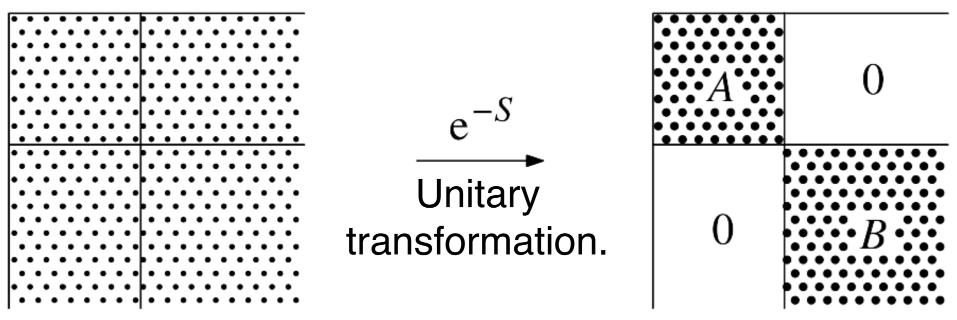
Since a balanced mixture is considered, only the quadratic Zeeman field takes effect. This favors certain configurations depending on the sign of the field.



$q < 0$ $q = 0$ $q > 0$

Effective Hamiltonian

Van Vleck quasi degenerate perturbation theory is used to retrieve the effective Hamiltonian. The tunneling term is taken as the perturbation.



Full Hamiltonian. Block Hamiltonian.

The effective Hamiltonian is a bilinear biquadratic Heisenberg model.

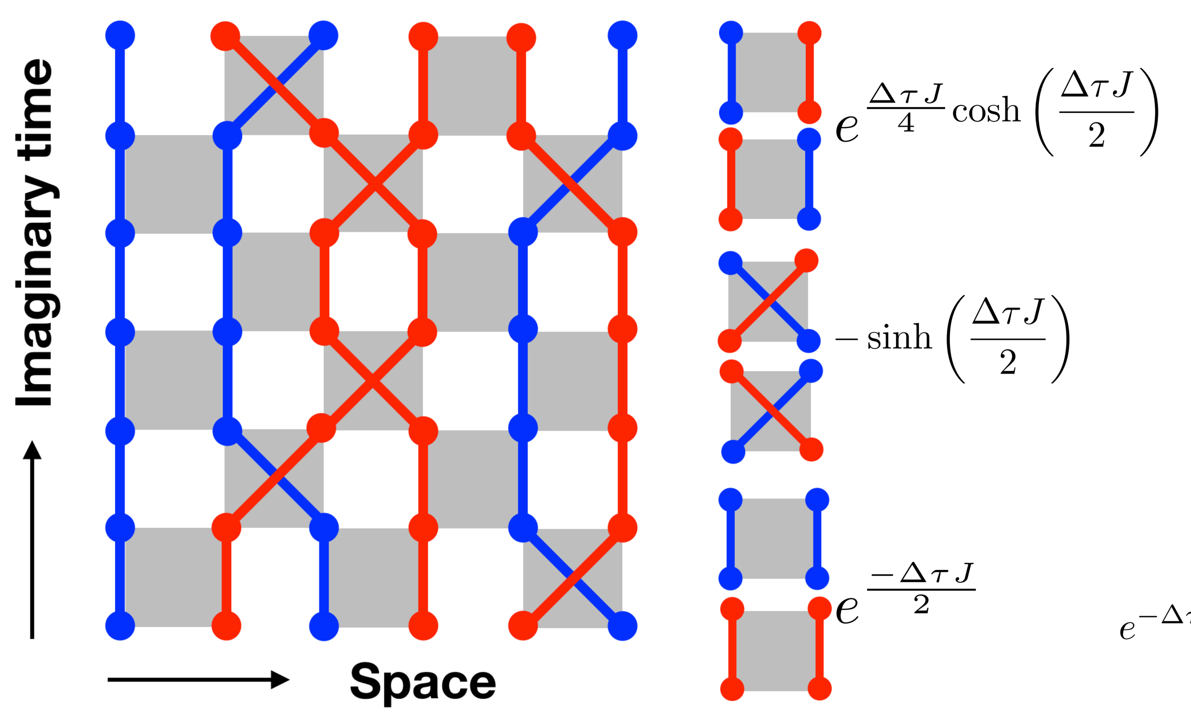
$$\hat{H}_{eff} = J\sum_{\langle i,j\rangle}\left[\cos\theta\left(\hat{S}_i\cdot\hat{S}_j\right) + \sin\theta\left(\hat{S}_i\cdot\hat{S}_j\right)^2\right] + DJ\sum_i\left(\hat{S}_i^z\right)^2$$

The goal is to develop a method to study the ferromagnetic phases of this model in a 1D optical lattice filled with spin-1 bosons.

Winkler R., Spin-Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems, Springer, Berlin, 201-206 (2003).

Spin-1/2 Heisenberg model and world lines

The spin-1/2 Heisenberg model is presented for a better understanding of the partition function and the world lines after the Suzuki-Trotter decomposition.



$M = 3;\ L = 6$

$$\hat{H} = J\sum_{\langle i,j\rangle}\hat{\vec{S}}_i\cdot\hat{\vec{S}}_j$$

$$\hat{H} =: \begin{pmatrix} \frac{J}{4} & 0 & 0 & 0\\ 0 & \frac{-J}{4} & \frac{J}{2} & 0\\ 0 & \frac{J}{2} & \frac{-J}{4} & 0\\ 0 & 0 & 0 & \frac{J}{4}\end{pmatrix} \quad \text{(basis } |\uparrow,\uparrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\downarrow,\downarrow\rangle)$$

$$e^{-\Delta\tau\hat{H}_i} =: e^{\frac{\Delta\tau J}{4}}\begin{pmatrix} e^{-\frac{\Delta\tau J}{2}} & 0 & 0 & 0\\ 0 & \cosh\left(\frac{\Delta\tau J}{2}\right) & -\sinh\left(\frac{\Delta\tau J}{2}\right) & 0\\ 0 & -\sinh\left(\frac{\Delta\tau J}{2}\right) & \cosh\left(\frac{\Delta\tau J}{4}\right) & 0\\ 0 & 0 & 0 & e^{-\frac{\Delta\tau J}{2}}\end{pmatrix} \quad \text{(basis } |\uparrow,\uparrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\downarrow,\downarrow\rangle)$$

The quantum partition function is mapped into the one of an effective model with one extra dimension. The extra dimension is given by the world lines, which restrict the possible configurations.

Suzuki-Trotter decomposition

First, one needs the Trotter approximation.

$$e^{x\hat{A}}e^{x\hat{B}} = e^{x(\hat{A}+\hat{B})+\mathcal{O}(x^2)}$$

A Hamiltonian with nearest neighbor interactions at most such as the one of interest, may be divided into bond Hamiltonians of neighboring sites.

$$\hat{H} = \sum_{i\ even}\hat{H}_i + \sum_{i\ odd}\hat{H}_i = \hat{H}_A + \hat{H}_B \quad \left[\hat{H}_A, \hat{H}_B\right] \neq 0 \quad \left[\hat{H}_i, \hat{H}_j\right] = 0$$

The quantum partition function of the Hamiltonian becomes:

$$Z = \mathrm{tr}\, e^{-\beta\hat{H}} = \mathrm{tr}\, e^{-\beta\left(\hat{H}_A+\hat{H}_B\right)} \approx \mathrm{tr}\, e^{-\beta\hat{H}_A}e^{-\beta\hat{H}_B}$$

The Trotter number is introduced to get rid of the error.

$$Z = \mathrm{tr}\left[e^{-\frac{\beta}{M}\left(\hat{H}_A+\hat{H}_B\right)}\right]^M = \lim_{M\to\infty}\mathrm{tr}\left[e^{-\Delta\tau\hat{H}_A}e^{-\Delta\tau\hat{H}_B}\right]^M$$

Expanding the partition function explicitly and adding completeness relations between the products of exponentials.

$$Z = \lim_{M\to\infty}\sum_{\sigma^0}\langle\sigma^0|\underbrace{e^{-\Delta\tau\hat{H}_A}}_{0}\underbrace{e^{-\Delta\tau\hat{H}_B}}_{1}\cdots\underbrace{e^{-\Delta\tau\hat{H}_A}}_{2M-2}\underbrace{e^{-\Delta\tau\hat{H}_B}}_{2M-1}|\sigma^0\rangle$$
$$= \lim_{M\to\infty}\sum_{\{\sigma\}}\underbrace{\langle\sigma^0|e^{-\Delta\tau\hat{H}_A}|\sigma^1\rangle}_{0}\underbrace{\langle\sigma^1|e^{-\Delta\tau\hat{H}_B}|\sigma^2\rangle}_{1}\cdots\underbrace{\langle\sigma^{2M-2}|e^{-\Delta\tau\hat{H}_A}|\sigma^{2M-1}\rangle}_{2M-2}\underbrace{\langle\sigma^{2M-1}|e^{-\Delta\tau\hat{H}_B}|\sigma^0\rangle}_{2M-1}$$

The partition function is transformed into the summation of world lines weights given by the imaginary time evolution plaquettes [2, 3].

$$Z = \sum_W\prod_P\Omega(W|P) = \sum_W\Omega(W)$$

Observables and Metropolis scheme

The observables that can be measured must be 1-site or 2-site separable operators and they need to conserve the basis locally. Some correlations can not be measured. Now, the observables are calculated explicitly by taking advantage of the trace properties and the world lines weights.

$$\left\langle\hat{O}\right\rangle = \frac{1}{Z}\mathrm{tr}\left[\left(e^{-\Delta\tau\hat{H}_A}e^{-\Delta\tau\hat{H}_B}\right)^M\left(\hat{O}_A+\hat{O}_B\right)\right]$$
$$= \frac{1}{Z}\mathrm{tr}\left[\left(e^{-\Delta\tau\hat{H}_A}e^{-\Delta\tau\hat{H}_B}\right)^{M-1}\left(e^{-\Delta\tau\hat{H}_A}\hat{O}_Ae^{-\Delta\tau\hat{H}_B} + e^{-\Delta\tau\hat{H}_A}e^{-\Delta\tau\hat{H}_B}\hat{O}_B\right)\right]$$
$$= \frac{1}{Z}\sum_W\Omega(W)\left[\frac{\langle\sigma^0|e^{-\Delta\tau\hat{H}_A}\hat{O}_A|\sigma^1\rangle}{\langle\sigma^0|e^{-\Delta\tau\hat{H}_A}|\sigma^1\rangle} + \frac{\langle\sigma^0|e^{-\Delta\tau\hat{H}_A}\hat{O}_A|\sigma^1\rangle}{\langle\sigma^0|e^{-\Delta\tau\hat{H}_A}|\sigma^1\rangle}\right]$$

This measures the observables in one time slice, to obtain better statistics, one must average over all the time slices.

$$\left\langle\hat{O}\right\rangle = \frac{1}{Z}\sum_W\Omega(W)\underbrace{\left[\frac{1}{M}\sum_n\frac{\langle\sigma^n|e^{-\Delta\tau\hat{H}_A}\hat{O}_A|\sigma^{n+1}\rangle}{\langle\sigma^n|e^{-\Delta\tau\hat{H}_A}|\sigma^{n+1}\rangle}\right]}_{o(W)}$$
$$= \frac{1}{Z}\sum_W\Omega(W)o(W) = \frac{\sum_W\Omega(W)o(W)}{\sum_W\Omega(W)}$$

Now one can proceed to use a classical stochastic method to do the measurements. A Metropolis like algorithm is chosen.

"Metropolis" algorithm:

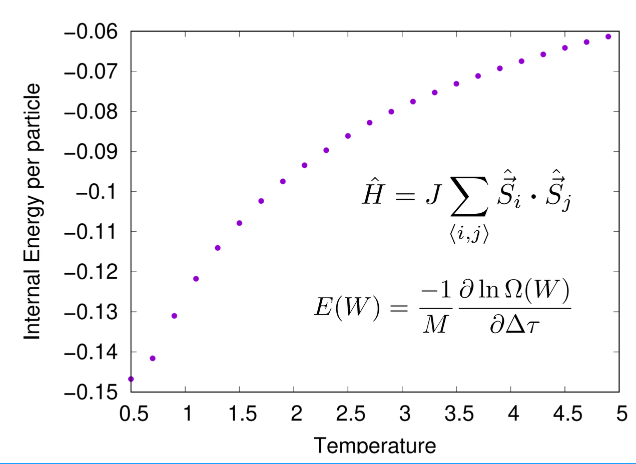
1. Markov process.
2. Ergodicity.
3. Detailed balance:

$$\frac{P_{\mu\to\nu}}{P_{\nu\to\mu}} = \frac{P_\nu}{P_\mu} = \underbrace{e^{-\beta(E_f-E_i)}}_{\text{classical}} = \underbrace{\frac{\Omega(W_\nu)}{\Omega(W_\mu)}}_{\text{quantum}}$$

Transition rate:

$$P_{\mu\to\nu} = \begin{cases}\frac{\Omega(W_\nu)}{\Omega(W_\mu)} & \Omega_\nu < \Omega_\mu\\ 1 & \Omega_\nu \geq \Omega_\mu\end{cases}$$

Results for the energy as a function of the temperature for the spin-1/2 Heisenberg model were measured.



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[1] L. de Forges de Parny, V. G. Rousseau, *Phys. Rev. A* **97**, 023628 (2018).
[2] M. Suzuki, *Progr. Theor. Exp. Phys.* **56**, 1454 (1976).
[3] F. F. Assaad, H. G. Evertz, World-line and Determinantal Quantum Monte Carlo Methods for Spins, Phonons and Electrons, Springer, Berlin (2008).

Perspectives

Measure quantum and thermodynamical observables, such as magnetization and von Neumann entropy, using the QMC developed to characterize the ferromagnetic phases of the spin-1 system.