Semi-definite programming for solving the local Hamiltonian problem

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The power of semidefinite programmes (SDPs) for solving quantum ground state problems has been hardly explored so far. This is a veritable deficiency given that they have great potential to outperform and complement existing methods. SDPs, in contrast to any other known method, give lower bounds on the ground state energy, rather than upper bounds. Thereby they yield benchmarks for other successful methods such as those based on tensor networks. What is more, SDPs, unlike quantum Monte-Carlo techniques, do not suffer from the sign problem that prevents application in many interesting situations.

Convex optimization

- A general convex optimization problem is of the form:
  With f, g_i convex and h_i affine

$$\begin{aligned} & \min_{\mathbf{x}\in\mathbb{R}^m} f(\mathbf{x}) \\ \text{such that} \quad & \forall i : g_i(\mathbf{x}) \geq 0 \\ & \forall i : h_i(\mathbf{x}) = 0 \end{aligned}$$

- A simple example:

$$\begin{aligned} & \min_{\mathbf{x}\in\mathbb{R}^2} x_1 x_2 \\ \text{such that} \quad & -x_2^2 + x_2 + 1/2 \geq 0 \\ & x_1^2 - x_1 = 0 \end{aligned}$$

Semi-definite relaxation

We can relax any convex problem to a semi-definite one. The latter is easier to solve and yields an approximate solution of the former. There is a hierarchy (Lasserre hierarchy) of relaxations that yield better and better approximations [1].

- A general semi-definite optimization problem is of the form:
  With a cost vector $\mathbf{c} \in \mathbb{R}^m$ and constrain matrices $(F_i)_{i=0}^m$

$$\begin{aligned} & \min_{\mathbf{y}\in\mathbb{R}^m} \mathbf{c}\cdot\mathbf{y} \\ \text{such that} \quad & \sum_{i=1}^m F_i y_i - F_0 \geq 0 \end{aligned}$$

- Level 2 relaxation of the example:
  1. Construct all oder 2 monomials: $x := (1, x_1, x_2, x_1x_2, x_1^2, x_2^2)$
  2. Introduce SDP variables $y_1, y_2, \ldots, y_8$ for all distinct elements in $x\,x^T$ after applying the substitution rule $x_1^2 \mapsto x_1$.
  3. Rewrite everything in terms of the SDP variables:

$$\begin{aligned} & \min y_3 \\ \text{such that} \quad & \begin{pmatrix} 1 & y_1 & y_2 & y_3 & y_4 \\ y_1 & y_1 & y_3 & y_3 & y_5 \\ y_2 & y_3 & y_4 & y_5 & y_6 \\ y_3 & y_3 & y_5 & y_5 & y_7 \\ y_4 & y_5 & y_6 & y_7 & y_8 \end{pmatrix} \geq 0 \\ & \begin{pmatrix} -y_4 + y_2 + 1/2 & -y_5 + y_3 + y_1/2 & -y_6 + y_4 + y_2/2 \\ -y_5 + y_3 + y_1/2 & -y_5 + y_3 + y_1/2 & -y_7 + y_5 + y_3/2 \\ -y_6 + y_4 + y_2/2 & -y_7 + y_5 + y_3/2 & -y_8 + y_6 + y_4/2 \end{pmatrix} \geq 0 \end{aligned}$$

Non-commutative generalizations

In a non-commutative convex optimization problem the vector $\mathbf{x}$ of numbers is replaced by a vector of operators.

- A similar hierarchy of semi-definite relaxations still exists [2]
- SDP variable become expectation values of local observables
- The hierarchy can be proven to converge if the constraints force the operators to be bounded (satisfied for fermions and spins) [3]

Benchmarking with the Fermi-Hubbard model

The Fermi-Hubbard model is the paradigmatic model of condensed matter physics. It describes electrons hopping on a lattice.

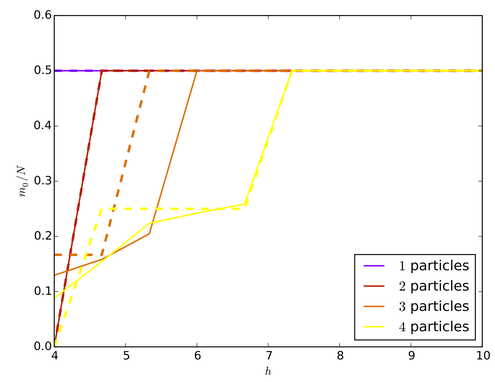
$$H := \underbrace{-t \sum_{\langle j,k\rangle,\sigma\in\{\uparrow,\downarrow\}} f_{j,\sigma}^\dagger f_{k,\sigma}}_{\text{hopping}} + \underbrace{U \sum_j f_{j,\uparrow}^\dagger f_{j,\downarrow}^\dagger f_{j,\downarrow} f_{j,\uparrow}}_{\text{on-site interaction}} - \underbrace{\frac{h}{2} \sum_j f_{j,\uparrow}^\dagger f_{j,\uparrow} - f_{j,\downarrow}^\dagger f_{j,\downarrow}}_{\text{magnetic field}}$$

- Exactly solvable in 1D by Bethe ansatz
- Difficult to solve in 2D
  - ! No analytic solution
  - ! Hilbert space grows fast ⇒ exact diagonalization only for $\lessapprox 12$ sites
  - ! Fermions ⇒ sign problem ⇒ no Monte Carlo
  - ! 2D ⇒ tensor networks not efficiently contactable

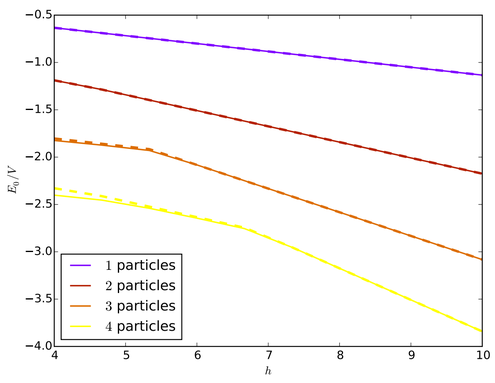
Work in progress: very first preliminary numerical results

We are implementing a pair of python libraries [4, 5] that make formulating and solving semi-definite relaxations of ground-state problems of local Hamiltonians easy.

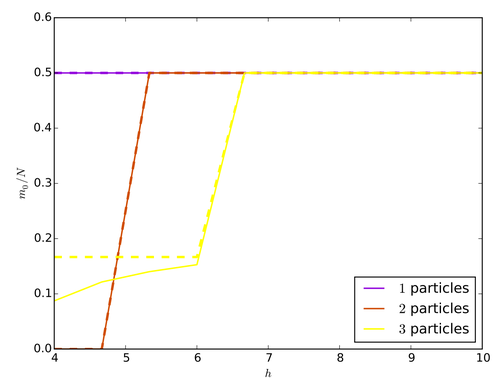
- Magnetization $m_0 := \left\langle \sum_j a_{\uparrow,j}^\dagger a_{\uparrow,j} - a_{\downarrow,j}^\dagger a_{\downarrow,j} \right\rangle_0$



- Energy $E_0 := \langle H \rangle_0$



- Energy $E_0 := \langle H \rangle_0$ in 2D



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[4] ncpol2sdpa, URL: https://github.com/peterwittek/ncpol2sdpa.

[5] sdpqpy, URL: https://github.com/cgogolin/sdpqpy.

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