Dimensional reduction procedure in Hilbert space. Application to strongly correlated systems

Tarek Khalil

Laboratoire de Physique Théorique, Université Louis Pasteur, Strasbourg
In collaboration with Jean Richert :

J. Phy. A:Math. Gen. 37(2004) 4851-4860
arxiv:quant-ph/0606056

Les Houches, June 2006

Introduction

Strongly correlated systems $\Rightarrow$
Techniques based on Perturbation theory breaks down

- Renormalization in real or momentum space.

  (Kadanoff et al. Rev. Mod. Phys. **19** (1967) 395)

  (K. G. Wilson, Phys. Rev. Lett. **28** (1972) 548; Rev. Mod. Phys. **47** (1975) 773)

  (S. R. White and R. M. Noack, P.R.L. **68** (1992) 3487)

- Exact diagonalization methods like Lanczos technique.

  (Lanczos Algorithms, J.K.Cullum and R. A. Willoughby)

Motivation

In Practice:

Diagonalization of the Hamiltonian of strongly correlated systems in large Hilbert space $\mathcal{H}^{(N)}$.

- **Alternative** : Use a projection technique to reduce the size of Hilbert space. Practically reduce the size of the Hamiltonian matrix.

  (H. Feshbach, Nuclear Spectroscopy part B (1960), Academic Press)
- Study the properties of the low excited states of microscopic strongly correlated systems at $T = 0$.
- Study the properties of the system near the first or higher critical points in the spectrum.

  (W.D.Heiss, Phy.Rev.E61(2000), 929)

  (Sachdev, Quantum Phase Transition, Cambridge)

Outline

- Renormalization in Hilbert space at T$= 0$
- Algorithm
- Application to spin ladders
- Conclusions
- Perspectives

Renormalization in Hilbert space at $T = 0$

The Hamiltonian:
$H = H_0 + gH_1$, with $H_0|\Phi_i^{(N)}\rangle = \epsilon_i|\Phi_i^{(N)}\rangle$, $i = 1, \ldots, N$

Using the feshbach formalism, we can write the Hilbert space $\mathcal{H}^{(N)}$

$\mathcal{H}^{(N)} = P\mathcal{H}^{(N)} + Q\mathcal{H}^{(N)}$

$\dim P\mathcal{H}^{(N)} = N - 1, \quad \dim Q\mathcal{H}^{(N)} = 1$

with P and Q are the projection operators.

In the projected subspace $P\mathcal{H}^{(N)}$:

$$H_{eff}(E) = PHP + PHQ(E - QHQ)^{-1}QHP$$

with, $P|\Psi_1^{(N)}\rangle = \sum_{i=1}^{N-1} a_{1i}^{(N)}(g^{(N)})|\Phi_i^{(N)}\rangle$

So, $H_{eff}(E_1^{(N)})P|\Psi_1^{(N)}\rangle = E_1^{(N)}P|\Psi_1^{(N)}\rangle$

H_{eff} is projected on $\langle\Phi_1|$:

$$\langle\Phi_1|H_{eff}(E_1^{(N)})|P\Psi_1^{(N)}\rangle = E_1^{(N)}(g^{(N)})a_{11}^{(N)}(g^{(N)}) \qquad (I)$$

- At this point, we begin the reduction procedure $\mathcal{H}^{(N)} \longrightarrow \mathcal{H}^{(N-1)}$
- We renormalize g by defining $H^{(N-1)} = H_0 + g^{(N-1)}H_1$ acting on $\mathcal{H}^{(N-1)}$.
- we impose the constraint: $E_1^{(N-1)} = E_1^{(N)}$

Developing Eqt.(I). One gets a discret quadratic flow equation:

$$a^{(N-1)}g^{(N-1)^2} + b^{(N-1)}g^{(N-1)} + c^{(N-1)} = 0$$

where

$a^{(N-1)}$, $b^{(N-1)}$ and $c^{(N-1)}$ are functions of $\{E_1^{(N)}, a_{1i}$ and $\langle \Phi_i | H | \Phi_j \rangle$, $i = 1, \ldots, N\}$

- **This method could give information about the excited states**

Algorithm :

1− Compute the elements of the Hamiltonian matrix $H^{(N)}$ by arranging the diagonal ones in increasing order.

2− Use the Lanczos technique to determine $E_1^{(N)}$ and $|\Psi_1^{(N)}(g^{(N)})\rangle$.

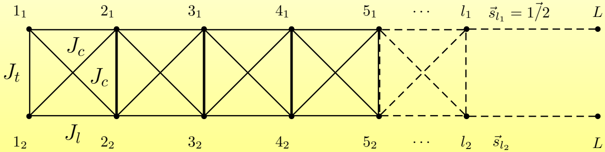
3− Compute the flow equation of $g^{(N-1)}$ and take the value nearest to $g^{(N)}$ by continuity.

4− Build $H^{(N-1)}$ by elimination of the element $H^{(N)}$ corresponding to the state $|\Phi_N\rangle$.

5− Repeat the same procedure 2, 3 and 4 by fixing at each step $E_1^{(K)} = E_1^{(K-1)}$.

6− Continue the iterations up to a low dimensional $k = N_{min}$.

Application to spin ladders



The Hamiltonian of $s = 1/2$:

$H^{(s,s)} = J_t \sum_{i=1}^{L} s_{i_1} s_{i_2} + J_l \sum_{<ij>} s_{i_1} s_{j_1} + J_l \sum_{<ij>} s_{i_2} s_{j_2} + J_c \sum_{(ij)} s_{i_1} s_{j_2} + J_c \sum_{(ij)} s_{i_2} s_{j_1}$

Here: $H_0 = 0$ and $g^{(N)} = J_t$

- The renormalization is restricted to a unique coupling strength.

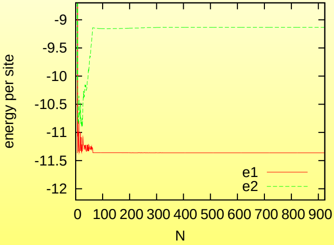
$$H^{(N)} = g^{(N)} H_1$$

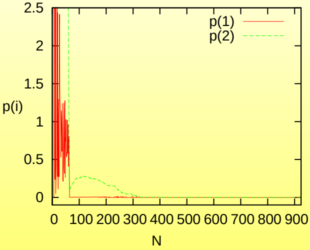
$$H_1 = \sum_{i=1}^{L} s_{i_1} s_{i_2} + \gamma_{tl} \sum_{<ij>} (s_{i_1} s_{j_1} + s_{i_2} s_{j_2}) + \gamma_{1c} \sum_{<ij>} s_{i_1} s_{j_2} + \gamma_{2c} \sum_{<ij>} s_{i_2} s_{j_1}$$

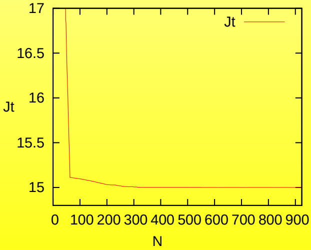
where $\gamma_{tl} = J_l/J_t$, $\gamma_{1c} = J_c/J_t$ and $\gamma_{2c} = J_c/J_t$.

- These quantities are kept constant and $g^{(N)} = J_t$ will be subject to renormalization in the reduction process.

$L = 12$ sites, $J_t = 15$, $J_l = 5$, $J_c = 3$, $S^z_{tot} = 0$







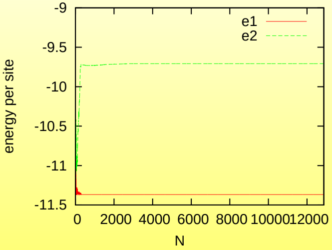
$$p(i) = \left|\frac{(e_i^{(N)} - e_i^{(n)})}{e_i^{(N)}}\right| \times 100$$

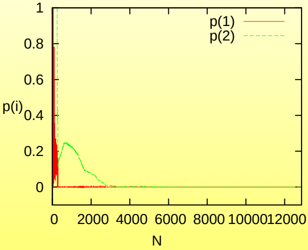
$$n/N \sim 0.067$$

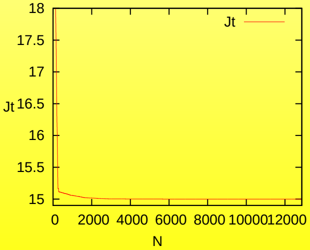
$$p(1) \sim 0.8\%$$

$$p(2) \sim 0.8\%$$

$L = 16$ sites, $J_t = 15$, $J_l = 5$, $J_c = 3$, $S^z_{tot} = 0$

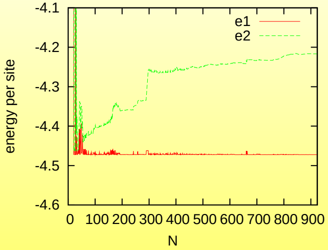


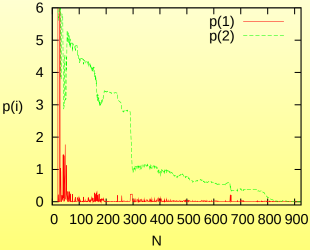


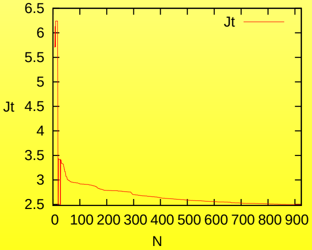


$$n/N \sim 0.007 \Rightarrow$$
$$p(1) \sim 0.8\%$$
$$n/N \sim 0.02$$
$$p(2) \sim 0.53\%$$

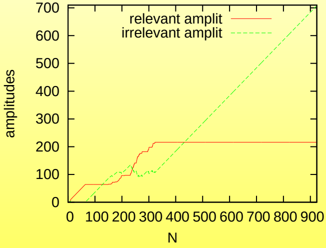
$L = 12$ sites, $J_t = 2.5$, $J_l = 5$, $J_c = 3$, $S^z_{tot} = 0$

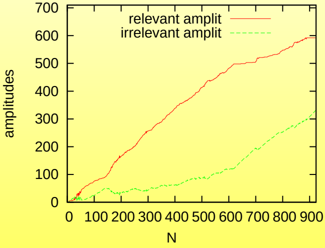






$L = 12$ sites, $J_t = 15, 2.5,\ J_l = 5,\ J_c = 3,\ S^z_{tot} = 0$





N is the dimension of the Hilbert space. *Amplitudes* show the number of relevant -irrelevant amplitudes in the ground state eigenfunction. Relevant amplitudes are those for which $\{a_{1i} > \epsilon$, (here $\epsilon = 10^{-2}$), $i = 1, \ldots, n\}$

Conclusions

- The stability of the low-lying states of the spectrum in the course of the reduction procedure depends on the relative values of the coupling strengths.
- The evolution of the spectrum depends on the initial size of Hilbert space.
- Local spectral instabilities appearing in the course of the reduction procedure are correlated with the elimination of basis states with sizable amplitudes in the ground state wavefunction.

Perspectives

- Study the efficiency of the reduction procedure for the same system in different symmetry schemes.

  K. Kikoin, Y. Avishai and M. N. kiselev, PRB 68 (2003)

- Study higher dimensional systems(2D).

- Use the method in the neighborhood of first and higher order critical points for realistic systems.

  J. Phy. A:Math. Gen. 37(2004) 4851-4860

- Use the criteria of decreasing amplitudes of the ground state wave function to arrange the elements of the matrix.