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

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Introduction

Strongly correlated systems ⇒ Techniques based on Perturbation theory breaks down

- Renormalization in real or momentum space.
  
  (Kadanoff et al. Rev. Mod. Phys. 19 (1967) 395)
  (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.
  

- 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.


  (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:

$$H = H_0 + gH_1, \text{ with } H_0|\Phi_{i}^{(N)}\rangle = \epsilon_i|\Phi_{i}^{(N)}\rangle, \ i = 1, \ldots, N$$

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 $P\mathcal{H}^{(N)}$:

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

with, $P|\Psi_{1}^{(N)}\rangle = \sum_{i=1}^{N-1} a_{1i}^{(N)}(g^{(N)})|\Phi_{i}^{(N)}\rangle$
So, \( H_{\text{eff}}(E^{(N)}_1)P|\psi^{(N)}_1\rangle = E^{(N)}_1 P|\psi^{(N)}_1\rangle \)

\( H_{\text{eff}} \) is projected on \( \langle \Phi_1 | \):

\[
\langle \Phi_1 | H_{\text{eff}}(E^{(N)}_1) | P \psi^{(N)}_1 \rangle = E^{(N)}_1 (g^{(N)}) a^{(N)}_{11} (g^{(N)}) \quad (I)
\]

- At this point, we begin the reduction procedure \( \mathcal{H}^{(N)} \rightarrow \mathcal{H}^{(N-1)} \)

- 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: \( E^{(N-1)}_1 = E^{(N)}_1 \)
Developing Eqn. (1). One gets a discrete quadratic flow equation:

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

where

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

- 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 $s = 1/2$:

$$\mathcal{H}^{(s,s)} = J_t \sum_{i=1}^{L} s_i s_{i+1} + J_l \sum_{<ij>} s_i s_j + J_l \sum_{<ij>} s_j s_i + J_c \sum_{(ij)} s_i s_{j+1} + J_c \sum_{(ij)} s_j s_{i+1}$$

Here: $H_0 = 0$ and $g^{(N)} = J_t$
The renormalization is restricted to a unique coupling strength.

\[ H^{(N)} = g^{(N)} H_1 \]

\[ H_1 = \sum_{i=1}^{L} s_i s_j + \gamma_{tl} \sum_{<ij>} (s_i s_j + s_i s_j) + \gamma_{1c} \sum_{<ij>} s_i s_j + \gamma_{2c} \sum_{<ij>} s_i s_j \]

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, $J_t = 15$, $J_l = 5$, $J_c = 3$, $S_{\text{tot}}^z = 0$

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

$n/N \approx 0.067$

$p(1) \approx 0.8\%$

$p(2) \approx 0.8\%$
$L = 16$ sites, $J_t = 15$, $J_l = 5$, $J_c = 3$, $S_{tot}^z = 0$

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

$n/N \sim 0.02$
$p(2) \sim 0.53\%$
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$L = 12$ sites, $J_t = 2.5$, $J_i = 5$, $J_c = 3$, $S^z_{tot} = 0$
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$L = 12$ sites, $J_t = 15, 2.5$, $J_I = 5$, $J_C = 3$, $S_{tot}^Z = 0$

$N$ 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 $\{a_{1i} > \epsilon, (\text{here } \epsilon = 10^{-2}), i = 1, \ldots, n\}$
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.
  

- Study higher dimensional systems (2D).

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

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