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Introduction to quantum spin systems

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Abstract

This manuscript is the collection of lectures given in the summer school on strongly correlated electron systems held at Isfahan university of technology, June 2007. A short overview on quantum magnetism and spin systems is presented. The numerical exact diagonalization (Lanczos) alghorithm is explained in a pedagogical ground. This is a method to get some ground state properties on finite cluster of lattice models. Two extensions of Lanczos method to get the excited states and also finite temperature properties of quantum models are also explained. The basic notions of quantum phase transition is discussed in term of Ising model in transverse field. Its phase diagram and critical properties are explained using the quantum renormalization group approach. Most of the topics are in tutorial level with hints to recent research activities.

Keywords: quantum magnetism, exact diagonalization, quantum renormalization group

1. Introduction

The field of quantum spin system or *quantum magnetism* has been originated since some decades ago. The Ising [1] and Heisenberg models [2] are the original ones introduced in this field. For Ising model the ground state on a hyperqubic lattice is an ordered configuration of the spins. However, the ground state of Heisenberg model is not just a simple configuration of spins but a linear combination of several configurations. Although the ground state of Ising model on the hyperqubic lattice can be represented simply by a configuration of spins the ground state of Heisenberg model is not known exactly on two and three dimensional lattice. Even for one dimensional antiferromagnetic Heisenberg model the ground state of N spin 1/2 is given by a set of N-coupled linear equations via Bethe anzats [3]. The main difference between the two models is related to the non-commuting terms which exisit in Heisenberg model. In this sence the Ising model is a classical one and the Heisenberg model is a quanum one.

Quantum magnetism becomes more interesting since the discovery of high-T_c superconductors. Part of the phase diagram of cuprate superconductors is a quantum antiferromagnet. Understanding the ground state of this part might help to understand the mechanism of superconductivity at higher doping in these materials. This is one of the enigma of the last two decades in condensed matter physics. Many other novel effects have also been discoverd in the category which is called strongly correlated electron systems like colossal magnetoresistance [4] and heavy fermions [5, 6].

Quantum phase transition [7, 8] is the other play ground where quantum magnetism models have an important role. A phase transition which takes place at zero temperature upon change of a parameter like pressure or impurity concentration is a quantum phase transition. It is a qualitative change in the ground state of the model. The Ising model in transverse field (ITF) is a generic model which shows the quantum phase transition upon change of the trnasverse field. The non-analytic behvaiour of some ground state expectation value at the quantum critical point, the universality class at this point and critical exponents are those information which classifies the quantum critical point [9].

This articel is the collection of three lectures given in the first summer school on strongly correlated electron systems held at Isfahan university of technology. The summer school was initiated for graduate students and young researchers. Thus, I have tried to present the lectures in a pedagogical ground. I have presented a short overview on strongly correlated systems and its definition. Then, the model Hamiltonians in this category have been introduced with more emphasis on some novel effects in quantum magnetism. The exchange interaction in terms of Heisenberg model which is the most known model in quantum magnetism is also driven to represent the combination of coulumb interaction plus the Pauli exclusion principle. The next

part is devoted to the introductin of Lanczos exact diagonalization and some of its extensions to calculate the ground state, excited states and finite temperature properties of lattice models. Finally, the quantum phase transition is discussed for ITF model by introducing and implementing the quantum renormalization group. We have introduced the block renormalization group which is suitable for lattice models. The quantum renormalization group can be used to find the phase diagram at zero temperature. Moreover, it can also be extended to get the quantum information properties of quantum lattice models.

2. Strongly correlated electron systems

A system of elctrons and nuclei can be described by the following Hamiltonian

$$H = H_e + H_n + H_{e-n},$$
$$H_e = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j}^{N} \frac{e^2}{|r_i - r_j|},$$
$$H_n = \sum_{i=1}^{N'} \frac{P_i^2}{2M} + \sum_{i<j}^{N'} \frac{(Ze)^2}{|R_i - R_j|}, \quad (1)$$
$$H_{e-n} = -\sum_{i<j}^{N,N'} \frac{Ze^2}{|r_i - R_j|},$$

where p_i, r_i, m, e are electron momentum, position, mass and elecctric charge respectively and the corresponding ones for the nuclei are P_i, R_i, M, Ze. In the adiabatic approximation we assume the nuclei to be fixed at their equillibrium positions and the dynamic is considered for the electrons in the presence of nuclei lattice. In this case, the Hamiltonian is the sum of electronic and electron-nuclei parts

$$H \simeq H_e + H_{e-n}. \quad (2)$$

This is a many body Hamiltonian composed of coupled differential equations for N electrons. Several approaches and approximations have been introduced to find some information on this system. In *weakly correlated electron systems* the many body Hamiltonian can be approximated with a sum on the single particle Hamiltonians where the many body effects (i.e. correlation effects) has been represented by an effective potential,

$$H \simeq \sum_{i=1}^{N} [h(r_i) + V_{eff}(r_i)],$$
$$h(r_i) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i<j}^{N,N'} \frac{Ze^2}{|r_i - R_j|}. \quad (3)$$

The effective potential ($V_{eff}(r_i)$) can be found in different approximations [10], for instance by density functional theroy. This is the case when the kinetic energy of electrons is stronger than their potential energy.

However, most of **d** and **f** electrons which contribute to the electronic and magnetic property of some materials have the converse situation. Among them are the transition metals, mixed valence rare earth compounds, Lactanides and Actanids in the periodic table. For this electrons the kinetic energy of electrons is less than their interacting potential energy. In such cases, the approximation of many body Hamiltonian to single particle ones plus an effective potential fails. This approximation may even lead to wrong results. Such cases are called *strongly correlated electron systems* [11, 12].

2.1. Model Hamiltonians

As discussed in the previous section some of **d** and **f** electrons are strongly correlated which should be studied by a many body Hamiltonian. A simple model which mimics several features of metalic, magnetic and insulating phases of such materials is the Hubbard model [13]. A detailed introduction to this model is given by S. A. Jafari in an article in this issue. The one band Hubbard model is defined by considering a lattice of atoms where each atom contribute a single orbital for the electrons. The electrons can hop between nearest neighbour atoms which can be modeled by the following Hamiltonian

$$H_0 = \sum_{<ij>,\sigma} (t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + t_{ji} c_{j\sigma}^{\dagger} c_{i\sigma}), \quad (4)$$

where $c_{j\sigma}^{\dagger}$ ($c_{j\sigma}$) creates (annihilates) an elctron in a single-particle orbital ϕ_j with spin σ localized at site j. The hopping strength is given by t_{ij} which is usually nonzero for the nearest neighbour atoms and zero for the others. Those electrons which reside on a single orbital with different spins have a large columb repulsion energy. Therefore, the one-band Hubbard model on a lattice is defined by the following Hamiltonian

$$H_{Hubbard} = H_0 + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (5)$$

where $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ is the occupation operator at the i-th orbital. U is the scale of coulumb repulsion energy. In Hubbard model each orbital has four degrees of freedom: no occupation, singly occupied (up or down) and double occupation.

In some cases U is very large, i.e. $U/t \gg 1$, the double occupied states have large energy and reside in the upper part of the spectrum. The contribution of these configurations to the ground state and low energy behaviour of the model is weak. Thus, the Hamiltonian can be mapped to the subspace without double occupation. This is called the t-J model. The Hamiltonian of t-J model is composed of two terms: a hopping term for electrons and an exchange interaction between the spin of electrons,

$$H_{t-J} = \Im[\sum_{<ij>,\sigma} (t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + t_{ji} c_{j\sigma}^{\dagger} c_{i\sigma})$$
$$+ J \sum_{<ij>} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j)]\Im, \quad (6)$$

where $\Im$ is the projection to subspace without double occupation, $J = 4t^2/U$ is the exchange coupling, S is the electron spin operator and $n_i = \sum_{\sigma} n_{i\sigma}$. If the

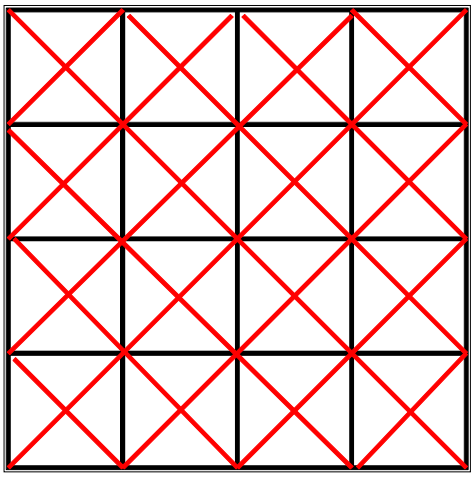

Figure 1. Square lattice with diagonal bonds.

number of electrons are equal to the number of lattice sites (half-filling) the hopping term in the t-J model is suppressed and the Hamiltonian is effectively described only by the exchange term which represents the interaction between the spin of frozen electrons. Apart from a constant this is the Heisenberg Hamiltonian

$$H = J \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j . \qquad (7)$$

If $J > 0$ the model describes the antiferromagnetic interaction and for $J < 0$ the ferromagnetic one. The magnetic property of several materials at low temperature can be described by the Heisenberg Hamiltonian. This branch of research is called *quantum magnetism.* This includes different extensions of the Heisenberg model. A very good reference on this topic is Ref.[14].

2. 2. Some novel effect

Several novel and exotic phenomena have been observed in quantum magnetism. Among them is the seminal work of Haldane [15] which defines different universality classes for antiferromagnetic ($J > 0$) Heisenberg (AFH) Hamiltonian (7) in one-dimensional models (chains). It has been conjectured by Haldane that an integer spin AFH chain is gapful and its correlation functions decay exponentialy versus distance, while the half-integer ones are gapless with algebraic decay of correlations. However, the bond alternating spin chain is gapful even for small value of bond alternation [16].

Another surprising investigation deals with spin ladders which have attracted a considerable amount of attention [18]. They consist of coupled one-dimensional chains and may be regarded as interpolating truly one and two-dimensional systems. These models are useful to study the properties of the high-Tc superconductor materials. Theoretical studies have suggested that there are two different universality classes for the uniform-spin ladders, i.e., the antiferromagnetic spin-1/2 ladders are gapful or gapless, depending on whether n_l (the number of legs) is even or odd [18]. These predictions have been confirmed experimentally by compounds like $SrCu_2O_3$ and $Sr_2Cu_3O_5$. However, again bond-alternation changes this universality. It has been shown that a gapless line which depends on the staggered bond-alternation parameter, divides the gapful phase of a 2-leg antiferromagnetic spin-1/2 ladder into two different phases [19, 20]. Moreover, there are some other configurations, like the columnar bond-alternation that introduces new phases for the antiferromagnetic ladders [21, 22]. The appearance of the magnetization plateaus for both chains [23, 24] and ladders [25, 26] and the appearance of the new phases for spin ladders [27], are also some of the consequences of the bond-alternations.

Before going to the next section, let us briefly discuss an example of a recent study in this field. The magnetic property of two family of materials, Li_2VOXO_4 with X=Si, Ge and $AA'VO(PO_4)_2$ with A, A'=Pb, Zn, Sr, Ba can be described by the Heisenberg Hamiltonian on a square lattice. The magnetic ions reside on the vertex of the lattice and is represented by a spin. The nearest neighbour spins and those on the diagonal of each plaquette interact with each other, see Fig.1.
The Hamiltonian for this model is given by

$$H = J_1 \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\ll i,j \gg} \vec{S}_i \cdot \vec{S}_j , \qquad (8)$$

where $< i, j >$ represents the horizontal and vertical bonds and $<< i, j >>$ is for the diagonal ones. J_1 is the strength of exchange interaction in horizontal and vertical directions and J_2 is the corresponding one along the diagonal ones. Depending on the ratio of J_1/J_2 and its sign the ground state of Hamiltonian (8) shows different ordering (more details can be found in Ref.[28] and the article by P. Thalmeier in this issue). A classical picture gives the antiferromagnetic Neel ordered phase for $J_1 > 0$ and $J_2 < J_1/2$, ferromagnetic ordering for $J_1 < 0$ and $J_2 < J_1/2$, and canted-antiferromagnetic phase for $|J_2| > |J_1/2|$. The ratio of J_1/J_2 is fixed by the components defined in the two family of materials mentioned before.

I have just mentioned few number of novel effects in quantum magnetism. There are other aspects of this field which are part of current research activities like frustrated spin systems, disorded models and also quantum information properties of spin models.

2. 3. Exchange interaction

Magnetism is a quantum property of matter which can not be explained by a pure classical model. It is stated in the Bohr van Leeuwen theorem that "The magnetic susceptibility is zero for a pure classical model". This can be easily proofed by considering a classical partition function which is

$$Z_{classic} = \int e^{-\beta H(q_i, p_i)} \prod_i d^3 q_i d^3 p_i , \qquad (9)$$

where $\beta = 1/k_B T$, k_B is the Boltzmann constant, T is absolute temperature, q_i are position coordinate of particles and p_i are their momentums. The effect of magnetic field on this system can be considered by simply change of momentums to the following ones

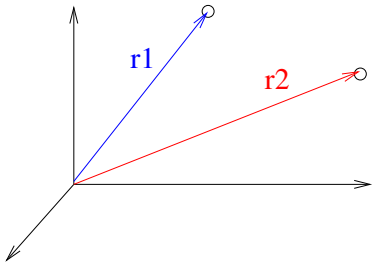

Figure 2. Two electrons at positions r1 and r2.

$$p_i \to p_i' = p_i + \frac{e}{c} A(q_i), \tag{10}$$

where p_i' are the new momentums, e is the electric charge of particles (electrons here), c is the speed of light and $A(q_i)$ is the magnetic potential. Replacing the new momentums in the partition function describe the system in the presence of magnetic field. However, p_i' is a dummy variable in the integral and a change of this variable to p_i leaves the Jacobian equal to one. Hence the classical partition function is independent of A which gives the zero value for the magnetic susceptibility.

Moreover, the dipole-dipole interaction between magnetic moments of atoms is very small which gives the critical temperature of magnetic transition some orders of magnetiude incorrect.

To get an impression of the magnetic exchange interation consider a simple model which consists of two electrons (see Fig. 2) each represented by a state which is an atomic orbital. Each orbital can be occupied by only one electron. The Hamiltonian of an independent electron is $h_0(r_i)$ with the following energy for each mentioned orbitals

$$\begin{aligned} &h_0(r_1)\,|\,\phi_a\,\rangle = \varepsilon_a\,|\,\phi_a\,\rangle; \\ &h_0(r_2)\,|\,\phi_b\,\rangle = \varepsilon_b\,|\,\phi_b\,\rangle; \\ &\langle\,\phi_a\,|\,\phi_b\,\rangle = 0. \end{aligned} \tag{11}$$

Now let the electrons being close to each other and interact via the Columb repulsion potential. Thus the Hamiltonian of the two electrons model is

$$H_{2e} = h_0(r_1) + h_0(r_2) + \frac{e^2}{|\,r_1 - r_2\,|}. \tag{12}$$

The state of two electrons system is the Slater determinant of the single electron states which also considers the spin configuration of each electron

$$\begin{aligned} |\,\psi_1\,\rangle &= \frac{1}{\sqrt{2}} \det\begin{pmatrix} \phi_a(r_1)\alpha(s_1) & \phi_a(r_2)\alpha(s_2) \\ \phi_b(r_1)\alpha(s_1) & \phi_b(r_2)\alpha(s_2) \end{pmatrix}, \\ |\,\psi_2\,\rangle &= \frac{1}{\sqrt{2}} \det\begin{pmatrix} \phi_a(r_1)\alpha(s_1) & \phi_a(r_2)\alpha(s_2) \\ \phi_b(r_1)\beta(s_1) & \phi_b(r_2)\beta(s_2) \end{pmatrix}, \\ |\,\psi_3\,\rangle &= \frac{1}{\sqrt{2}} \det\begin{pmatrix} \phi_a(r_1)\beta(s_1) & \phi_a(r_2)\beta(s_2) \\ \phi_b(r_1)\alpha(s_1) & \phi_b(r_2)\alpha(s_2) \end{pmatrix}, \\ |\,\psi_4\,\rangle &= \frac{1}{\sqrt{2}} \det\begin{pmatrix} \phi_a(r_1)\beta(s_1) & \phi_a(r_2)\beta(s_2) \\ \phi_b(r_1)\beta(s_1) & \phi_b(r_2)\beta(s_2) \end{pmatrix}. \end{aligned} \tag{13}$$

where α and β represent the $\uparrow$ and $\downarrow$ state of spin configuration, respectively. In the slater determinant states the Hamiltonian is represented in the following form

$$H_{2e} = (\varepsilon_a + \varepsilon_b)1 + \begin{pmatrix} C_{ab} - J_{ab} & 0 & 0 & 0 \\ 0 & C_{ab} & -J_{ab} & 0 \\ 0 & -J_{ab} & C_{ab} & 0 \\ 0 & 0 & 0 & C_{ab} - J_{ab} \end{pmatrix}, \tag{14}$$

where

$$0 < C_{ab} = e^2 \iint d^3r_1 d^3r_2 \frac{|\,\phi_a(r_1)\,|^2\,|\,\phi_b(r_2)\,|^2}{|\,r_1 - r_2\,|}, \tag{15}$$

$$0 < J_{ab} = e^2 \iint d^3r_1 d^3r_2 \frac{\phi_a(r_1)^*\phi_b(r_2)^*\phi_a(r_2)\phi_b(r_1)}{|\,r_1 - r_2\,|}. \tag{16}$$

The Hamiltonian has two distinct energy energy levels, a triple degenerate level

$$e_{triplet} \equiv (\varepsilon_a + \varepsilon_b) + C_{ab} - J_{ab}, \tag{17}$$

and a singlet

$$e_{singlet} \equiv (\varepsilon_a + \varepsilon_b) + C_{ab} + J_{ab}. \tag{18}$$

The distinction between the two energy levels is related to the spin configurations of the two electrons. Thus, an effective Hamiltonian based on the spin of electrons (S_1, S_2) is responsible to represent the energy levels of the system.

$$H = \frac{e_{singlet} + e_{triplet}}{2} - \left(\frac{e_{singlet} - e_{triplet}}{2}\right)\left(2S_1 \cdot S_2 + \frac{1}{2}\right). \tag{19}$$

Apart from an additive constant the effective Hamiltonian which represent the interaction between two electrons is given by the ferromagetic Heisenberg Hamiltonian with the exchange coupling $J = -2J_{ab} < 0$,

$$H_{eff} = constant - 2J_{ab} S_1 \cdot S_2. \tag{20}$$

It can be shown that if the atomic orbitals are not orthogonal $(\langle\,\phi_b\,|\,\phi_a\,\rangle \neq 0)$ the effective spin Hamiltonian is antiferromagnetic, $J > 0$.

3. Numerical approaches

It has been discussed in the previous sections that correlation effects are important in strongly correlated systems. In such cases the single particle picture is not able to capture the true behaviour of the model. Most of the correlation effects can be discovered by numerical approaches on finite clusters. The finite size scaling is then implemented to extend the results of finite cluster to the thermodynamic limit. Quantum Monte Carlo (QMC) and Exact Diagonalization (ED) Lanczos method are the most known numerical approaches to study the strongly correlated systems. QMC is the implementation of Monte-Carlo approach to quantum systems which is composed of two steps. In the first step the quantum system on D-dimensional lattice is mapped to a classical one on a $D+1$-dimensional model. This can be

done by Trotter expansion [29]. The second step is a MC simulation to find the equillibrium state of system. An advantage of QMC is the large size of lattice which can be implemented in computations. The finite temperature properties is usually gained with good accuracy. However, the critical slowing down and the sign problem in fermionic models are usually the disadvantage of QMC close to zero temperature (see also the article by J. Zaanen et.al in this issue). The ground state properties which are the dominant ones at zero temperature mimic the main quanutm effects in strongly correlated systems. The ground state of a quatum model can be found exactly by ED method. However, the size of lattice which can be considered is rather smaller than the case of QMC. Finite size scaling is usually necessary to be done for getting the thermodynamic information of the quantum model. In the next section we will introduce the Lanczos method to get the ground state and some low lying eigenstates of a quatum lattice model.

3. 1 Lanczos method

Let us introduce the Lanczos method by a concrete example, the spin $1/2$ Heisenberg model. The general Heisenberg model Hamiltonian can be written as,

$$\mathcal{H} = \sum_{i,j}^{N} \left\{ J_{ij}^{xy} \left(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y \right) + J_{ij}^z \sigma_i^z \sigma_j^z \right\}, \qquad (21)$$

One can represent the Hamiltonian on N sites in the configuration space,

$$\mathcal{H}_{ij} = \langle i | \mathcal{H} | j \rangle, \qquad (22)$$

where $|i\rangle$ is a configuration of spins, e.g. $|\uparrow\downarrow\uparrow\cdots\downarrow\downarrow\uparrow\rangle$. The spins can be labeled as their binary form; say 0 for $\downarrow$ and 1 for $\uparrow$. So the configuration with all spins down, $|\downarrow\downarrow\cdots\downarrow\downarrow\rangle$ will be $|00\cdots00\rangle$ or $|0\rangle$, $|\downarrow\downarrow\cdots\downarrow\uparrow\rangle$ will be $|00\cdots01\rangle$ or $|1\rangle$ and the last configuration with all spins up, $|\uparrow\uparrow\cdots\uparrow\uparrow\rangle$, will be $|11\cdots11\rangle$ or $|2^N - 1\rangle$. Hence,

$$i = \sum_{n=1}^{N} 2^{n-1} S_n, \quad S_n = 0,1. \qquad (23)$$

Any vector in our Hilbert space is a linear combination of these basis vectors,

$$|\psi\rangle = \sum_{i=0}^{2^N-1} c_i |i\rangle \qquad (24)$$

To store a vector, a one dimensional array is sufficient for storing c_i in index i. One can employ symmetries of the Hamiltonian, such as rotational invariance, conservation of total spin or translational invariance for reduction of the Hilbert space and therefore calculating higher dimension matrices. As a consequence, the binary labeling scheme must change to another (optional, but not always optimal) labeling system, which can led to utilization of more CPU time or memory (due to converting the indices to configurations and vice versa). One approach is using a hashing function,

$h(i) = (i \bmod K) + 1,$

K is a prime number greater than 2^N which is commonly used in practice. A simpler approach is to sort the configurations of the same total spin, and then use their sorted index as their label. This method requires computing (or storing) the indices, which can be inefficient for large values of N. For a discussion on good labeling schemes, see [30].

The operation of σ^α ($\alpha = x, y, z$) on a specific site j is

$$\sigma_j^x |\uparrow\uparrow\cdots s\cdots\downarrow\uparrow\rangle = |\uparrow\uparrow\cdots\bar{s}\cdots\downarrow\uparrow\rangle$$

$$\sigma_j^y |\uparrow\uparrow\cdots s\cdots\downarrow\uparrow\rangle = (2s-1)\, I\, |\uparrow\uparrow\cdots\bar{s}\cdots\downarrow\uparrow\rangle,$$

$$I = \sqrt{-1}$$

$$\sigma_j^z |\uparrow\uparrow\cdots s\cdots\downarrow\uparrow\rangle = (2s-1)|\uparrow\uparrow\cdots s\cdots\downarrow\uparrow\rangle$$

The operation of σ^x and σ^y operators can be implemented as a simple flip of the associated bit in the binary representation of all configurations of the vector. Now we can completely work out the operation of $\mathcal{H}$ on a vector and therefore doing the Lanczos algorithm.

It is instructive first to explain the Lanczos method [31, 32] as an improvement of the power method. The power method is a simple way to calculate the eigenvalue of a matrix with the largest absolute value; one starts from an arbitrary initial vector $|v_0\rangle$ and multiplies the matrix $\mathcal{H}$ repeatedly until the resulting vector converges to the desired eigenvector. More precisely, when the eigenvalues and eigenvectors of an m-dimensional matrix $\mathcal{H}$ are E_j and $|\psi_j\rangle$, the arbitrary vector $|v_0\rangle$ can be written as,

$$|v_0\rangle = \sum_{j=1}^{m} a_j |\psi_j\rangle.$$

Multiplying the initial vector k times by $\mathcal{H}$, one obtains

$$|v_k\rangle \equiv \mathcal{H}^k |v_0\rangle = \sum_{j=1}^{m} a_j E_j^k |\psi_j\rangle,$$

$$E_1 > E_2 > E_3 > \cdots$$

$$|v_k\rangle = a_1 E_1^k |\psi_1\rangle + \sum_{j=2}^{m} a_j E_j^k |\psi_j\rangle =$$

$$E_1^k \left[a_1 |\psi_1\rangle + \sum_{j=2}^{m} a_j \left(\frac{E_j}{E_1} \right)^k |\psi_j\rangle \right]$$

It is apparent that the relative weight of the eigenvector corresponding to the eigenvalue with the largest absolute value increases exponentially with k among terms appearing in the above sum.

Acceleration of convergence over the simple power method is achieved by subtracting components of previous vectors ($|v_{k-1}\rangle$, $|v_{k-2}\rangle$, …) from $|v_k\rangle$ so

that one can eliminate the effects of the arbitrarily chosen initial vector as rapidly as possible.

This subtraction of components of previous vectors is incidentally equivalent to tridiagonalization. If the tridiagonal matrix $\mathcal{T}$ is obtained from the original matrix $\mathcal{H}$ by a transformation matrix $\mathcal{V}$, one has the relation $\mathcal{T} = \mathcal{V}^{-1}\mathcal{H}\mathcal{V}$, or $\mathcal{V}\mathcal{T} = \mathcal{H}\mathcal{V}$. Let the column vectors of $\mathcal{V}$ be $|v_1\rangle, |v_2\rangle,$, and the diagonal elements of $\mathcal{T}$ be $\alpha_1, \alpha_2,$, and the sub diagonal elements $\beta_1, \beta_2,$, Then the relation $\mathcal{V}\mathcal{T} = \mathcal{H}\mathcal{V}$ is written as

$\mathcal{H}|v_1\rangle = \alpha_1|v_1\rangle + \beta_1|v_2\rangle$,

$\mathcal{H}|v_2\rangle = \beta_1|v_1\rangle + \alpha_2|v_2\rangle + \beta_2|v_3\rangle$,

$\mathcal{H}|v_3\rangle = \beta_2|v_2\rangle + \alpha_3|v_3\rangle + \beta_3|v_4\rangle$,

…

$\mathcal{H}|v_{m-1}\rangle = \beta_{m-2}|v_{m-2}\rangle + \alpha_{m-1}|v_{m-1}\rangle + \beta_{m-1}|v_m\rangle$

$\mathcal{H}|v_m\rangle = \beta_{m-1}|v_{m-1}\rangle + \alpha_m|v_m\rangle$

If one rewrites previous equations into a form to calculate $|v_k\rangle$ successively,

$|v_2\rangle = (\mathcal{H}|v_1\rangle - \alpha_1|v_1\rangle)/\beta_1$

$|v_3\rangle = (\mathcal{H}|v_2\rangle - \beta_1|v_1\rangle - \alpha_2|v_2\rangle)/\beta_2$

…

In order to have a vanishing $(m+1)$ th vector in the series of $|v_k\rangle$, it is sufficient to choose $|v_k\rangle$ so that it is orthogonal to all previous vectors, since $m+1$ vectors cannot be orthogonal to each other in the m-dimensional space. It is useful here to regard latter equations as an iterative orthogonalization process by subtracting components of previous vectors. Actually, it turns out that by choosing

$\alpha_i = \langle v_i|\mathcal{H}|v_i\rangle$,

$\beta_i = \| \mathcal{H}|v_i\rangle - \beta_{i-1}|v_{i-1}\rangle - \alpha_i|v_i\rangle \|$,

all $|v_k\rangle$ are orthogonal to each other. Since this process can be regarded as an improvement of the power method, it is not necessary to execute all of $m-1$ steps if one wishes to evaluate only several low-lying eigenvalues; one may calculate the eigenvalues of the intermediate tridiagonal matrix of dimension l $(< m)$ by the bisection method to see whether or not the low-lying eigenvalues have reached sufficiently converged values. It can be done by comparing the low-lying eigenvalues for two successive *m* values, for example *m* and *m*+10.

To get the eigenvectors, one first calculates the eigenvectors of the tridiagonal matrix when convergence of eigenvalues is confirmed. One then transforms the eigenvectors of the tridiagonal matrix into the original representation by use of the transformation matrix $\mathcal{V}$. That is, the eigenvectors in the original representation are obtained by summing up the products of the components $c_1^i, c_2^i, ...$ of the eigenvector i in the tridiagonal representation and the column vectors $|v_1\rangle, |v_2\rangle, ...$, of $\mathcal{V}$

$$|\psi_i\rangle = \sum_{j=1}^{m} c_j^i |v_j\rangle.$$

However, it is difficult to store the sequence $|v_1\rangle, |v_2\rangle, ...$ generated until convergence since convergence usually results after tens of iterations (and tens of the vectors should be stored in memory). A simple way is to store $c_1, c_2, ...$ real numbers) in the first run, and repeat the Lanczos process to generate $|v_1\rangle, |v_2\rangle, ...$ and sum up the products of the vectors and $c_1, c_2, ...$.

Using the eigenvectors of the Hamiltonian, calculation of correlation functions and the static structure factor are quite similar to the calculation of the operation of $\mathcal{H}$ on a vector.

$$g^{\alpha}(r) \equiv \left\langle \sigma_0^{\alpha}\sigma_r^{\alpha} \right\rangle = \left\langle \psi_0 \right| \ \sigma_0^{\alpha}\sigma_r^{\alpha} \ \left| \ \psi_0 \right\rangle,$$

and for a translationally invariant system the structure factor is

$$G^{\alpha}(k) \equiv \sum_r \cos\left(\frac{2\pi k}{N}\right) g^{\alpha}(r).$$

3. 2. Getting an arbitrary excited state by Lanczos method

The Lanczos method applied to a Hamiltonian $(\mathcal{H})$ converges to the ground state with a very high accuracy. However, the excited states which can be obtained from the m-dimensional tridiagonal matrix have less accuracy than the ground state. Moreover, the eigenvectors of the m-dimensional tridiagonal matrix do not have the correct sequence of excited states of the Hamiltonian, since the Lanczos method converges to the extreme limit of the spectrum. The m-eigenvalues are a collection of random excited eigenvalues between the extreme limits depending on the initial random vector in the Lanczos process.

If we are interested to get an excited state close to an eigenvalue as accurare as the ground state, one can use an auxiliary operator, $\mathcal{A}$. Suppose we want to get the eigenvector close to E_t in the energy spectrum. The auxiliary operator is defined by

$$\mathcal{A} = (\mathcal{H} - E_t)^2. \qquad (25)$$

The ground state of $\mathcal{A}$ is the closest eigenvector of $\mathcal{H}$ to energy E_t. Thus, the Lanczos algorithm applied to $\mathcal{A}$ converges to an eigenstate of $\mathcal{H}$ which is close to energy E_t. It is called modified Laczos method [33] which changes the sequece of eigenstates as depicted in Fig.3.

3. 3. Finite temperature Lanczos method

As a general definition in the canonical ensemble the thermal average of a physical quantity A is defined

$$\langle A\rangle = \frac{\sum_{n=1}^{N_S}\langle n|e^{-\beta H}A|n\rangle}{\sum_{n=1}^{N_S}\langle n|e^{-\beta H}|n\rangle}, \qquad (26)$$

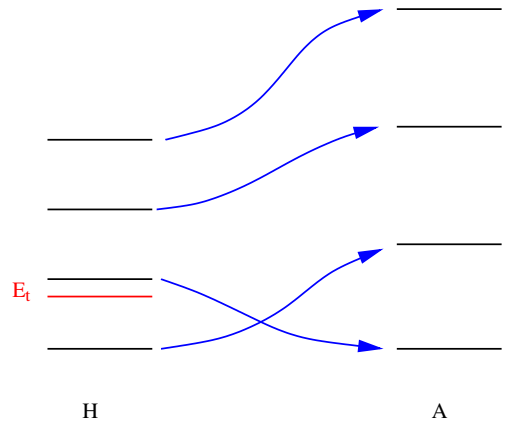

Figure 3. The sequece of spectrum in the modified Lanczos method.

where N_s is the dimension of Hilbert space, $\beta = (k_B T)^{-1}$ and $|n\rangle$ represent the bases of Hilbert space. The above equation can be rewritten in the following form by expanding the exponential (high temperature expansion)

$$\langle A\rangle = \frac{1}{Z}\sum_{n=1}^{N_s}\sum_{k=0}^{\infty}\frac{(-\beta)^k}{k!}\langle n|H^k A|n\rangle,$$

$$Z = \sum_{n=1}^{N_s}\sum_{k=0}^{\infty}\frac{(-\beta)^k}{k!}\langle n|H^k|n\rangle. \qquad (27)$$

The Lanczos process enable us to calculate $\langle n|H^k B H^l A|n\rangle$ exactly by using M-steps such as $M > k,l$; A and B are two arbitrary operators [32]. For $B=1$ and $l=0$ we get

$$\langle n|H^k A|n\rangle = \sum_{i=0}^{M}\langle n|\psi_i\rangle\langle\psi_i|A|n\rangle\varepsilon_i^k. \qquad (28)$$

Thus ,

$$\langle n|H^k A|n\rangle = \sum_{i=0}^{M}\langle n|\psi_i^{(n)}\rangle\langle\psi_i^{(n)}|A|n\rangle(\varepsilon_i^{(n)})^k. \qquad (29)$$

Note that the superscript $^{(n)}$ reminds that the eigenvectors ($|\psi_i^{(n)}\rangle$) and the corresponding eigenvalues $\varepsilon_i^{(n)}$ are obtained in the Lanczos process which starts with the initial vector $|n\rangle$. The above equation (Eq.(29)) is replaced in the high temperature expansion (Eq.(27)) which gives an exact expression for $k < M$. However, k is running from zero to infinity where we extend the result obtained in Eq.(29) for $k > M$. In this respect we get the following approximate expression

$$\langle A\rangle \simeq \frac{1}{Z}\sum_{n=1}^{N_s}\sum_{i=0}^{M}e^{-\beta\varepsilon_i^{(n)}}\langle n|\psi_i^{(n)}\rangle\langle\psi_i^{(n)}|A|n\rangle,$$

$$Z \simeq \sum_{n=1}^{N_s}\sum_{i=0}^{M}e^{-\beta\varepsilon_i^{(n)}}\langle n|\psi_i^{(n)}\rangle\langle\psi_i^{(n)}|n\rangle. \qquad (30)$$

The next step of approximation comes from the replacement of the whole sum on the full Hilbert space by a sum over some random number of states in the procedure of calculating the thermal average of a physical quantity. This step of approximation is inevitably done because the summation on the full Hilbert space is a massive time consuming procedure and causes the whole idea impossible. In this respect the thermal average of the physical quantity A is approximated by $\tilde{A}$,

$$\tilde{A} = \frac{\sum_{r=1}^{R}\langle r|e^{-\beta H}A|r\rangle}{\sum_{r=1}^{R}\langle r|e^{-\beta H}|r\rangle}, \qquad (31)$$

where R is the number of random sampling with initial states $|r\rangle$.

If $[H,A]=0$ an estimated argument for the error can be obtained by the following relation,

$$\tilde{A} = \langle A\rangle + O(\frac{1}{\sqrt{R\bar{Z}}}),$$

$$\bar{Z} = e^{-\beta E_0}\sum_{n=1}^{N_s}\langle n|e^{-\beta H}|n\rangle, \qquad (32)$$

where E_0 is the ground state energy.

Summing up, the general formula in finite temperature Lanczos method (FTLM) to get the thermal average of a physical quantity is

$$\langle A\rangle = \frac{1}{Z}\sum_{r=1}^{R}\sum_{i=0}^{M}e^{-\beta\varepsilon_i^{(r)}}\langle r|\psi_i^{(r)}\rangle\langle\psi_i^{(r)}|A|r\rangle,$$

$$Z = \sum_{r=1}^{R}\sum_{i=0}^{M}e^{-\beta\varepsilon_i^{(r)}}|\langle r|\psi_i^{(r)}\rangle|^2. \qquad (33)$$

3. 3. 1. Low temperature Lanczos method

In the previous FTLM approach, the limit of $T\to 0$ does not lead to ground state expectation value which should be the case. To solve this problem a similar approach but with one more Lanczos procedure for each sampling is proposed [3].

$$\langle A\rangle = \frac{1}{Z}\sum_{r=1}^{R}\sum_{i,j=0}^{M}e^{\frac{-\beta}{2}(\varepsilon_i^{(r)}+\varepsilon_j^{(r)})}\times$$

$$\langle r|\psi_j^{(r)}\rangle\langle\psi_j^{(r)}|A|\psi_i^{(r)}\rangle\langle\psi_i^{(r)}|r\rangle,$$

$$Z = \sum_{r=1}^{R}\sum_{i=0}^{M}e^{-\beta\varepsilon_i^{(r)}}|\langle r|\psi_i^{(r)}\rangle|^2. \qquad (34)$$

In the limit of zero temperature the above equation approaches the ground state expectation value.

$$T\to 0 \Rightarrow \langle A\rangle = \langle\psi_0|A|\psi_0\rangle. \qquad (35)$$

The price of solving this problem is to implement more RAM capacity and CPU time. However, the accuracy of this mothod is appreciable at low temperatures [35].

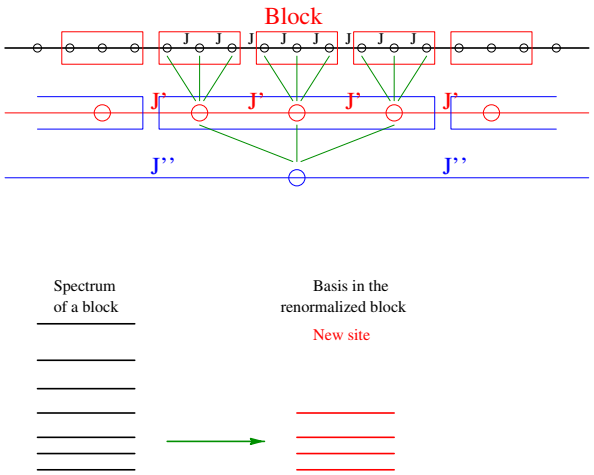

Figure 4. The block renormalization group procedure.

4. Quantum renormalization group

Quantum phase transition has been one of the most interesting topics in the area of strongly correlated systems in the last decade. It is a phase transition at zero temperature where the quantum fluctuations play the dominant role [8]. Suppression of the thermal fluctuations at zero temperature introduces the ground state as the representative of the system. The properties of the ground state may be changed drastically shown as a non-analytic behaviour of a physical quantity by reaching the quantum critical point. This can be done by tuning a parameter in the Hamiltonian, for instance the magnetic field or the amount of disorder. The study of the ground state and its energy is thus of central importance for understanding the critical behaviour of such systems.

The technique of renormalisation group (RG) has been so devised to deal with these multi-scale problems [36, 37, 38]. In the momentum space RG which is suitable for studying the continuous systems, one iteratively integrates out small scale fluctuations and renormalizes the Hamiltonian. In the real space RG, which is usually performed on the lattice systems with discrete variables (i.e quantum spin chain), an original Hamiltonian is replaced with an effective one for a lower energy subspace, iteratively. In this approach the Hamiltonian is divided into inter-block (H^{BB}) and intra-block parts (H^{B}), see Fig.4. H^{B} is diagonalized exactly and then H^{BB} is projected into the low energy subspace of H^{B} [39]. The accuracy of this method is determined by the number of states kept in the H^{B} subspace and the approach to consider the effect of neglected subspace. The Ising model in a transverse field [40] and the anisotropic Heisenberg model [41] have been studied by quantum renormalisation group (QRG) approach which gives the correct phase diagram. Moreover, the recent study on a more general model, XYZ in a transverse field, supports the power of this method to study the collective behaviour of the spin models [42].

To be concrete let us consider the Ising model in Transverse Field (ITF) [39] The Hamiltonian of ITF

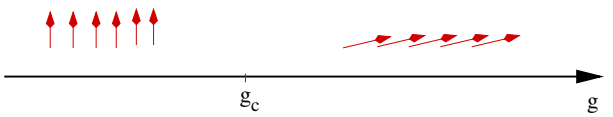

Figure 5. Two extreme limits of ITF model and its ground state configuration versus control parameter g .

model on a periodic chain of N sites is

$$H = -J[\sum_{i=1}^{N}(\sigma_i^z\sigma_{i+1}^z + g\sigma_i^x]. \qquad (36)$$

Two extreme limits give us the insight of two different phases in this model. For $g = 0$ the ground state is a ferromagnet in the z direction. However, as $g \to \infty$ the paramagnetic term is dominant and the ground state shows a paramagnet in the x direction, see Fig.5.

We have considered the two-site block with the following Hamiltonian:

$$h_I^B = -J(\sigma_{1,I}^z\sigma_{2,I}^z + g\sigma_{1,I}^x + g\sigma_{2,I}^x) \qquad (37)$$

The inter-block (H^{BB}) and intra-block (H^{B}) Hamiltonian for the two sites decomposition are

$$H^B = -J\sum_{I=1}^{N/2}(\sigma_{1,I}^z\sigma_{2,I}^z + g\sigma_{1,I}^x + g\sigma_{2,I}^x)$$

$$H^{BB} = -J\sum_{I=1}^{N/2}(\sigma_{2,I}^z\sigma_{1,I+1}^z) \qquad (38)$$

where $\sigma_{j,I}^{\alpha}$ refers to the α-component of the Pauli matrix at site j of the block labeled by l. The matrix form of h_I^B in the σ^x basis ($\sigma^x|\uparrow\rangle = |\uparrow\rangle, \sigma^x|\downarrow\rangle = -|\downarrow\rangle, \sigma^y|\uparrow\rangle = i|\downarrow\rangle, \sigma^y|\downarrow\rangle = -i|\uparrow\rangle$) is

$$h_I^B = -J\begin{pmatrix} 2g & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & -2g \end{pmatrix}$$

The exact treatment of this Hamiltonian leads to four distinct eigenvalues. The ground state, first, second and third excited state energies have the following expressions in terms of the coupling constants.

$$|\psi_0\rangle = \frac{1}{\sqrt{1+q^2}}(|\uparrow\uparrow\rangle - q|\downarrow\downarrow\rangle) \quad , \quad e_0 = -J\sqrt{4g^2+1}$$

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \quad , \quad e_1 = -J$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad , \quad e_1 = J$$

$$|\psi_4\rangle = \frac{1}{\sqrt{1+p^2}}(|\uparrow\uparrow\rangle + p|\downarrow\downarrow\rangle) \quad , \qquad (39)$$

$$e_4 = J\sqrt{4g^2+1}$$

where q, p are

$$q = \sqrt{4g^2+1} - 2g \quad , \quad p = -(\sqrt{4g^2+1} + 2g). \tag{40}$$

The effective (renormalized) Hamiltonian in first order RG approximation is

$$H^{eff} = H_0^{eff} + H_1^{eff}. \tag{41}$$

One can consider higher order RG treatment. As an example, the second order RG treatment of XXZ model can be found in Ref.[43,44]. The effective Hamiltonians are expressed by the following relations in terms of projcetion operator.

$$H_0^{eff} = P_0 H^B P_0 \quad , \quad H_1^{eff} = P_0 H^{BB} P_0 \quad . \tag{42}$$

The first order projection operator is

$$P_0 = |\psi_0\rangle\langle\psi_0| + |\psi_1\rangle\langle\psi_1|. \tag{43}$$

To get the effective Hamiltonian we need to know the projection of each operators in the renormalized space

$$P_0^I \sigma_{1,I}^z P_0^I = \frac{1+q}{\sqrt{2(1+q^2)}} \sigma_I^z \ ,$$

$$P_0^I \sigma_{2,I}^z P_0^I = \frac{1+q}{\sqrt{2(1+q^2)}} \sigma_I^z \ ,$$

$$P_0^I \sigma_{1,I}^z \sigma_{2,I}^z P_0^I = \frac{(1+q)^2}{2(1+q^2)} - \frac{(1-q)^2}{2(1+q^2)} \sigma_I^x ,$$

$$P_0^I \sigma_{1,I}^x P_0^I = \frac{1-q^2}{2(1+q^2)} (1+\sigma_I^x),$$

$$P_0^I \sigma_{2,I}^x P_0^I = \frac{1-q^2}{2(1+q^2)} (1+\sigma_I^x). \tag{44}$$

Based on the above equations the projection of block Hamiltonian and inter-block Hamiltonian are as the following

$$P_0^I h_I^B P_0^I = -J\{[\frac{(1+q)^2}{2(1+q^2)} 1 - \frac{(1-q)^2}{2(1+q^2)} \sigma_I^x] + g \frac{1-q^2}{(1+q^2)} (1+\sigma_I^x)\},$$

$$P_0^{I+1} P_0^I (h_{I,I+1}^{BB}) P_0^I P_0^{I+1} = -J\{(\frac{1+q}{\sqrt{2(1+q^2)}})^2\} \sigma_I^z \sigma_{I+1}^z. \tag{45}$$

The effective Hamiltonian for $N/2$ sites is given by the self-similar Hamiltonian

$$H = -J'[\sum_{i=1}^{N} (\sigma_i^z \sigma_{i+1}^z + g' \sigma_i^x], \tag{46}$$

where the renormalized coupling constants are given by the following equations,

$$J' = J \frac{(1+q)^2}{2(1+q^2)},$$

$$g' = 2g \frac{1-q^2}{(1+q^2)} - \frac{(1-q)^2}{(1+q)^2}. \tag{47}$$

The exchange coupling J which is an overall factor defines the scale of energy. However, the control parameter g determines the ground state property of the model. The fixed points, $g' = g \equiv g^*$ are two types. $g^* = 0$ and $g^* = \infty$ are stable fixed points and define two stable phases ferromaget and paramagnet, respectively. The unstable fixed point $g^* \simeq 1.27 \equiv g_c$ is the quantum critical point which divides two different ferromagnet and paramagnet behvaiour. The value of $g_c \simeq 1.27$ is different from the exact result $g_c^{exact} = 1$ which can be obtained by the Jordan-Wigner transformation of the ITF model to free fermions. This difference is originated from the quantum RG approximation which is related to the finite number of sites in the block (in our case $n_B = 2$), the finte number of states kept in the projection operator (two from four in our case) and the boundary condition which is adopted for the block. However, the quantum RG gives the correct qualitative picture of the phase diagram. One can also obtain the critical exponents using quantum RG [39]. The effect of boundary conditions and an improvement of quantum RG, the density matrix renormalization group (DMRG) can be found in Ref.[45, 46].

We can combine the idea of renormalization group and quantum information theory. It can be shown how the entanglement or concurrence evolve as the size of the system being large, i.e. the finite size scaling is obtained. Moreover, It introduces how the renormalization group approach can be implemented to obtain the quantum information properties of a many body system. We have obtained the concurrence as a measure of entanglement, its derivatives and their scaling behavior versus the size of system for the one dimensional Ising model in transverse field [47] and the anisotropic spin 1/2 Heisenberg model [48]. We have found that the derivative of concurrence between two blocks each containing a fraction of the system size diverges at the critical point with the exponent which is directly associated with the divergence of the correlation length.

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