# Numerical methods for quantum magnets

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Methods for studies on quantum magnets are overviewed. In the classical picture, spin can be regarded as a vector of magnetic moment. But, various interesting properties due to the quantum effects have been studied as the so-called 'quantum spin systems'[1]. Quantum mechanical effect in spin systems is originated in the non-commutative property of spin operators: $[S_x, S_y] = i\hbar S_z$ , etc. In order to take into account the quantum effect, we need to treat the Hamiltonian matrix $\mathcal{H}$ of the system whose matrix is of $2^N$x$2^N$ for a system consisting of $N$ spins of $S$=1/2. The straightest way to study the system is a diagonalization method to obtain the eigenvalues and eigenvectors of the matrix. To study finite temperature properties, we calculate Tr exp($-\beta\mathcal{H}$), and we need all the eigenvalues and eigenvectors[2]. However, often we are interested in low temperature properties of the system, in particular the ground system. There, we may use iterative methods for the low energy states, such as the Lanczos method. For such purpose, TIT-pack was released[3], which encouraged studies in this field in Japan, and several method to extrapolate the data has been developed.[4]. But, the system size is still limited.

To study a large system a quantum Monte Carlo (QMC) method by making use of the Suzuki-Trotter method[5] has been introduced. This method has been developed with the idea of the loop algorithm and the continuous imaginary time algorithm[6], and methods to take into account effects of lattice distortion have been also developed. Now QMC is the one of the most reliable methods for quantum many body systems. However, the method consists of a sampling of the so called world lines (paths in the path-integral method) [7], and suffers from the so-called 'negative sign' problem, and cannot be applied to frustrated system efficiently.

As an efficient method to study large systems in one dimension (1D), the so-called DMRG (density matrix renormalization group) method was invented[8]. The idea of this method has been developed and is now one of the most powerful method for 1D systems. This method is extended to higher dimensions[9] also to finite temperatures. The similar idea has been introduced as the matrix-product method[10], and recently it has been studied extensively as tensor-network methods.[11]

Magnetic resonance is also an important subject of the study of magnetism. The ESR spectrum is given by Kubo formula. As a microscopic approach, a direct calculation of the formula by making use of full diagonalization has been introduced[12], which gives precise information of the spectrum for given systems, e.g., the effect of spatial configuration of the lattice, the dependence on the field direction. Application of this method is also limited to small sizes because it uses diagonalization of the system Hamiltonian. For the ESR spectrum in the ground state, we may use the idea of Lanczos method, and also DMRG (dynamical DMRG)[13,14]. For finite temperatures we can make use of the time evolution of the so-called typical state.[15,16,17] The field and temperature dependent in 1D systems has been studied bay making use of field theoretical informations[18]. The typical state would give a seminal method to give temperature dependent thermal properties[17].

Moreover quantum dynamics is also an important issue in quantum magnets. The dynamics of magnetization under time dependent field reflects the energy level structure of the system. Such effect was observed in single molecular magnets (SMM) such as Mn12, Fe8, and V15, etc. [19] The importance of the Landau-Zener process was pointed out.[20] The dynamics in dissipative environments is treated by the quantum master equation[21]. The combination of quantum dynamics and dissipative effects provides interesting phenomena, such as the phonon-bottleneck effect or magnetic Foehn effect[22]. Recently the hybridization between magnetic state and photon state in a cavity attracts interests in the context of manipulation of quantum state. The quantum master equation is also used to emulate such quantum dynamics[23]. In quantum systems, the so-called quantum fluctuation plays an important role. By making this fact, the so-called quantum annealing method was invented[24]. This method is used in a quantum computing of the D-wave machine.[25]

With the development of super-computer such as the K-computer, massive parallel algorithm allows us to use a large memory. Such technique has been established, and now systems with more than 40 spins ($S$=1/2), can be calculated.[26) ] Recently the system ALPS is released for non-specialists, in which some of the above methods are prepared in user-friendly way[27)].


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