# Monte Carlo Calculation of Elementary Excitation of Spin Chains

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An efficient Monte Carlo method is proposed to calculate the elementary excitation spectrum of quantum systems. The lowest energy with arbitrary momentum is obtained by the projector Monte Carlo method. This is applied to the spin-$\frac{1}{2}$ and -1 Heisenberg antiferromagnetic chains with length 32. For the $S=\frac{1}{2}$ case, the spectrum coincides completely with that of des Cloiseaux and Pearson. For the $S=1$ case, the spectrum has a gap at momentum $\pi$ as was predicted by Haldane. The value of the gap coincides with the calculation of Nightingale and Blote. The spectrum satisfies a variational relation with the structure factor.

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For the calculation of quantum systems the exact diagonalization method is used in many cases. But in this method the size of the system is very restricted. So quantum Monte Carlo methods are used for larger systems. The partition function approach is used widely for finite temperature properties.[1] On the other hand, the projector Monte Carlo (PMC) method[2-5] is also powerful especially for the investigation of the ground state. The Green's-function Monte Carlo method[6] can be regarded as a kind of PMC method.

We assume that all the off-diagonal elements of the Hamiltonian $H$ are zero or negative. Then all the elements of the ground-state wave vector have the same sign. The ground state is represented by a distribution of random walkers. In many cases the Hamiltonian $H$ has translational symmetry and there is the translation operator $T$ which satisfies

$$HT=TH, \quad T^N=I, \tag{1}$$

where $N$ is the length of the system. All the eigenvectors of $H$ can be classified by the momentum $K$:

$$\begin{aligned} &H|l;K\rangle=E_l(K)|l;K\rangle, \quad T|l;K\rangle=e^{iK}|l;K\rangle, \\ &K=2\pi k/N, \quad k=0,1,2,\ldots,N-1, \\ &E_1(K)\le E_2(K)\le\cdots, \end{aligned} \tag{2}$$

where $|l;K\rangle$ and $E_l(K)$ are the $l$th eigenvector and eigenvalue in $K$-momentum states. Usually the ground state of $H$ belongs to the subspace $K=0$. If one can calculate the lowest-energy eigenvalue for a given momentum, it is just the elementary excitation. The exact diagonalization method can calculate the elementary excitation spectrum of small systems. But no one has succeeded in calculating the elementary excitation spectrum by the Monte Carlo method.

In the PMC method the ground-state energy is given by the following formula:

$$E_1(0)=\lim_{\tau\to\infty}\frac{\langle\psi_0|He^{-\tau H}|\xi_0\rangle}{\langle\psi_0|e^{-\tau H}|\xi_0\rangle}, \tag{3}$$

where $|\xi_0\rangle$ and $\langle\psi_0|$ are some arbitrary vectors. If $|\xi_0\rangle$ and $\langle\psi_0|$ are states with momentum $K$, we will have the lowest-energy eigenvalue of momentum $K$. The operator $e^{-\tau H}$ serves as a projector to the lowest-energy states with momentum $K$. So it may be possible to get the excitation spectrum in the PMC method. One choice of $\langle\psi_0|$ and $|\xi_0\rangle$ with momentum $K$ is as follows:

$$\langle\psi_0|=\langle\psi|R(-K), \quad |\xi_0\rangle=R(K)|0;1\rangle. \tag{4}$$

Here $\langle\psi|$ is the vector whose elements are all 1 and $R(K)$ is a diagonal operator which satisifies

$$TR(K)=e^{iK}R(K). \tag{5}$$

As $|0;1\rangle$ and $\langle\psi|$ are zero-momentum states, $|\xi_0\rangle$ and $\langle\psi_0|$ are $K$-momentum states. Corresponding to Eq. (3) we should consider the following function:

$$B(K,\tau)=\frac{\langle\psi|R(-K)He^{-\tau H}R(K)|0;1\rangle}{\langle\psi|R(-K)e^{-\tau H}R(K)|0;1\rangle}. \tag{6}$$

The function $B(K,\tau)$ should approach the lowest-energy eigenvalue of momentum $K$ unless $\langle\psi_0|$ and $|\xi_0\rangle$ are orthogonal to this state. In the PMC method $|0;1\rangle$ is given as a distribution of walkers. As $R(K)$ is a diagonal operator, each walker has a value of $R(K)$. After time $\tau$ it should be multiplied by a new $R(-K)$.

Hereafter we restrict ourselves to the Heisenberg antiferromagnetic chain (HAC):

$$\begin{aligned} &\tilde{H}=J\sum_{i=1}^{N}S_i^xS_{i+1}^X+S_i^yS_{i+1}^y+S_i^zS_{i+1}^z, \\ &\mathbf{S}_{N+1}=\mathbf{S}_1, \quad N=\text{even}. \end{aligned} \tag{7}$$

This commutes with the true translation operator $\tilde{T}$ ($\tilde{T}\mathbf{S}_l=\mathbf{S}_{l+1}$) and the total spin in the $z$ direction $S^z=\sum_l S_l^z$. In the PMC calculation of spin systems a walker is represented by a set of $z$-component spin values on $N$ sites:

$$(s_1^z,s_2^z,\ldots,s_N^z), \quad s_l^z=S,S-1,\ldots,-S. \tag{8}$$

In this representation off-diagonal elements of $\tilde{H}$ are non-negative. By making the unitary transformation $U$

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$=\exp(\pi i \sum_{l=\text{even}} S^z)$, Eq. (7) and $\tilde{T}$ become as follows:

$$H = U\tilde{H}U^{-1} = \sum_{l=1}^{N} h_l , \tag{9a}$$

$$h_l = J(-S_l^x S_{l+1}^x - S_l^y S_{l+1}^y + S_l^z S_{l+1}^z) ,$$

$$T = U\tilde{T}U^{-1} = \exp[\pi i (NS - S^z)]\tilde{T} . \tag{9b}$$

Then all the off-diagonal elements of $H$ become nonpositive and the PMC method is applicable. It should be noted that the true momentum shifts by $\pi$ from $K$, if $NS - S^z$ is odd. To get the ground-state energy we use Eq. (3). At the beginning of the calculation $|\xi_0\rangle$ is approximated by a set of $L$ random walkers and the weights of the walkers are assumed to be the same. The wave function is approximated by

$$e^{-\tau H}|\xi_0\rangle = \sum_{i=1}^{L} w(i,\tau)\,|i,\tau\rangle . \tag{10}$$

Here $|i,\tau\rangle$ and $w(i,\tau)$ are the $i$th walker and its weight at time $\tau$.

The calculation of the ground-state wave function is done by the following two processes:

*(1) Operation of $\exp(-\Delta\tau H)$ for walkers.*—Here $\Delta\tau$ is some small time interval. Repeating this we get $e^{-\tau H}$. The operator $\exp(-\Delta\tau H)$ is approximated by

$$[\exp(-\Delta\tau H_1/2r)\exp(-\Delta\tau H_2/r)\exp(-\Delta\tau H_1/2r)]^r , \tag{11a}$$

$$H_1 = \sum_{l=\text{even}} h_l , \quad H_2 = \sum_{l=\text{odd}} h_l . \tag{11b}$$

The matrix $\exp(-\Delta\tau H_1/2r)$ is decomposed to a product of a stochastic matrix and a diagonal matrix:

$$\{\exp(-\Delta\tau H_1/2r)\}_{lj} = p_{lj} q_j , \quad \sum_l p_{lj} = 1 . \tag{12}$$

The operation of the diagonal matrix multiplies the weight by $q_j$. The stochastic matrix $\{p_{lj}\}$ makes a jump from $j$ to $l$ with probability $p_{lj}$. The spin configuration of a walker is changed by this process. As $H_1$ is decomposed into $N/2$ pairs, the change of spin configuration is done for each spin pair. The operations of $\exp(-\Delta\tau H_2/r)$ are also done in the same way.

*(2) Reconfiguration of weights.*—As time proceeds some walkers become very heavy and the others very light. We should make a new set of walkers so that the existence probability is proportional to the weight in the old set:

$$e^{-(\tau+0)H}|\xi_0\rangle = \sum_i^L a\,|i,\tau+0\rangle , \quad a = \sum_{l=1}^{L} w(l,\tau)/L , \tag{13a}$$

$$|i,\tau+0\rangle = |j(i),\tau\rangle . \tag{13b}$$

Here $j(i)$ should be determined by

$$h(j-1) \le i - \alpha < h(j) , \quad h(j) \equiv \sum_{i=1}^{j} w(i,\tau)/a , \tag{13c}$$

where $\alpha$ is a random number between 0 and 1. So, light walkers are eliminated and heavy walkers breed. The total number of walkers is the same. A walker $l$ after the reconfiguration has an ancestor $j(l)$ before the reconfiguration. The necessity of a reconfiguration process was pointed out by Hetherington.[3] We sometimes do the reconfiguration process when the variance of weights becomes large.

By repeating the above processes many times we get an approximate ground-state wave function:

$$|0;1\rangle = \lim_{\tau'\to\infty} \sum_{i=1}^{L} |i,\tau'\rangle \tilde{w}(i,\tau') ,$$

$$\tilde{w}(i,\tau') \equiv w(i,\tau') \Big/ \sum_l w(l,\tau') , \tag{14}$$

where $\tilde{w}$ is the normalized weight. Taking the long-time average with respect to $\tau'$ we have a more accurate wave function. From Eq. (3) $E_1(0)$ is

$$E_1(0) = \sum_{\tau'} \sum_{i=1}^{L} \langle\psi|H|i,\tau'\rangle \tilde{w}(i,\tau') \Big/ \sum_{\tau'} 1 . \tag{15}$$

To calculate Eq. (6) we adopt the following operator as $R(K)$:

$$R(K) = \sum_{l=1}^{N} (S_l^z - S)\exp(iKl) . \tag{16}$$

Apparently this is diagonal and satisfies (5). The $i$th walker at time $\tau_1$ has the $j$th walker at time $\tau_2$ as its ancestor. We call $j(i;\tau_1,\tau_2)$ the *ancestor function.* It satisfies

$$j(i;\tau_1,\tau_3) = j(j(i;\tau_1,\tau_2);\tau_2,\tau_3), \quad \tau_1 > \tau_2 > \tau_3 . \tag{17}$$

The ancestor function can be constructed by successive substitution of $j(i;\tau,\tau-\Delta\tau)$. The wave function $e^{-\tau H} \times R(K)\,|0;1\rangle$ is represented as follows:

$$\lim_{\tau'\to\infty} \sum_{i=1}^{L} \tilde{w}(i,\tau') R(j(i;\tau',\tau'-\tau),K,\tau'-\tau)\,|i,\tau'\rangle , \tag{18}$$

where $R(i,K,\tau') \equiv \langle i,\tau'|R(K)|i,\tau'\rangle$. Taking the average with respect to $\tau'$ we have a more accurate wave function. Then $B(K,\tau)$ defined in (6) becomes

$$\frac{\sum_{\tau'}\sum_{i=1}^{L}\langle\psi|R(-K)H|i,\tau'\rangle\tilde{w}(i,\tau')R(j(i;\tau',\tau'-\tau),K,\tau'-\tau)}{\sum_{\tau'}\sum_{i=1}^{L}\tilde{w}(i,\tau')R(i,-K,\tau')R(j(i;\tau',\tau'-\tau),K,\tau'-\tau)} . \tag{19}$$

So we can calculate $B(K,\tau)$ by a small modification of the ground-state energy calculation. We only need to store the complex value $R(i,K,\tau')$ for each walker $i$ and ancestor function $j(i;\tau',\tau'-\Delta\tau)$. Very old data of these quantities are not needed because we do not calculate $B(K,\tau)$ at very large $\tau$.

Here we show some results of our calculation for $S^z = 0$.

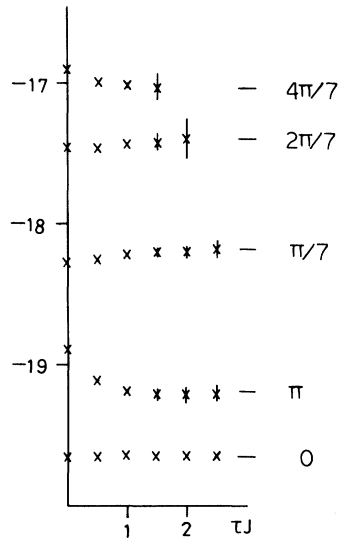


FIG. 1. Function $B(K,\tau)/J$ for $N=14$, $S=1$ HAC at $K=0$, $\pi/7$, $2\pi/7$, $4\pi/7$, and $\pi$. $E_1(K)/J$ values are plotted as horizontal bars (Ref. 7). MC results and exact diagonalization results are compared. The coincidence of $E_1(K)$ and $B(K,\tau)$ at $\tau J=1$–2 is very good. But the statistical error grows exponentially as $\tau$ becomes large..

*(A) HAC with $S=1$, $N=14$.*—For this system the results of the exact diagonalization method are given in Ref. 7. In Fig. 1, $B(K,\tau)$ is plotted for $K=0$, $\pi/7$, $2\pi/7$, $4\pi/7$, and $\pi$. In the case $K=0$ it is very stable and gives the ground-state energy. For other momenta the error bar increases exponentially as $\tau$ increases. But $B(K,\tau)$ approaches $E_1(K)$ even at $\tau J=1$–2. We put $L=4096$, $\Delta\tau=0.5/J$, and $r=8$. We take the time average over $6000\Delta\tau$.

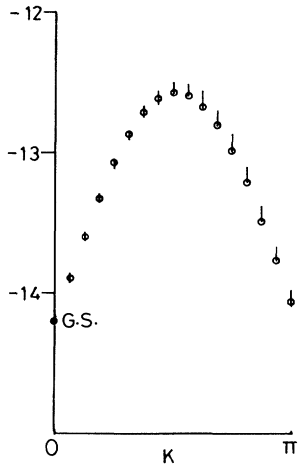


FIG. 2. $E_1(K)/J$ for $N=32$, $S=\frac{1}{2}$ HAC. Circles are results of the Bethe-*Anstaz* equation (Ref. 8). Bars are results of the MC calculation. Length of the bar represents error of MC calculation.

TABLE I. Estimated values of $-E_1(K)/J$ of $S=\frac{1}{2}$ and 1 HAC with $N=32$. For $S=\frac{1}{2}$, the exact value is calculated by the Bethe-*Ansatz* equation in Ref. 8. The agreement is very good. For $S=1$, the value 44.45 at $k=16$ should be compared with $-$(lowest energy)$/J$ in $S^z=1$ subspace. According to NB (Ref. 5) it is 44.4364(40).

| | $S=\frac{1}{2}$ | | $S=1$ |
|---|---|---|---|
| $k$ | Estimated | Bethe-*Ansatz* | Estimated |
| 0 | 14.202(1) | 14.2065 | 44.875(3) |
| 1 | 13.891(30) | 13.8953 | 43.93(16) |
| 2 | 13.595(28) | 13.5972 | 43.56(12) |
| 3 | 13.314(34) | 13.3204 | 43.18(11) |
| 4 | 13.061(44) | 13.0753 | 42.84(12) |
| 5 | 12.852(59) | 12.8712 | 42.55(14) |
| 6 | 12.698(77) | 12.7159 | 42.35(16) |
| 7 | 12.572(95) | 12.6153 | 42.23(18) |
| 8 | 12.52(11) | 12.5732 | 42.22(19) |
| 9 | 12.55(11) | 12.5913 | 42.26(19) |
| 10 | 12.61(11) | 12.6688 | 42.42(18) |
| 11 | 12.748(92) | 12.8026 | 42.67(16) |
| 12 | 12.923(77) | 12.9876 | 42.99(15) |
| 13 | 13.163(62) | 13.2165 | 43.38(14) |
| 14 | 13.442(52) | 13.4804 | 43.81(15) |
| 15 | 13.740(49) | 13.7688 | 44.22(19) |
| 16 | 14.053(82) | 14.0683 | 44.46(36) |

*(B) HAC with $S=\frac{1}{2}$, $N=32$.*—This system is too big for exact diagonalization. But we can calculate $E_1(K)$ by solving numerically the Bethe-*Ansatz* equation as was done by des Cloiseaux and Pearson.[8] The results of the PMC and the Bethe-*Ansatz* are shown in Fig. 2 and Table I.

*(C) HAC with $S=1$, $N=32$.*—It is expected that the system has an energy gap.[9] Nightingale and Blote[5] (NB) determined the lowest energy of $S^z=0$, 1, and 2 using the PMC method. In Table I we show $E_1(K)$ obtained by our method. In Fig. 3 it is compared with the upper bound calculated in Ref. 10. $E_1(0)$ is the ground-state energy and $E_1(\pi)$ is the first excited energy. The value of $E_1(\pi)$, $-44.45(36)J$, coincides with NB's lowest energy, $-44.4364(40)J$, in $S^z=1$ subspace. The energy gap is about $0.4J$. It is noteworthy that the spectra for the $S=\frac{1}{2}$ and 1 cases are completely different. The former has the shape $c|\sin k|$, while the latter has the shape $c(\sin^2 K+\xi^{-2})^{1/2}$ as was proposed in Ref. 10. From Fig. 3 we find that spectrum is asymmetric about the axis $K=\pi/2$. So this is not correct in detailed points. It seems that the gap at $K=0$ is twice of that at $K=\pi$:

$$\lim_{K\to 0}[E_1(K)-E_1(0)]=2[E_1(\pi)-E_1(0)]. \qquad (20)$$

This may be explained by regarding the low-momentum excited state as a scattering state of two excitations with momenta near $\pi$.

In summary I have proposed a new Monte Carlo method which calculates the excitation energy as a func-

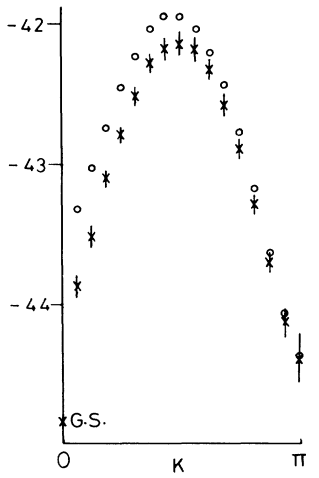


FIG. 3. $E_1(K)/J$ for $N=32$, $S=1$ HAC. The spectrum has a gap at $K=\pi$. The value of the gap is about $0.4J$ and coincides with NB's calculation. Small circles are the upper bound of $E_1(K)/J$ given in Ref. 10. This upper bound was calculated from the structure factor and variational relation.

tion of momentum. This method may be generalized if the Hamiltonian has some other symmetry.[11] We are able to get the lowest-energy state in each subspace if an appropriate diagonal operator is found. By this method elementary excitation spectra of the $N=32$ HAC with spin $\frac{1}{2}$ and 1 are obtained. The exact diagonalization method is almost impossible for such long chains. The result of the $S=\frac{1}{2}$ case agrees with the theory of des Cloiseaux and Pearson.[8] In the $S=1$ case the spectrum of elementary excitations has an energy gap. The energy gap is about $0.4J$. This agrees with Haldane's prediction[9] and NB's numerical calculation.[5] This excitation spectrum satisfies the variational relation with the structure factor $S(K)$ as shown in Fig. 3.

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