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RELATION BETWEEN ISOTROPIC HEISENBERG MODELS AND SYMMETRIC GROUP

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*Institute of Theoretical Physics, University of Wroclaw, Poland.

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Соотношение между изотропными моделями Гейзенберга и симметрической группой

Найдена связь между изотропными моделями Гейзенберга и неприводимыми представлениями симметрической группы. На основе этого результата может быть получен любой гамильтониан Гейзенберга в квазидиагональном виде. Предложен класс простых "обрезанных" моделей Гейзенберга, у которых сохраняется много свойств точных гамильтонианов Гейзенберга.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1978

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Relation Between Isotropic Heisenberg Models and Symmetric Group

Using the relation between symmetric group and isotropic Heisenberg Hamiltonian, we propose the quasidiagonal form of this Hamiltonian. The class of the model Hamiltonians is proposed and the properties of these models are illustrated by the example of a one-dimensional Heisenberg model.

The investigations has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1978

Introduction.

It is well known that the problem of exact calculation of the thermodynamic quantities for quantum spin models is notoriously complicated. There exists huge literature devoted to both exact and approximate methods of solving this problem [6].

Even in rather special classical problem of solving the isotropic Heisenberg model the progress is really small, despite a great effort made in this field. Thus, it remains worthwhile to study simple models, still containing most important properties of realistic models.

In this paper we propose the class of such "restricted" models following from the relation between the isotropic Heisenberg Hamiltonian for spin 1/2 and the irreducible representations of the symmetric group S_N. This allows to reduce the Hamiltonian of the Heisenberg model to a quasidiagonal form. We believe that the discovered relation between the Heisenberg models and the symmetric group, opens a new possibility for such a classical field of studies.

It seems that the above-mentioned relation is simply a mathematical formulation of the basic ideas underlying this model.

1.Isotropic Heisenberg Hamiltonians.

In this section we shall derive the relation between the isotropic Heisenberg model and the symmetric group S_N.

The isotropic Heisenberg Hamiltonians for spin 1/2 have the following form

$$H = -\sum_{\dots} \tfrac{1}{4} J_{ij} \left(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z\right), \qquad /1/$$

where $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, are the Pauli matrices and summation depends on the considered model.

We can rewrite the operator $\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z$ in the form

$$\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z = 2\left[\tfrac{1}{2}\left(\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z + 1\right)\right] - 1 =$$
$$= 2\, P_{ij} - 1 . \qquad /2/$$

The matrices P_{ij} have many interesting and nice properties

i/ All P_{ij} have the dimensionality 2^N./N is the number of sites/

ii/Their elements are equal to either 0 or 1.

iii/In each row and column there is only one element not equal to 0.

iv/ $\mathrm{Tr}\, P_{ij} = 2^{N-1}$

v/ $P_{ij}^2 = 1$

vi/ $P_{ij} A_i P_{ij} = A_j$, where $A_k = 1_1 \otimes \cdots \otimes 1_{k-1} \otimes \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \otimes 1_{k+1} \otimes \cdots \otimes 1_N$

$$1_i = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_i \qquad \alpha, \beta, \gamma, \delta \in \mathbb{C} .$$

From the properties v/ and vi/ it follows,that to each matrix there corresponds a permutation p_{ij}

$$P_{ij} \Longleftrightarrow \begin{pmatrix} 1 & 2 & 3 & \cdots & i & \cdots & j & \cdots & N \\ 1 & 2 & 3 & \cdots & j & \cdots & i & \cdots & N \end{pmatrix} = p_{ij} . \qquad /3/$$

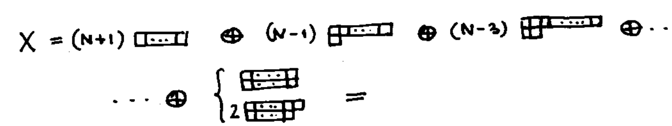
The permutations p_{ij} /so-called transpositions/ are the generators of the group of permutations of N elements S_N.

Thus,the P_{ij} matrices generate a reducible representation X of the symmetric group S_N.

The Hamiltonian /1/ expressed in terms of P_{ij}

$$H = -\sum_{\dots} \tfrac{1}{2} J_{ij} P_{ij} + \sum_{\dots} \tfrac{1}{4} J_{ij} \mathbf{1} \qquad /1a/$$

is a linear combination of the S_N-group elements in the X-representation.This X-representation can be reduced by the use of standard methods [3,4]



$$= \sum_{k=0}^{[\frac{N}{2}]} (N-2k+1)\, [N-k, k] \qquad [\tfrac{N}{2}] = \begin{cases} \frac{N-1}{2} & N \text{ odd} \\ \frac{N}{2} & N \text{ even} . \end{cases} \qquad /4/$$

Formula /4/ is a proposal,we are able to check its validity up to $N \leqslant 12$.However,one can show that the dimensionality of X is the sum of the dimensionalities of r.h.s. representations in /4/

$$\dim X = 2^N = \sum_{k=0}^{[\frac{N}{2}]} (N-2k+1) \dim [N-k, k] = \qquad /5/$$
$$= \sum_{k=0}^{[\frac{N}{2}]} (N-2k+1) \frac{N!\,(N-2k+1)}{(N-k+1)!\,k!} .$$

Since every term of Hamiltonian /1a/ reduces to the quasidiagonal form, we obtain the Hamiltonian /1a/ in a quasidiagonal form.

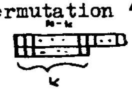
The problem of diagonalization of the Heisenberg Hamiltonians as well as the evaluation of the partition function is still not solved. We have shown that using the Trotter formula [2] and the transfer matrix method [5,6] the above problems can be reduced to finding the maximal eigenvalue of some matrix, which is the function of P_{ij}. Thus, from Eq./4/ it follows that only one of the r.h.s. irreducible representations plays the essential role. Unfortunately, it is not known which one.

Summing up, every isotropic Heisenberg Hamiltonian may be reduced to the quasidiagonal form

$$H = \bigoplus_{k=0}^{[\frac{N}{2}]} H_k (N-2k+1), \qquad /6/$$

where

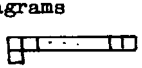
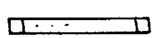
$$H_k = -\sum_{\dots} \tfrac{1}{2} J_{ij} P_{ij}^{k} + \sum_{\dots} \tfrac{1}{4} J_{ij} 1 ,$$

P_{ij}^{k} are the representatives of permutation p_{ij} in the irreducible representation $[N-k,k] \equiv$  .

2. Restricted Heisenberg models

The problem of calculation of the thermodynamic functions is a very complicated task. For this reason we shall study simplified models, which still contain many properties of real Heisenberg models.

From the set of irreducible representations in Eq./4/ the most simple are those connected with the following Young diagrams

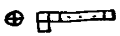
 $= [N-1,1]$ and  $= [N]$

For these representations the Hamiltonian /1a/ may be diagonalized, and thus, some of the energy eigenstates of the Heisenberg Hamiltonian can be derived.

The Heisenberg models limited to those representations shall be called the restricted models. Singularities which will appear in such models will also appear in the familiar models, although the critical indices could differ.

For illustration, let us consider the isotropic one-dimensional restricted Heisenberg model with the following Hamiltonian

$$H = -\frac{J}{2} \sum_{i=1}^{N} P_{i\,i+1} + \frac{1}{4} J N 1 \qquad P_{N,N+1} \equiv P_{1N} . \qquad /7/$$

The representation which is the sum of  $\oplus$  is of the dimensionality N, and it is isomorfic to the natural permutation representation of S_N.

Since the matrix $P_{i\,i+1}$

$$P_{i\,i+1} = \begin{array}{c} \qquad\quad i \;\; i+1 \\ \begin{pmatrix} 1 & 0 & \cdots & & & 0 \\ 0 & 1 & \cdots & & & \vdots \\ \vdots & & \ddots & & & \\ & & & 0 & 1 & \\ & & & 1 & 0 & \\ & & & & & 1 \\ & & & & & & \ddots \\ 0 & & \cdots & & & & 1 \end{pmatrix} \end{array} \qquad /8/$$

corresponds to the transposition $p_{i\,i+1}$, the restricted Hamiltonian /7/ takes the form

$$H = -\frac{J}{2} \begin{pmatrix} 0 & 1 & 0 & \cdots & & 0 & 1 \\ 1 & 0 & 1 & \cdots & & & 0 \\ 0 & 1 & 0 & 1 & \cdots & & 0 \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ & & & & 1 & 0 & \\ 0 & & & & 1 & 0 & 1 \\ 1 & 0 & \cdots & & 0 & 1 & 0 \end{pmatrix} - \frac{J}{4} N 1 + J 1 \qquad /9/$$

The Hamiltonian /9/ can also be written as

$$H = -\frac{J}{2}\left(T + T^{-1}\right) - \left(\frac{J}{4}N - J\right)\mathbb{1}\,, \qquad /10/$$

where T is the matrix corresponding to the permutation

$$T \Longleftrightarrow \begin{pmatrix} 1 & 2 & 3 & \dots & N \\ 2 & 3 & 4 & \dots & 1 \end{pmatrix}.$$

The permutation T obeys the relation

$$T^N = \mathbb{1}\,. \qquad /11/$$

Thus,all of the eigenvalues of the Hamiltonian /7/ are of the form

$$\lambda_k = -J\cos\frac{2\pi k}{N} - \frac{J}{4}N + J \qquad /12/$$

$$k = 0, 1, 2, \dots, N-1\,.$$

Let us study the partition function Z and internal energy E

$$Z = \mathrm{Tr}\, e^{-\beta H} = e^{\beta J\left(\frac{N}{4} - 1\right)} \sum_{k=0}^{N-1} e^{\beta J\cos\frac{2\pi k}{N}}\,, \qquad /13/$$

$$E = -\frac{\partial}{\partial\beta}\ln Z\,.$$

In the thermodynamic limit $N \to \infty$ for the internal energy and the specific heat C_v , we obtain,

$$E = -\frac{1}{4}J + J e^{-\beta J}\left(I_0 - I_1\right) \qquad /14/$$

$$\beta = \frac{1}{kT}$$

$$C_v = \frac{\partial E}{\partial T} = k(\beta J)^2 e^{-\beta J}\left(\frac{3}{2}I_0 - 2I_1 + \frac{1}{2}I_2\right) \qquad /15/$$

$$I_k = \frac{1}{\pi}\int_0^{\pi} \cos kx\, e^{\beta J\cos x}\, dx\,,$$

where I_k are the Bessel functions of imaginary argument [7] . Our results for E and C_v are shown in Fig.1 and compared with both results for Ising model and Bonner and Fisher results for Heisenberg model for 11 sites [1] .

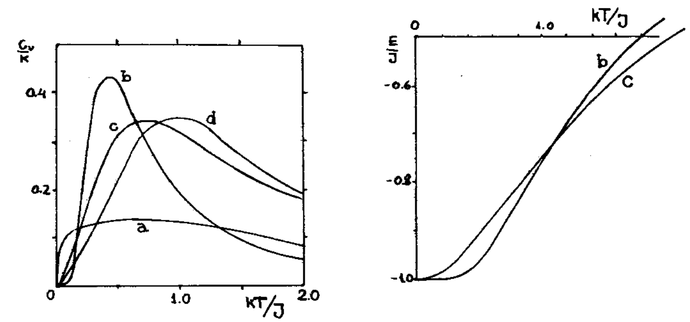


Fig.1
Comparision of specific heats and internal energy for
/a/ s = 1/2 Heisenberg ferromagnetic coupling /Bonner,Fisher/
/b/ s = 1/2 Ising coupling,ferro - or antiferromagnetic
/c/ s = 1/2 Restricted model coupling ferro - or antiferromagnetic
/d/ s = 1/2 Heisenberg antiferromagnetic coupling /Bonner,Fisher/

One can see that the obtained results are quite reasonable. Since the physical nature of restricted models is not clear yet, we hope to devote the forthcoming papers to this problem.

Evaluation

The basic result of the paper is formula /4/.As we already have mentioned, there is a strong support for a belief that this formula is generally valid for any N.Since the symmetric group is the best known one,one can hope that the existing powerful methods can be applied to the spin models.Further,we expect that these irreducible representations are not accidental but there exists a deep physical reason for their occurence.It seems that restricted models,especially those with the long range interactions,exhibiting the phase transition in non-zero temperature could help to clarify this point.

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Referencies

[1] J.C.Bonner,M.E.Fisher,Phys.Rev,135,No 3A,640 /1964/.

[2] H.F.Trotter,Proc.Am.Math.Soc., 10,545,/1959/.

[3] D.E.Littlewood ,The Theory of Group Characters,Oxford 1950.

[4] M.Hamermesh, Group Theory and its Application to Physical Problems,Pergamon Press,New York

[5] C.J.Thompson,Mathematical Statistical Mechanics,New York 1972.

[6] C.Domb,M.S.Green, Phase Transition and Critical Phenomena Vol.1,2,3,4,5,5a,6.London.

[7] E.Jahnke,F.Emde,Tables of Functions with Formulea and Curves, Dover 1945.

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