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TWO EXACTLY SOLVABLE ISOTROPIC HEISENBERG MODELS

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Две точнорешаемые изотропные модели Гайзенберга

На основе связи между представлениями группы перестановок и изотропными моделями Гайзенберга решаются две модели Гайзенберга: квантовая модель Кюри-Вейсса и модель ближайших соседей.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1978

Strycharski Z. E17 - 11197

Two Exactly Solvable Isotropic Heisenberg Models

The connection between the permutation group representation and the isotropic Heisenberg models is used for the solution of two of them: the quantum Curie-Weiss model and the model with the nearest neighbour interaction.

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

Communication of the Joint Institute for Nuclear Research. Dubna 1978

Introduction

The basic problem of the statistical mechanics is the calculation of the partition function Z_N

$$Z_N = \sum_{a} e^{-\beta E(a)}, \qquad /1/$$

where $E(a)$ are the eigenvalues of the Hamiltonian. So, in order to perform such calculations one should diagonalize the Hamiltonian. This is not easy task and in the case of the Heisenberg spin model

$$H = -\sum_{\langle ij \rangle} J_{ij} \vec{\sigma}_i \cdot \vec{\sigma}_j \qquad /2/$$

this problem is still unsolved. In our previous paper [3] we have found the relation between irreducible representations of symmetric group S_N and any isotropic Heisenberg Hamiltonian for spin 1/2 for the lattice with N sites.

This relation allows one to reduce any of these Hamiltonians to the quasidiagonal form.

In this paper we shall describe the exact solution for two models based on our previous results. One of them is the quantum Curie-Weiss model [1] with Hamiltonian

$$H = -\frac{J}{N} \sum_{1 \le i < j \le N} \vec{\sigma}_i \cdot \vec{\sigma}_j , \qquad /3/$$

and the second one is the N nearest neighbours model/NNNM/

$$H = -J \sum_{i=1}^{N} \vec{\sigma}_i \cdot \vec{\sigma}_N \, . \qquad /4/$$

The quantum Curie-Weiss model is especially interesting since it is the simplest model exhibiting the phase transition [1] .

1.The relation between symmetric group and Heisenberg Hamiltonian

We can write any isotropic Heisenberg Hamiltonian for s=1/2 in the following form

$$H = -\sum_{...} J_{ij}\, \vec{\sigma}_i \cdot \vec{\sigma}_j = -\sum_{...} 2J_{ij}\, P_{ij} + \sum_{...} J_{ij}\, 1 \, , \qquad /5/$$

where P_{ij} are elements of symmetric group S_N in some reducible representation X with the dimensionality 2^N.

The X representation can be reduced in the following way:

$$X = (N+1)\ \square\square\cdots\square \ \oplus\ (N-1)\ \begin{array}{l}\square\square\cdots\square\\ \square\end{array} \ \oplus\ (N-3)\ \begin{array}{l}\square\square\square\cdots\square\\ \square\square\end{array} \ \oplus \cdots$$

$$= \bigoplus_{k=0}^{[\frac{N}{2}]} (N-2k+1)\ [N-k,k] \, , \qquad \left[\tfrac{N}{2}\right] = \begin{cases} \frac{N-1}{2} & N \text{ odd} \\ \frac{N}{2} & N \text{ even ,} \end{cases} \qquad /6/$$

where $[N-k,k] \equiv \begin{array}{l}\overbrace{\square\square\square\cdots\square}^{N-k}\\ \underbrace{\square\cdots\square}_{k}\end{array}$ denotes the irreducible representation S_N, and $\bigoplus$ means the direct sum of representations.

From formula /6/ it follows that our general Hamiltonian /5/ can be reduced to the quasidiagonal form.

$$H = \bigoplus_{k=0}^{[\frac{N}{2}]} (N-2k+1)\ H_K \, , \qquad /7/$$

where

$$H_K = -\sum_{...} 2J_{ij}\, P_{ij}^{k} + \sum_{...} J_{ij}\, 1^{k} \, , \qquad /8/$$

P_{ij}^{k} are the representatives of the transpositions of the i-th and j-th sites in the representation $[N-k,k]$ .We denote the unit matrix in the same representation by 1^{k} .

2.The N nearest neighbours Heisenberg model /NNNM/

The Hamiltonian /4/ can be rewritten in the form containing transposition operators

$$H = -J\sum_{i=1}^{N-1} \vec{\sigma}_i \cdot \vec{\sigma}_N = -2J\sum_{i=1}^{N-1} P_{iN} + J(N-1)1 =$$

$$= \left\{-2J\sum_{i=1}^{N-1} P_{iN} + 2J(N-1)1\right\} - J(N-1)1 = H' - J(N-1) \, . \qquad /9/$$

Such a partition of the Hamiltonian is worthwhile since the ground state energy of H' vanishes.

Now we shall calculate the eigenvalues of H' and their degenerations.The use of /8/ yields

$$H' = \bigoplus_{k=0}^{[\frac{N}{2}]} H'_k\ (N-2k+1) \, ,$$

$$H'_k = -2J\sum_{i=1}^{N-1} P_{iN}^{k} + 2J(N-1)\, 1^{k} . \qquad /10/$$

Hence we see that this Hamiltonian can be represented by the quasidiagonal matrix

$$\begin{pmatrix} \boxed{H_0'} & & & & & & & 0 \\ & \boxed{H_1'} & & & & & & \\ & & \ddots & & & & & \\ & & & \boxed{H_1'} & & & & \\ & & & & \boxed{H_2'} & & & \\ & & & & & \boxed{H_2'} & & \\ & & & & & & \ddots & \\ 0 & & & & & & & \boxed{H'_{[\frac{N}{2}]}} \end{pmatrix} . \qquad /11/$$

To each block there corresponds one of the Hamiltonians $\{H_k'\}$. Let us recall a few basic facts about the representations of the symmetric group. The diagonalization of H_k' is based on them.

i/ All transpositions P_{ij} belong to the one class $(1^{N-2}2)$.

ii/ For any irreducible representation the sum of elements of the $(1^{N-2}2)$ class is proportional to the unit matrix. The coefficient of proportionality is given by the formula

$$\lambda([\lambda_1,\lambda_2,\dots\lambda_n]) = \frac{1}{2}\sum_{i=1}^{n} \lambda_i(\lambda_i - 2i + 1), \qquad /12/$$

iii/ The dimensionality of representation $[N-k,k]$ is equal to

$$\frac{N!\ (N-2k+1)}{(N-k+1)!\ \ k!} \ . \qquad /13/$$

In the decomposition /6/ only the representations $\{[N-k,k]\}$ are present, thus

$$\lambda_1 = N-k \qquad \lambda_2 = k \qquad \lambda_3 = \lambda_4 = \dots = \lambda_n = 0 .$$

The proportionality coefficient λ is also the eigenvalue of the operator, being the sum of all transpositions

$$\Lambda_N^{[N-k,k]} = \sum_{1\le i<j\le N} P_{ij}^k \ .$$

For the class of representations $[N-k,k]$

$$\lambda([N-k,k]) = \frac{1}{2}(N-k)(N-k-1) + \frac{1}{2}k(k-3). \qquad /14/$$

Using the above informations we can transform the Hamiltonian /10/ to the form

$$H_k' = -2J\sum_{i=1}^{N-1} P_{iN}^k + 2J(N-1)\,1^k = \qquad /15/$$

$$= -2J\left\{\sum_{1\le i<j\le N} P_{ij}^k - \sum_{1\le i<j\le N-1} P_{ij}^k\right\} + 2J(N-1)\,1^k .$$

The operator $\sum_{1\le i<j\le N-1} P_{ij}$ contains only transpositions belonging to the subgroup S_{N-1}, so the representation $[N-k,k]$ becomes now reducible

$$[N-k,k] = [N-k-1,k] \oplus [N-k,k-1] . \qquad /16/$$

In these representations the operator $\sum_{1\le i<j\le N-1} P_{ij}$ is diagonal.

Using Eqs. /14,15,16/ the Hamiltonian /15/ can be cast in the final form

$$\begin{aligned} H_k' = -2J\Big[&\Big\{\tfrac{1}{2}(N-k)(N-k-1) + \tfrac{1}{2}k(k-3) - \tfrac{1}{2}(N-k-1)(N-k-2) - \\ &- \tfrac{1}{2}k(k-3) - N + 1\Big\}\,1([N-k-1,k]) \oplus \Big\{\tfrac{1}{2}(N-k)(N-k-1) + \\ &+ \tfrac{1}{2}k(k-3) - \tfrac{1}{2}(N-k)(N-k-1) - \tfrac{1}{2}(k-1)(k-4) - N + 1\Big\}\,1([N-k,k-1])\Big] = \\ = kJ\,&1([N-k-1,k]) \oplus (N-k+1)J\,1([N-k,k-1]) . \end{aligned} \qquad /17/$$

Thus, the Hamiltonian H_k' contains only two different eigenvalues $E_k^1 = kJ$ and $E_k^2 = (N-k+1)J$ with the degenerations

$$\frac{(N-1)!\,(N-2k)}{(N-k)!\ \ k!} \quad \text{and} \quad \frac{(N-1)!\,(N-2k+2)}{(N-k+1)!\ (k-1)!}$$ respectively.

Our results for the whole Hamiltonian H' are presented in fig.1.

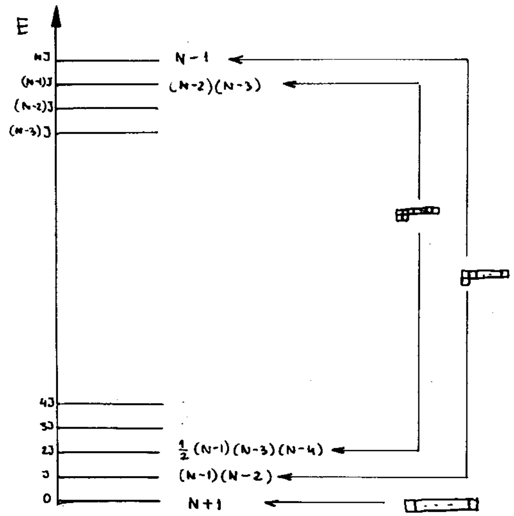

Fig.1.
Energy spectrum and degenerations for NNNM.

Using the eigenvalues and their degenerations, one can easily calculate the partition function and the free energy.

$$Z_N = \mathrm{Tr}\, e^{-\beta H} = e^{\beta J(N-1)}\, \mathrm{Tr}\, e^{-\beta H'} = e^{\beta J(N-1)} \Big[\sum_{k=0}^{[\frac{N}{2}]} (N-2k+1) \frac{(N-1)!\,(N-2k)}{(N-k)!\;k!}\, e^{-\beta J k} +$$

$$+ \sum_{k=0}^{[\frac{N}{2}]} (N-2k+1) \frac{(N-1)!\,(N-2k+2)}{(N-k+1)!\,(k-1)!}\, e^{-\beta J(N-k+1)} \Big] = e^{\beta J(N-1)} \sum_{k=1}^{N} \frac{1}{N} (N-2k+1)(N-2k) \binom{N}{k} e^{-\beta J k} =$$

$$= e^{\beta J(N-1)} \left(N+1 + \left(4 + \frac{2}{N}\right) \frac{\partial}{\partial \beta J} + \frac{4}{N} \frac{\partial^2}{\partial (\beta J)^2} \right) \sum_{k=0}^{N} \binom{N}{k} e^{-\beta J k} =$$

$$= 2^N e^{\frac{\beta J}{2}(N-1)} \mathrm{ch}^N \frac{\beta J}{2} \left\{ N+1 + 4N \left[(1+e^{-\beta J})^{-2} - (1+e^{-\beta J})^{-1} \right] - 2(1+e^{-\beta J})^{-1} \right\} =$$

$$= 2^N e^{\frac{1}{2}\beta J(N-1)} \mathrm{ch}^N \frac{\beta J}{2} \left\{ 1 - 2(1+e^{-\beta J})^{-1} + N\left(1 + 4(1+e^{-\beta J})^{-2} - 4(1+e^{-\beta J})^{-1}\right) \right\} .$$

These formulas allow one to study the thermodynamic limit

$$-\frac{\Psi}{kT} = \lim_{N\to\infty} \frac{1}{N} \ln Z_N = \ln 2 + \frac{1}{2}\beta J + \ln \mathrm{ch} \frac{\beta J}{2} .$$

In this limit the free energy of this model coincides with the free energy for one-dimensional Ising model. It means that in both models the thermodynamical functions are the same.

3. The quantum Curie-Weiss model /QCWM/

Now we shall diagonalize the Hamiltonian for QCWM. There exists many exact results for this model, but only in the thermodynamic limit [4,5]. In particular, it was shown that the mean-field approximation is exact in this limit. But nobody succeeded in the calculation of the energy spectrum and partition function for finite N for this model. We shall show that using the results of sections 1 and 2 we can solve this problem.

In terms of the transposition operators the Hamiltonian reads

$$H = -\frac{J}{N} \sum_{1 \le i < j \le N} \vec{\sigma}_i \cdot \vec{\sigma}_j = -\frac{2J}{N} \sum_{1 \le i < j \le N} P_{ij} + \frac{J}{2}(N-1)\,\mathbb{1} =$$

$$= \bigoplus_{k=0}^{[\frac{N}{2}]} (N-2k+1) \left(-\frac{2J}{N}\right) \Lambda_N^{[N-k,\,k]} + \frac{J}{2}(N-1)\,\mathbb{1} . \qquad /18/$$

We see that Hamiltonian /18/ contains the whole sum.

Helpfully from /11/ it follows that this sum is already diagonal in irreducible representations $\{[N-k,k]\}$. Hence, in fact we have found the solution of our problem.

Similarly as in the case of NNNM we can visualize the properties of the energy spectrum in figure 2.

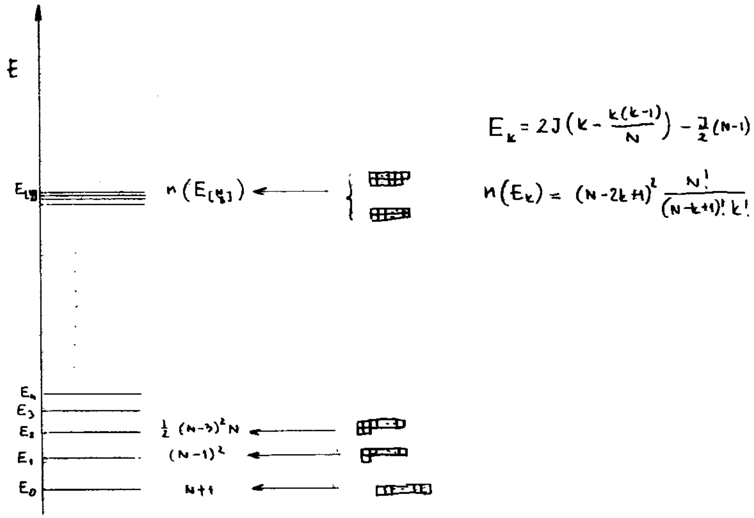

Fig. 2

Energy spectrum and degenerations for QCWM.

The partition function can be transformed to the form

$$Z_N = \sum_{k=0}^{[\frac{N}{2}]} n(E_k) e^{-\beta E_k} = e^{\frac{\nu}{2}(N-1)} \sum_{k=0}^{[\frac{N}{2}]} (N-2k+1)^2 \frac{N!}{(N-k+1)!\,k!}\, e^{2\nu\left(k - \frac{k(k-1)}{N}\right)} =$$

$$= e^{-\frac{\nu}{2}(3+\frac{1}{N})} \sum_{k=0}^{[\frac{N}{2}]} \frac{(N-2k+1)^2}{N+1} \binom{N+1}{k} e^{\frac{\nu}{2N}(N-2k+1)^2} =$$

$$= e^{-\frac{\nu}{2}(3+\frac{1}{N})} \frac{2N}{N+1} \frac{\partial}{\partial \nu} \sum_{k=0}^{N} \binom{N}{k} e^{\frac{\nu}{2N}(N-2k+1)^2} \qquad /19/$$

$$\nu = \beta J .$$

This form resembles the Kac result [1] .Hence we can use his ingenious method of calculating the term under derivative.

Using the identity

$$e^{a^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\tfrac{1}{2}\xi^2 + \sqrt{2}\,a\,\xi\right) d\xi \qquad /20/$$

one has

$$Z_N = e^{-\frac{\nu}{2}(3+\frac{1}{N})} \frac{2N}{N+1} \frac{\partial}{\partial \nu} \sum_{k=0}^{N} \binom{N}{k} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left(-\tfrac{1}{2}\xi^2 + \sqrt{\tfrac{\nu}{N}}\,\xi\,(N-2k+1)\right) d\xi =$$

$$= e^{-\frac{\nu}{2}(3+\frac{1}{N})} \frac{2N}{N+1} \frac{1}{\sqrt{2\pi}} \frac{\partial}{\partial \nu} \int_{-\infty}^{\infty} e^{-\frac{1}{2}\xi^2} \left(\sum_{k=0}^{N} \binom{N}{k} e^{\xi \sqrt{\frac{\nu}{N}}(N-2k+1)}\right) d\xi . \qquad /21/$$

One can now perform the sum over the k independently of the result that

$$Z_N = e^{-\frac{\nu}{2}(3+\frac{1}{N})} \frac{2N}{N+1} \frac{1}{\sqrt{2\pi}} 2^N \frac{\partial}{\partial \nu} \int_{-\infty}^{\infty} e^{-\frac{1}{2}\xi^2 + \xi\sqrt{\frac{\nu}{N}}} \operatorname{ch}^N\left(\xi \sqrt{\tfrac{\nu}{N}}\right) d\xi . \qquad /22/$$

The change of variables $\xi - \sqrt{\frac{\nu}{N}} = \eta\sqrt{N}$ gives

$$Z_N = e^{-\frac{\nu}{2}(3+\frac{1}{N})} \frac{2N}{N+1} 2^N \frac{\sqrt{N}}{\sqrt{2\pi}} \frac{\partial}{\partial \nu} \left[\int_{-\infty}^{\infty} e^{-\frac{1}{2}\eta^N} \operatorname{ch}^N\left(\eta\sqrt{\nu} + \tfrac{\nu}{N}\right) d\eta\, e^{\frac{\nu}{2N}} \right], \qquad /23/$$

and application of Laplace's method /i.e., the saddle-point method / shows that for large N

$$Z_N = e^{-\frac{v}{2}(3+\frac{1}{N})} \frac{2N}{N+1} 2^N \frac{\sqrt{N}}{\sqrt{2\pi}} \frac{\partial}{\partial v} e^{\frac{v}{2N}} \max_{-\infty<\eta<\infty} \left(e^{-\frac{\eta^2}{2}} ch\, \eta\sqrt{N}\right)^N =$$

$$= e^{-\frac{v}{2}(3+\frac{1}{N})} \frac{\sqrt{N}}{N+1} \frac{1}{\sqrt{2\pi}} 2^N e^{\frac{v}{2N}} \mathcal{K}^N\left(\frac{v}{2}\right) \left[1 + 2N^2 \frac{\frac{\partial \mathcal{K}}{\partial v}}{\mathcal{K}}\right]. \qquad /24/$$

Therefore

$$-\frac{\Psi}{kT} = \lim_{N\to\infty} \frac{1}{N} \ln Z_N = \ln 2 + \ln \mathcal{K}\left(\frac{v}{2}\right), \qquad /25/$$

where $\mathcal{K}(\frac{v}{2})$ is the Kac function for classical Curie-Weiss model

$$\mathcal{K}\left(\frac{v}{2}\right) = \max_{-\infty<\eta<\infty} \left[e^{-\frac{1}{2}\eta^2} ch\, \eta\sqrt{v}\right].$$

The equation for maximum of $\mathcal{K}$ gives the well-known solution for mean-field approximation.

$$\eta = \sqrt{v}\ th\, \eta\sqrt{v} \qquad /26/$$

Let us mention that in quantum case the argument $\frac{v}{2}$ of $\mathcal{K}$ is equal to half of classical argument of $\mathcal{K}$. It means that in quantum case the critical temperature is twice as large as in classical one.

Summary

We have shown that using some results of the symmetric group one can rather easily diagonalize the Hamiltonians of a class of Heisenberg models. Our results are valid not only in thermodynamic limit but also for any number of sites. In particular, the comparison of the results for both considered models and the corresponding to them classical Ising models, shows that these,

quite different for N finite, models coincide in the thermodynamic limit. Thus, we are faced with astonishing properties of the thermodynamic limit. We believe that the symmetric group, one of the best known in mathematics, could give solutions for more sophisticated models which does not correspond to the mean-field theory.

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