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Fermi-Liquid Theory of Linear Antiferromagnetic Chains

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An attempt has been made to understand various results obtained so far in the one-dimensional isotropic antiferromagnetic spin system from the point of view of the Fermi liquid theory. Specific heat thus obtained is very close to the value given by Bonner and Fisher by the numerical calculation. A brief discussion is made on the exact solution of the magnetic susceptibility.

§ 1. Introduction

Recently, one-dimensional Heisenberg spin systems have attracted much attention theoretically[1] as well as experimentally.[2] In these systems many interesting behaviours can be expected since the short-range order develops greatly at low temperatures.

For various properties in the Heisenberg linear chains, many works have been published since Bethe's work. It seems to us that there are roughly three different approaches to attack this problem, namely,

(1) a method to diagonalize the Hamiltonian exactly,[3),4)]
(2) a method to perform the numerical calculation on finite chains and extrapolate the results to infinite chains,[5)]
(3) approximate methods.[6),7)]

In one-dimensional spin systems, on account of their simplicity various exact solutions are obtained by the method (1), but on the other hand a simple approximation seems to fail. For instance, in the Z^{-1} expansion[8)] of Brout, where Z is the number of the nearest neighbour spins, higher order correlations are discarded in comparison with the lower order ones, Z^{-1} being the expansion parameter. But since $Z=2$ in one-dimensional systems, a simple decoupling scheme can hardly be adopted.

In various approximate methods there is a comparatively satisfactory theory which makes use of the Fermi representation for one-dimensional spin systems with spin $S=\frac{1}{2}$.[9)] With this representation even the simplest Hartree-Fock approximation gives the values for the magnetic susceptibility and the specific heat which are close to the results of the numerical calculation of reference 5).[6)] Use of this representation gives rise to many advantages, for instance

(1) a clear physical picture can be obtained in the Fermi representation,
(2) a connection with the conventional many-body theory can be examined,

(3) calculation is simplified in comparison with using the original spin operator.

In this paper we try to understand the results obtained by the exact and numerical calculations in terms of the Landau quasi particles, whereby we use the Fermi representation.

For simplicity here we only consider the isotropic case.

In § 2 the des Cloizeaux and Pearson spin waves[10] are shown to be extended to the case when more than one spin wave are excited. In § 3 the obtained energy spectrum is represented by the energy of the quasi-particles, and then with the aid of this consideration the specific heat and the magnetic susceptibility at low temperatures are discussed. Section 4 is devoted to the summary and the future problems in our work are briefly mentioned.

§ 2. The des Cloizeaux and Pearson solution

In this section we obtain the states when more than one des Cloizeaux and Pearson spin wave[10] are excited. Since a treatment in this section is almost the same as theirs, we only write down what is needed below.

We consider the linear isotropic Heisenberg chain with spin $\frac{1}{2}$. Its Hamiltonian is written as

$$H=\sum_{i=1}^{N}(\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1}-\tfrac{1}{4}). \tag{2·1}$$

Schrödinger equation for this system is

$$H\Psi=E\Psi, \tag{2·2}$$

where Ψ is a wave function and E the energy eigenvalue. Bethe first attempted to solve this equation exactly, and the eigenvalue E is obtained as follows,

$$E=-\sum_{j=1}^{N/2-S}(1-\cos k_j), \tag{2·3}$$

where S is a spin quantum number specifing the state and N is assumed to be an even number.

In order to obtain E, we must know the values of k_j's. This can be done by solving the following coupled equations,

$$2\cot(\varphi_{jl}/2)=\cot(k_j/2)-\cot(k_l/2), \tag{2·4}$$

where

$$-\pi<\varphi_{jl}\leq\pi,$$
$$Nk_j=2\pi\lambda_j+\sum_l\varphi_{jl}, \tag{2·5}$$

where the λ_j's are integers and we can solve Eq. (2·2) by specifying $(N/2-S)$ integers λ_j. A set of $(N/2-S)$ integers λ_j corresponds to a state whose spin

quantum number is S. By Bethe's hypothesis a set $\{\lambda_j\}$ which belongs to "class C" gives the lowest energy state for a given wave number k.[4),11)]

Now λ_j which belongs to "class C" must satisfy the following additional conditions,

$$0<\lambda_j<N, \qquad \lambda_{j+1}\geq\lambda_j+2. \tag{2·6}$$

This hypothesis which is based on a plausible argument[11)] is not yet given a rigorous proof. However, the same hypothesis is here accepted and the consideration is restricted to the "class C" solutions. In the ground state C. N. Yang and C. P. Yang gave[12)] a proof of this hypothesis.

By using these λ_j's the wave number of this state is given by

$$k=\sum_j k_j=\frac{2\pi}{N}\sum_j \lambda_j. \tag{2·7}$$

The ground state is a singlet[13)] and $S=0$. Then, its wave number is 0 for $N/2$ even and π for $N/2$ odd.[4)]

Next the excited states with $S=1$ are obtained. These excited states are given by a set of $(N/2-1)$ integers λ_j which belong to "class C".[10),*)] Most general sets of λ_j which belongs to "class C" and have $S=1$ are given by the following,

$$\{\lambda_j\};\ 1, 3, 5, \cdots, 2m-1, 2m+2, 2m+4, \cdots, 2n, 2n+3,$$
$$2n+5, \cdots, N-1. \tag{2·8}$$

The wave numbers of these states are given as follows,

$$q=2\pi\left(M-\frac{m+n+1}{N}\right), \tag{2·9}$$

where M is an appropriate integer taken such as $-\pi<q\leq\pi$ and q is measured from the ground state wave number.

Now we introduce a new variable x[10)] as

$$x=\frac{2j-1}{N}, \qquad 0<x<1,$$
$$j=1, 2, \cdots, \frac{N}{2}. \tag{2·10}$$

Furthermore we define $k(x)=k_j$, $\lambda(x)=\lambda_j/N$, $\varphi(x, y)=\varphi_{jl}$, and take a limit $N\to\infty$ to rewrite Eqs. (1·3), (1·4) and (1·5) as follows,

$$E=-\frac{N}{2}\int_0^1[1-\cos k(x)]dx, \tag{2·11}$$

*) If $\lambda=0$ is included in "class C", the problem becomes a little embarrassing. This question also arises in the ground state and we do not here go into details. (See reference 11).)

$$2\cot\frac{\varphi(x,y)}{2}=\cot\frac{k(x)}{2}-\cot\frac{k(y)}{2}, \tag{2·12}$$

$$k(x)=2\pi\lambda(x)+\frac{1}{2}\int_0^1\varphi(x,y)\,dy. \tag{2·13}$$

Here $\lambda(x)$ is given by

$$\lambda(x)=(2j-1)/N=x, \qquad j\leq m, \tag{2·14}$$

$$\lambda(x)=2j/N=x+\frac{1}{N}, \qquad m<j\leq n, \tag{2·15}$$

$$\lambda(x)=(2j+1)/N=x+\frac{2}{N}, \qquad n<j. \tag{2·16}$$

We define two variables x_1 and x_2,

$$x_1=\frac{2m+1}{N}, \qquad x_2=\frac{2n+1}{N}. \tag{2·17}$$

By making use of these variables, $\lambda(x)$ is written shortly as

$$\lambda(x)=x+\frac{1}{N}\theta(x;\,x_1,\,x_2), \tag{2·18}$$

where

$$\theta(x;\,x_1,\,x_2)=\begin{cases}0, & x<x_1,\\ 1, & x_1\leq x<x_2,\\ 2, & x_2\leq x,\end{cases} \tag{2·19}$$

and the wave number q is

$$q=2\pi\left(M-\frac{x_1+x_2}{2}\right). \tag{2·20}$$

$\lambda(x)$ for the ground state is given by

$$\lambda(x)=x. \tag{2·21}$$

Then, eliminating $\varphi(x,y)$ between (2·12) and (2·13) we obtain

$$k(x)=2\pi\left[x+\frac{1}{N}\theta(x;\,x_1,\,x_2)\right]+\int_0^1\operatorname{arccot}\left\{\frac{1}{2}\cot\left[\frac{k(x)}{2}\right]-\frac{1}{2}\cot\left[\frac{k(y)}{2}\right]\right\}dy. \tag{2·22}$$

Differentiating both sides of this equation with respect to k, we have

$$1=\pi\frac{dx}{dk}\left[1+\frac{2}{N}\delta(x-x_1)+\frac{2}{N}\delta(x-x_2)\right]$$
$$+\left\{\sin\left[\frac{k(x)}{2}\right]\right\}^2\times\int_0^1 dy\left\{4+\left[\cot\left[\frac{k(x)}{2}\right]-\cot\left[\frac{k(y)}{2}\right]\right]^2\right\}^{-1}. \quad (2\cdot23)$$

Now we change the variables as follows,

$$\xi\equiv\cot\left[\frac{k(x)}{2}\right], \quad (2\cdot24)$$

$$-\frac{dx}{d\xi}=f(\xi). \quad (2\cdot25)$$

ξ_1 and ξ_2 are variables that correspond to x_1 and x_2, respectively. Then, Eq. (2·23) becomes

$$f(\xi)+\frac{2}{\pi}\int_{-\infty}^{\infty}d\eta f(\eta)[4+(\xi-\eta)^2]^{-1}$$
$$=\frac{2}{\pi}(1+\xi^2)^{-1}-\frac{2}{N}\delta(\xi-\xi_1)-\frac{2}{N}\delta(\xi-\xi_2). \quad (2\cdot26)$$

This equation can be solved in the same manner as des Cloizeaux and Pearson,[10] and we obtain the excitation energy ϵ as

$$\epsilon=E-E_0=\frac{\pi}{2}\left[\frac{1}{\cosh(\pi/2)\xi_1}+\frac{1}{\cosh(\pi/2)\xi_2}\right], \quad (2\cdot27)$$

where E_0 is the ground state energy. There is a relation between ξ and x as

$$\sinh\left(\frac{\pi}{2}\xi\right)=\cot(\pi x). \quad (2\cdot28)$$

After all, Eq. (2·27) becomes

$$\epsilon=\frac{\pi}{2}[|\sin\pi x_1|+|\sin\pi x_2|]. \quad (2\cdot29)$$

Since $0<x_1+x_2<2$, we divide this interval into two sections, i.e. $0<x_1+x_2<1$ and $1<x_1+x_2<2$. For $0<x_1+x_2<1$, we have $q=-\pi(x_1+x_2)$, and for $1<x_1+x_2<2$, we have $q=2\pi(1-(x_1+x_2)/2)$.

We illustrate the spectrum thus obtained in Fig. 1. This spectrum is a continuous one, and for each q, the lower limit of this spectrum is given by $(\pi/2)\sin|q|$ which is the same as des Cloizeaux and

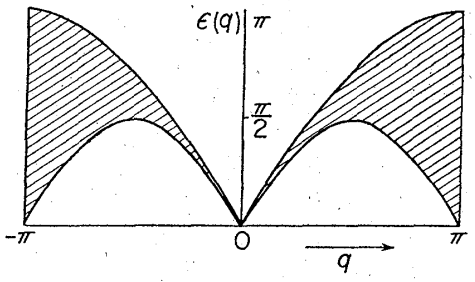

Fig. 1. Energy spectrum of the first excited states is represented by the shaded part.

Pearson spin wave spectrum, and the upper limit is $\pi \sin(|q|/2)$. Furthermore, this spectum has three-fold degeneracy corresponding to $S^z=1, 0, -1$ respectively.

§ 3. Fermi representation

It is well known that the linear Heisenberg spin system with spin 1/2 can be represented in terms of the Fermi operator.[9] Namely, the spin operators S_i^+, S_i^-, S_i^z are expressed by the Fermi operator c_i as $S_i^+=c_i^\dagger \exp[i\pi\sum_{j<i}c_j^\dagger c_j]$, $S_i^-=c_i\exp[-i\pi\sum_{j<i}c_j^\dagger c_j]$, $S_i^z=c_i^\dagger c_i-(1/2)$, where i, j denote the lattice sites, $c_i^\dagger c_j+c_jc_i^\dagger=\delta_{ij}$ and δ_{ij} is Kronecker's delta. Then, the spin system considered here is converted to the assembly of Fermi particles. For instance, the Hamiltonian (2·1) becomes

$$H=\sum_q(-\cos q-1)c_q^\dagger c_q-\frac{1}{4N}\sum_{q_1}\sum_{q_2}\sum_{q_3}\sum_{q_4}\Delta(q_1+q_2-q_3-q_4)$$
$$\times(e^{iq_1}-e^{iq_2})(e^{-iq_3}-e^{-iq_4})c_{q_1}^\dagger c_{q_2}^\dagger c_{q_3}c_{q_4}\,, \tag{3·1}$$

where c_q, etc. are the Fermi operators, $\Delta(k)=\sum_n^{0,\pm1,\cdots}\delta^{Kr}(k-K_n)$, $K_n=2\pi n$; reciprocal lattice vectors and δ^{Kr} denotes Kronecker's delta.[14] Thus, since the spin system and the assembly of the Fermi particles have one to one correspondence, the rigorous solutions obtained by Griffiths[18] and by Bonner and Fisher[5] and in the previous section can be understood also in the Fermi representation, as will be demonstrated in this section.

But, since this Hamiltonian represents a system of strongly coupled Fermi particles, it is not convenient to discuss it directly.

On the other hand, Landau has shown that at low temperatures an assembly of strongly interacting Fermi particles can be regarded as an assembly of weakly interacting quasi-particles. Thus it would be useful to apply Landau's idea in our Hamiltonian (3·1).[15),16]

Let us start with the interpretation of the spectrum shown in Fig. 1 on this basis. It is worth noting that an increase (a decrease) of one particle corresponds to an increase (a decrease) of spin one and the total spin $S^z=0$ corresponds to the assembly of $N/2$ particles. It is thus sufficient to consider this question for $S^z=0$ due to symmetry.

We assume the quasi-particle whose energy is given by

$$\epsilon(p)=\left(-\frac{\pi}{2}\right)\cos p\,, \tag{3·2}$$

where p is a momentum of this particle. Then, we consider the state filled with these quasi particles up to the Fermi surface $(\pi/2, -\pi/2)$ as is shown in Fig. 2.

A particle-hole excitation such as shown in Fig. 3 gives the excitation energy

$$\epsilon_q=\epsilon_{q_2}-\epsilon_{q_1}\,, \tag{3·3}$$

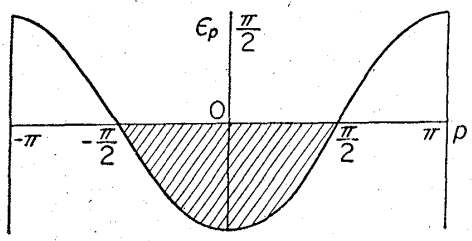

Fig. 2. Ground state of the Fermion quasi particles; shaded part is occupied by the quasi particles.

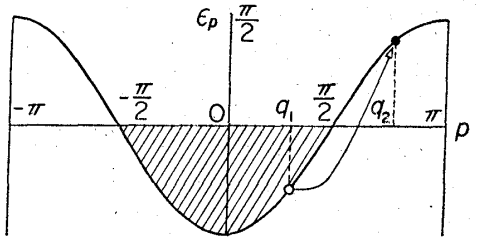

Fig. 3. Configuration of the particle-hole elementary excitation; one hole at q_1 and one particle at q_2 are created.

where

$$q = q_2 - q_1 + 2\pi n \,, \tag{3·4}$$

and n is an appropriate integer so determined as to satisfy $-\pi < q \leq \pi$.

It is easy to see that this excitation reproduces the excitation spectrum shown in Fig. 1. Therefore, the spectrum of Fig. 1 can also be represented as the excitation of the quasi-particles (3·2).*)

At low temperatures we can calculate various quantities by making use of this quasi-particle energy. We first make an assumption that this quasi particle is non-interacting.

Here we consider the quasi-particle energy in the magnetic field H. It is well known that the z-component of spin can be written by making use of the Fermi operator c_i as follows,[9]

$$S_i^z = c_i^\dagger c_i - (1/2), \tag{3·5}$$

where i represents the lattice site.

Since the total numbers of quasi-particles must be equal to the total numbers of bare-particles,[17] Zeeman term is invariant under the homogeneous magnetic field H when interaction between bare-particles are switched on and bare particles are dressed.

Therefore we first assume the quasi-particle energy in the magnetic field H of the following form,

$$\epsilon(p) = -\frac{\pi}{2}\cos p - h \,, \tag{3·6}$$

where $h = \mu H$, μ being a Bohr magneton.

Using Eq. (3·6), we obtain the specific heat at $H=0$. The internal energy of this system becomes

*) It is interesting to note how des Cloizeaux and Pearson's spin wave can be represented by the quasi-particle (3·2). It is easy to see that their spectrum corresponds to one particle or one excitation as a limiting case of Fig. 3.

hole

$$E=\frac{N}{2\pi}\int_{-\pi}^{\pi}dq\left(-\frac{\pi}{2}\cos p\right)f(q), \tag{3·7}$$

where $f(q)$ is a Fermi distribution function,

$$f(q)=(e^{-(\pi\cos q/2T)}+1)^{-1}, \tag{3·8}$$

and we put the Boltzmann constant $k_B=1$ for simplicity.

Differentiating Eq. (3·7) with respect to T, we have for the specific heat C_v at low temperatures,

$$C_v=\frac{\partial E}{\partial T}=\frac{N}{2\pi T^2}\int_{-\pi}^{\pi}dq\left(\frac{\pi}{2}\cos q\right)^2 e^{-(\pi\cos q/2T)}(e^{-(\pi\cos q/2T)}+1)^2$$

$$\simeq\frac{8TN}{\pi^2}\int_0^{\infty}dx\frac{x}{e^x+1}=\frac{2}{3}NT\,. \qquad (\text{as } T\to 0) \tag{3·9}$$

This result must be compared with that of Bonner and Fisher.[5] They obtained

$$C_v\simeq 0.70NT\,. \tag{3·10}$$

This value is very close to ours and it seems to us that the quasi-particle description in this section is fairly good. Various results so far are collected in Table I.

Table I. Results on the specific heat C_v.

Spin wave theory[21] (two sublattice model)	$\frac{2}{3}\pi NT$
Hartree-Fock approximation[6]	$\frac{\pi}{3(1+2/\pi)}NT$
Bonner & Fisher[5] (numerical calculation)	$\simeq 0.70\ NT$
ours	$\frac{2}{3}NT$

Next we consider the magnetic susceptibility. Using Eq. (3·6), the magnetic susceptibility at low temperatures becomes

$$\chi=\frac{1}{2\pi}\frac{\partial}{\partial h}\int_{-\infty}^{\infty}dq\,\{e^{[-(\pi\cos q/2)-h]/T}+1\}^{-1}$$

$$=\frac{2}{\pi^2}\,. \qquad (\text{as } T\to 0,\ h\to 0) \tag{3·11}$$

This value is twice larger than the exact one $1/\pi^2$ given by Griffiths.[18] This discrepancy may arise from ignoring the residual interaction between quasi-

particles.

When we take into account the residual interaction, the quasi-particle energy becomes[16]

$$\tilde{\epsilon}_p = \epsilon_p + \sum_{p'} f(p, p')\delta n_{p'}\,, \tag{3·12}$$

where ϵ_p is given by Eq. (3·2), $f(p, p')$ the residual interaction, and $\delta n_{p'}$ the deviation of the distribution function from the ground state distribution, namely the excitation. It is well known in the Fermi liquid theory that by introducing the residual interaction the specific heat given by Eq. (3·9) is not altered[16] because the second term of Eq. (3·12) adds only the higher order correction in T to the specific heat.

However, the situation is different for the magnetic susceptibility as compared with that for the specific heat. Since the magnetic susceptibility corresponds to the compressibility in the Fermi liquid theory,[16] the residual interaction is important.

When h is small, the deviation of the distribution function from that of $h=0$ is restricted around the Fermi surface. Thus $\tilde{\epsilon}_p$ with $p \simeq \pi/2$ becomes

$$\begin{aligned}\tilde{\epsilon}_p &= \epsilon_p + \sum_{p'} f(p, p')\delta n_{p'} - h \\ &\simeq \epsilon_p + \sum_{p' \simeq \pi/2} f(p, p')\delta n_{p'} + \sum_{p' \simeq -\pi/2} f(p, p')\delta n_{p'} - h \\ &\simeq \epsilon_p + f\left(\frac{\pi}{2}, -\frac{\pi}{2}\right)\sum_{p' \simeq \pi/2}\delta n_{p'} + f\left(\frac{\pi}{2}, -\frac{\pi}{2}\right)\sum_{p' \simeq -\pi/2}\delta n_{p'} - h\,.\end{aligned} \tag{3·13}$$

Because $\sum_{p \simeq -\pi/2}\delta n_p = \sum_{p \simeq -\pi/2}\delta n_p$ under the homogeneous disturbance h, we have

$$\begin{aligned}\tilde{\epsilon}_p &\simeq \epsilon_p + f\sum_{p'}\delta n_{p'} - h \\ &= \epsilon_p + f\langle s\rangle - h\,,\end{aligned} \tag{3·13′}$$

where $f = \{f(\pi/2, \pi/2) + f(\pi/2, -\pi/2)\}/2$, $\langle s\rangle$ the magnetization of the system due to the magnetic field h and we have used the relation $\langle s\rangle = \sum_{p'}\delta n_{p'}$. It is easy to check that the same relation is obtained for $p \simeq -\pi/2$ if we note $f(\pi/2, -\pi/2) = f(-\pi/2, \pi/2)$, $f(\pi/2, \pi/2) = f(-\pi/2, -\pi/2)$. By making use of the quasi-particle energy (3·13′), we can easily obtain the magnetic susceptibility χ as

$$\chi = [f + (\pi^2/2)]^{-1}. \tag{3·14}$$

Then, if f is positive (negative), χ tends to decrease (increase) and thus to approach (deviate from) the exact value. Therefore, in order to get the same result as the exact one, f must be equal to $\pi^2/2$. This quantity f corresponds to f_0 in the Fermi liquid theory.[16]

We may add that our system under discussion is a Fermi particle system

on a discrete lattice. Then it may contain a similar problem as the electron Fermi liquid in metals.*) It is interesting to study how the effective mass formula is obtained or modified, but this problem will be deffered to the future.

§ 4. Summary

In this paper attempts have been made to understand various results of the exact and numerical calculation from the point of view of a self-consistent Fermi liquid theory. In particular the specific heat obtained here has a satisfactory agreement with Bonner and Fisher's result obtained by numerical calculation.

But so far it can hardly be asserted that the system must be understood by the Fermi liquid theory since our results are so few. The author hopes that the Fermi liquid theory will be found to be useful by testing other quantities in the Heisenberg spin systems.

In order to make a progress in our Fermi liquid theory, it is necessary to clarify the following points, namely,

(1) according to the exact solution by C. N. Yang and C. P. Yang,[19] $\partial\chi/\partial h$ diverges as $h\to 0$ and $T=0$,

(2) the first excited states have three-fold degeneracy.[20],**)

After clarifing these points in connection with the Fermi liquid theory, it is interesting to investigate the response of the system for inhomogeneous or time dependent disturbances.

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*) cf. reference 16), p. 25 and Chap. 3.

**) This is true even in the X-Y model. See reference 20).

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