Effect of the Magnetic Field on the des Cloizeaux-Pearson Spin-Wave Spectrum

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The des Cloizeaux and Pearson's exact solution for the spin-wave spectrum of the $S=1/2$ antiferromagnetic Heisenberg chain is extended to the case of finite external field. It reproduces naturally the des Cloizeaux-Pearson spectrum in the zero-field limit as well as the spin-wave spectrum in the ferromagnetic state for fields larger than the critical field. The results are discussed by comparing them with predictions of other approximate theories.

§ 1. Introduction

For a long time one-dimensional (1D) systems were considered merely as mathematical test models for theorists. Recently, however, they have gotten their own rights even among experimentalists and many materials exhibiting one-dimensional characters have been found.[1]

One of the most impressive recent experiments is the work by Endoh et al.[2] on $CuCl_2 \cdot 2NC_5D_5$, which is a typical 1D antiferromagnetic Heisenberg spin system with $S=1/2$. They showed by neutron scattering that its spin-wave spectrum agrees quite well with the celebrated exact solution of des Cloizeaux and Pearson (dC-P),[2] and is in disagreement with the Anderson (molecular-field) theory. It clearly demonstrates the importance of exact theoretical studies of 1D systems. Although this experiment was made in the absence of external magnetic field, the magnetic-field dependence of elementary excitations in antiferromagnetic linear chains would be very interesting.

The purpose of this paper is to study exactly the magnetic-field dependence of the dC-P spin-wave spectrum. We hope that this work would stimulate further experimental studies on dynamics of 1D Heisenberg antiferromagnets in the presence of external field. The field dependence of spin waves of 1D Heisenberg antiferromagnets has previously been calculated by Pytte,[4] who applied the Bulaevskii (Hartree-Fock) approximation[5] based on the Fermion representation[5,6] of the 1D Heisenberg model. We later compare it with our result. We also show that the magnetic-field dependence of the dC-P spin wave is qualitatively different from that of the classical (Anderson) spin wave.

The details of the formulation and calculations are presented in § 2. Com-

parison with approximate theories and discussion of our results are made in the last section.

§ 2. Spin-wave spectrum in a magnetic field

The Hamiltonian of our system is given by

$$\mathcal{H} = 2J \sum_{j=1}^{N} \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} - g\mu_B H \sum_{j=1}^{N} S_j^{\,z} \tag{1}$$

with the cyclic boundary condition

$$\boldsymbol{S}_{N+1} = \boldsymbol{S}_1 , \tag{2}$$

where $\boldsymbol{S}_j$ is the spin operator of the j-th atom whose magnitude is $1/2$, and J is assumed to be positive.

2.1. *Ground state and des Cloizeaux-Pearson spin wave*

We follow the Bethe theory,[7] which is summarized as follows: A state ψ, whose z-component of the total spin is $N/2 - r$, is expanded as

$$\psi = \sum a(n_1, n_2, \cdots, n_r) \psi(n_1, n_2, \cdots, n_r), \tag{3}$$

where $\psi(n_1, n_2, \cdots, n_r)$ is the state, in which the spins at $n_1, n_2, \cdots, n_r$ are down and all other spins are up, and the summation in (3) is taken over all distinct sets of r indices $\{n_j\}$. According to Bethe the coefficient a is written as

$$a(n_1, n_2, \cdots, n_r) = \sum_P \exp\left[i\left(\sum_{j=1}^{r} k_{Pj} \cdot n_j + \frac{1}{2}\sum_{j<l} \phi_{Pj,Pl}\right)\right], \tag{4}$$

where the summation is performed over all permutations of the integers $1, 2, \cdots, r$. The wave vector k_j and phase shift ϕ_{jl} satisfy the relations:

$$Nk_j = 2\pi\lambda_j + \sum_{l(\neq j)} \phi_{jl} , \tag{5}$$

$$\cot \frac{\phi_{jl}}{2} = \frac{1}{2}\left[\cot \frac{k_j}{2} - \cot \frac{k_l}{2}\right], \tag{6}$$

where the λ_j's are integers between 0 and $N-1$. The energy of the state (3), which is measured from the exchange energy in the complete ferromagnetic state, is then given by

$$\varepsilon = \frac{1}{2J}[E - E_{\text{ex}}^{\text{Ferro}}]$$

$$= -\sum_{j=1}^{r}(1 - \cos k_j) - h\left(\frac{1}{2}N - r\right), \tag{7}$$

where $h = g\mu_B H / 2J$.

(i) Ground state:

Griffiths[8] showed that the ground state with $S^z = N/2 - r$ in an external field

corresponds to the set

$$\lambda_1 = \frac{N}{2} - r + 1, \quad \lambda_2 = \frac{N}{2} - r + 3, \cdots, \quad \lambda_r = \frac{N}{2} + r - 1. \tag{8}$$

Using Eq. (8) and taking the limit $N \to \infty$, we obtain from (5) $\sim$ (7) the following equations:[8]

$$k_0(x) = 2\pi x + \frac{1}{2} \int_{(1/2)-\rho}^{(1/2)+\rho} dy\, \phi_0(x, y), \tag{9a}$$

$$\cot \frac{\phi_0(x, y)}{2} = \frac{1}{2}\left[\cot \frac{k_0(x)}{2} - \cot \frac{k_0(y)}{2}\right], \tag{9b}$$

$$\varepsilon_{\mathrm{gr}} = -\frac{N}{2} \int_{(1/2)-\rho}^{(1/2)+\rho} dx[1 - \cos k_0(x)] - Nh\left(\frac{1}{2} - \rho\right), \tag{9c}$$

where λ_j, ϕ_{jl} and k_j have been replaced by Nx, $\phi(x, y)$ and $k(x)$, respectively. ρ is defined as

$$\rho = \frac{r}{N}. \tag{10}$$

(ii)   *des Cloizeaux-Pearson spin-wave state*:

The dC-P spin-wave state with one spin-flop $S^z = N/2 - r - 1$ in a magnetic field must be identified with a set $\{\lambda_j\}$, which differs from the ground-state set at only one point. Equation (8) and this assumption then lead to two branches of the excited state.[*]

(ii-a)   particle-like branch:

$$\lambda_0 = i, \quad \lambda_1 = \frac{N}{2} - r + 1, \quad \lambda_2 = \frac{N}{2} - r + 3, \cdots, \tag{11}$$

$$\lambda_r = \frac{N}{2} + r - 1. \qquad \left(0 \leq i \leq \frac{N}{2} - r - 1\right)$$

(ii-b)   hole-like branch:

$$\lambda_0 = \frac{N}{2} - r - 1, \quad \lambda_1 = \frac{N}{2} - r + 1, \quad \lambda_2 = \frac{N}{2} - r + 3, \cdots,$$

$$\lambda_n = \frac{N}{2} - r + 2n - 1, \quad \lambda_{n+1} = \frac{N}{2} - r + 2n + 2, \cdots,$$

$$\lambda_r = \frac{N}{2} + r. \qquad (0 \leq n \leq r - 1) \tag{12}$$

The set (12) is so chosen that two branches are connected with each other continuously.   It turns out that the sets (11) and (12) can reproduce the famous

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[*]   Here we restrict ourselves to the case, where the wave vector of the excitation is in $[0, \pi]$, since the spectrum is symmetric with respect to the origin.

dC-P spectrum in the zero-field limit as well as the well-known spin-wave spectrum of the ferromagnetic state for $H > H_{cr}$ (critical field). The wave vector of the excited state, which is the difference of the total wave vector from the ground-state value, is for each branch

$$q = \frac{2\pi}{N} \left(\sum_{\substack{j=0 \\ \text{(excited)} \\ \text{(state)}}}^{r} \lambda_j - \sum_{\substack{j=1 \\ \text{(ground)} \\ \text{(state)}}}^{r} \lambda_j \right) = \begin{cases} \dfrac{2\pi}{N} i: & \text{particle-like branch} \\[2ex] \pi - \dfrac{2\pi}{N} n: & \text{hole-like branch} \end{cases} \tag{13}$$

From $(5) \sim (7)$ and $(11) \sim (13)$ we may calculate the spin-wave spectrum.

2.2. *Particle-like branch*

Introducing $x_0 = \lambda_0 / N$, $x = \lambda_j / N (j \neq 0)$, $\phi(x, y) = \phi_{jl}$ and $k(x) = k_j$, and taking the $N \to \infty$ limit we obtain from $(5) \sim (7)$ and (11)

$$k(x_0) = 2\pi x_0 + \frac{1}{2} \int_{(1/2) - \rho}^{(1/2) + \rho} dy \, \phi(x_0, y), \tag{14a}$$

$$k(x) = 2\pi x + \frac{1}{N} \phi(x, x_0) + \frac{1}{2} \int_{(1/2) - \rho}^{(1/2) + \rho} dy \, \phi(x, y),$$

$$\left(\frac{1}{2} - \rho \leq x \leq \frac{1}{2} + \rho \right) \tag{14b}$$

$$\cot \frac{\phi(x, y)}{2} = \frac{1}{2} \left[\cot \frac{k(x)}{2} - \cot \frac{k(y)}{2} \right], \tag{14c}$$

$$\varepsilon = -(1 - \cos k(x_0)) - \frac{N}{2} \int_{(1/2) - \rho}^{(1/2) + \rho} dx [1 - \cos k(x)]$$

$$- hN \left(\frac{1}{2} - \rho \right) + h. \tag{14d}$$

To obtain the excitation energy $\varepsilon_p \equiv \varepsilon - \varepsilon_{gr}$, we put $k(x)$ and $\phi(x, y)$ as[*]

$$k(x) = k_0(x) + \frac{1}{N} k_1(x), \tag{15}$$

$$\phi(x, y) = \phi_0(x, y) + \frac{1}{N} \phi_1(x, y), \tag{16}$$

where $k_0(x)$ and $\phi_0(x, y)$ have already been introduced in (9a) and (9b). Substituting (15) and (16) into (14b) and (14c) and leaving the terms of order $1/N$, we obtain

$$k_1(x) = \phi(x, x_0) + \frac{1}{2} \int_{(1/2) - \rho}^{(1/2) + \rho} dy \, \phi_1(x, y), \tag{17}$$

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[*] Unlike the original dC-P formulation,[3] here we study directly the deviation of the wave vector $k(x)$ from its ground-state value.

$$\left(1+\cot^2\frac{\phi_0(x,y)}{2}\right)\phi_1(x,y)=\frac{1}{2}\left[\left(1+\cot^2\frac{k_0(x)}{2}\right)k_1(x)\right.$$
$$\left.-\left(1+\cot^2\frac{k_0(y)}{2}\right)k_1(y)\right]. \tag{18}$$

In (17) $\phi(x,x_0)$ may be replaced by $\phi_0(x,x_0)$, since it introduces differences of only $O(1/N)$. Equation (17) accompanied by (18) is the integral equation for $k_1(x)$, which eventually determines the excitation energy ε_p.

For convenience we use a variable $\hat{\xi}$ and a function $f(\hat{\xi})$ defined as[3),7),8)]

$$\hat{\xi}=\cot\frac{k_0(x)}{2}\,,\quad\frac{dx}{d\hat{\xi}}=-f(\hat{\xi})\,. \tag{19}$$

This simplifies Eqs. (9a) and (9b) into

$$f(\hat{\xi})=\frac{2}{\pi}\frac{1}{1+\hat{\xi}^2}-\frac{2}{\pi}\int_{-\alpha}^{\alpha}d\eta\,\frac{1}{4+(\hat{\xi}-\eta)^2}f(\eta)\,, \tag{20}$$

where α is related to the magnetization as

$$\rho=\frac{1}{2}\int_{(1/2)-\rho}^{(1/2)+\rho}dx=\frac{1}{2}\int_{-\alpha}^{\alpha}d\hat{\xi}\,f(\hat{\xi})\,. \tag{21}$$

The ground-state energy (9c) can be expressed in terms of $f(\hat{\xi})$ as

$$\varepsilon_{\mathrm{gr}}=-N\int_{-\alpha}^{\alpha}d\hat{\xi}\,\frac{1}{1+\hat{\xi}^2}f(\hat{\xi})-Nh\frac{1}{2}\left(1-\int_{-\alpha}^{\alpha}d\hat{\xi}\,f(\hat{\xi})\,\right). \tag{22}$$

Equations (17) and (18) for the excited state can also be written with the new variable as

$$k_1(\hat{\xi})=2\cot^{-1}\frac{\hat{\xi}-\hat{\xi}_0}{2}+\int_{-\alpha}^{\alpha}d\eta\,f(\eta)\,\frac{(1+\hat{\xi}^2)\,k_1(\hat{\xi})-(1+\eta^2)\,k_1(\eta)}{4+(\hat{\xi}-\eta)^2}\,, \tag{23}$$

where

$$\hat{\xi}_0=\cot\frac{k(x_0)}{2}\,. \tag{24}$$

In order to transform (23) into a simpler expression we put

$$k_2(\hat{\xi})\equiv(1+\hat{\xi}^2)f(\hat{\xi})k_1(\hat{\xi})\,. \tag{25}$$

Since $\hat{\xi}_0\geq\alpha\geq\hat{\xi}\geq-\alpha$ holds, (23) is then equivalent to

$$k_2(\hat{\xi})=-2+\frac{4}{\pi}\tan^{-1}\frac{\hat{\xi}_0-\hat{\xi}}{2}-\frac{2}{\pi}\int_{-\alpha}^{\alpha}d\eta\,\frac{1}{4+(\hat{\xi}-\eta)^2}k_2(\eta) \tag{26}$$

or

$$k_p(\hat{\xi})=\frac{2}{\pi}\left(\tan^{-1}\frac{\hat{\xi}_0-\hat{\xi}}{2}-\tan^{-1}\frac{\hat{\xi}_0+\hat{\xi}}{2}\right)-\frac{2}{\pi}\int_{-\alpha}^{\alpha}d\eta\,\frac{1}{4+(\hat{\xi}-\eta)^2}k_p(\eta)\,, \tag{27}$$

where $k_p(\tilde{\xi})$ is the odd part of $k_2(\tilde{\xi})$ and is needed to determine the excitation energy ε_p. In fact, from (9c) and (14d) we find

$$\varepsilon_p \equiv \varepsilon - \varepsilon_{gr}$$

$$= h - (1 - \cos k(x_0)) - \frac{1}{2} \int_{(1/2)-\rho}^{(1/2)+\rho} dx \sin k_0(x) \cdot k_1(x)$$

$$= h - \frac{2}{1+\tilde{\xi}_0^2} - \int_{-\alpha}^{\alpha} d\tilde{\xi} \frac{\tilde{\xi}}{(1+\tilde{\xi}^2)^2} k_p(\tilde{\xi}). \tag{28}$$

To derive the equation for the wave vector q of this excitation, we go back to (14a), which may be written as

$$k(x_0) = 2\pi x_0 + \int_{-\alpha}^{\alpha} d\eta \cot^{-1}\frac{\tilde{\xi}_0 - \eta}{2} f(\eta) \tag{29}$$

in the $N \to \infty$ limit. Using (13) and (29), we obtain

$$q = 2\pi x_0$$

$$= \pi(1-\rho) - 2\tan^{-1}\tilde{\xi}_0 + \int_{-\alpha}^{\alpha} d\eta \tan^{-1}\frac{\tilde{\xi}_0 - \eta}{2} f(\eta).$$

$$(0 \le q \le \pi(1-2\rho)) \tag{30}$$

The set, (28) and (30), supplemented with linear integral equations (27) and (20) determines the dispersion relation of the particle-like branch. What remains is to determine the relation between H and α. This can be achieved by minimizing ε_{gr} in (22) with respect to α to result in

$$h = \frac{2}{1+\alpha^2} + \int_{-\alpha}^{\alpha} d\tilde{\xi} \frac{\tilde{\xi}}{(1+\tilde{\xi}^2)^2} k_H(\tilde{\xi}), \tag{31}$$

where $k_H(\tilde{\xi})$ is an odd function defined by

$$\frac{\partial k_H(\tilde{\xi})}{\partial \tilde{\xi}} = \frac{4(\partial f(\tilde{\xi})/\partial\alpha)}{2f(\alpha) + \int_{-\alpha}^{\alpha} d\tilde{\xi}(\partial f(\tilde{\xi})/\partial\alpha)}. \tag{32}$$

Differentiating (20) with respect to α and rewriting the result we find the equation for $k_H(\tilde{\xi})$:

$$k_H(\tilde{\xi}) = \frac{2}{\pi}\left(\tan^{-1}\frac{\alpha-\tilde{\xi}}{2} - \tan^{-1}\frac{\alpha+\tilde{\xi}}{2}\right)$$

$$- \frac{2}{\pi}\int_{-\alpha}^{\alpha} d\eta \frac{1}{4 + (\tilde{\xi}-\eta)^2} k_H(\eta). \tag{33}$$

The relations (31) and (33) determine α as a function of H.

2.3. *Hole-like branch*

The analysis of the hole-like branch can be made in a way similar to the previous subsection: Define a continuous variable x by $x = 1/N((1/2)N - r + 2j - 1)$. Then $\lambda(x)$, which we called λ_j previously, can be written as

$$\lambda(x) = x + \frac{1}{N}\theta(x - x_n),\qquad (34)$$

where θ is the step function and

$$x_n = \frac{1}{N}\cdot\left(\frac{1}{2}N - r + 2n - 1\right) \simeq \frac{1}{2} - \rho + \frac{2n}{N}.\qquad (35)$$

With these quantities (5) and (12) are expressed as

$$k(x) = 2\pi\lambda(x) + \frac{1}{N}\phi(x, x_0) + \frac{1}{2}\int_{(1/2)-\rho}^{(1/2)+\rho}dy\,\phi(x, y),\qquad (36)$$

where $x_0 = (1/2) - \rho$. Again we put

$$\begin{cases} k(x) = k_0(x) + \dfrac{1}{N}k_1(x), \\[2mm] \phi(x, y) = \phi_0(x, y) + \dfrac{1}{N}\phi_1(x, y). \end{cases}\qquad (37)$$

Substituting (37) into (36) and leaving the terms of $O(1/N)$ we have

$$k_1(x) = 2\pi\theta(x - x_n) + \phi(x, x_0) + \frac{1}{2}\int_{(1/2)-\rho}^{(1/2)+\rho}dy\,\phi_1(x, y),\qquad (38)$$

where $\phi_1(x, y)$ is the same function as in (18). With the use of ξ defined in (19) Eq. (38) is replaced by

$$k_1(\xi) = 2\pi\theta(\xi_0 - \xi) + 2\cot^{-1}\frac{\xi - \alpha}{2}$$

$$+ \int_{-\alpha}^{\alpha}d\eta\,f(\eta)\,\frac{(1 + \xi^2)k_1(\xi) - (1 + \eta^2)k_1(\eta)}{4 + (\xi - \eta)^2},\qquad (39)$$

where

$$\xi_0 = \cot\frac{k_0(x_n)}{2}.\qquad (40)$$

With the introduction of a new function $k_2(\xi)$

$$k_2(\xi) = (1 + \xi^2)f(\xi)k_1(\xi) - 4\theta(\xi_0 - \xi) - 2k_H(\xi),\qquad (41)$$

Eq. (39) can be transformed to a simpler integral equation

$$k_2(\xi) = -2 - \frac{4}{\pi}\tan^{-1}\frac{\xi_0 - \xi}{2} - \frac{2}{\pi}\int_{-\alpha}^{\alpha}d\eta\,\frac{1}{4 + (\xi - \eta)^2}k_2(\eta).\qquad (42)$$

$k_H(\xi)$ in (41) is the same function as in (33).

It turns out that only the odd part of $k_2(\xi)$, which we define as $-k_h(\xi)$, is needed to calculate the hole-like branch of the excitation spectrum. From (42) we have

$$k_h(\xi) = \frac{2}{\pi}\left(\tan^{-1}\frac{\xi_0-\xi}{2} - \tan^{-1}\frac{\xi_0+\xi}{2}\right)$$

$$-\frac{2}{\pi}\int_{-\alpha}^{\alpha}d\eta\,\frac{1}{4+(\xi-\eta)^2}k_h(\eta), \tag{43}$$

which corresponds to (27) for the particle-like branch. The excitation energy is given by

$$\varepsilon_h \equiv \varepsilon - \varepsilon_{\mathrm{gr}}$$

$$= h - (1-\cos k(x_0)) - \frac{1}{2}\int_{(1/2)-\rho}^{(1/2)+\rho}dx\,\sin k_0(x)\cdot k_1(x)$$

$$= -h + \frac{2}{1+\xi_0^2} + \int_{-\alpha}^{\alpha}d\xi\,\frac{\xi}{(1+\xi^2)^2}k_h(\xi). \tag{44}$$

To derive the wave vector q of the excitation we employ the equation

$$-\int_{\alpha}^{\xi_0}d\xi\,f(\xi) = \int_{(1/2)-\rho}^{x_n}dx = x_n - \frac{1}{2} + \rho = 1 - \frac{q}{\pi}, \tag{45}$$

which leads to

$$q = \pi - \pi\int_{\xi_0}^{\alpha}d\xi\,f(\xi). \qquad (\pi(1-2\rho)\leq q\leq\pi) \tag{46}$$

The set, (44) and (46), supplemented with integral equations (43) and (20) determines the dispersion relation of the hole-like branch. The relation between h and α has already been given in (31).

Thus we have extended the calculation of the dC-P spectrum to the finite-field case. Notice the parallelism in the particle-like and hole-like branches: (28) vs (44) and (27) vs (43). Analytic solutions of the equations seem difficult in general. However some features of the spectrum can be analytically studied. Moreover numerical calculations of the spectrum are easy to perform. Those results will be presented in the next subsection.

2.4. *Analytic results and numerical calculations*

(i) $\alpha\to 0$ limit:

By letting α go to zero in (31) the critical field h_{cr} is obtained as $h_{\mathrm{cr}}=2$.[*] In this case ρ goes to zero; the hole-like branch vanishes and the particle-like branch extends over the whole Brillouin zone $[-\pi,\pi]$. From (28) and (30) the spectrum is given by $\varepsilon_p = h-1+\cos q$, which is the expected spin wave spectrum for the ferromagnetic state.

(ii) $\alpha\to\infty$ limit:

In this limit h goes to zero and ρ approaches $1/2$; the particle-like branch

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[*] Since the anisotropy energy is absent in (1), the spin-flop state is realized for finite magnetic fields. The critical field is defined here as a minimum field to obtain the complete ferromagnetic state.

is reduced to zero and the hole-like branch extends the whole interval $[-\pi, \pi]$. From (43), (44) and (46) we easily obtain the dC-P spectrum

$$\varepsilon_h = \frac{\pi}{2} |\sin q|. \tag{47}$$

(iii)   To see the spectrum near $q=0$ at intermediate field strengths, let us assume $\xi_0 \gg 1$. We find then from (30) and (27)

$$q \simeq 2(1-2\rho)\frac{1}{\xi_0} \tag{48}$$

and

$$k_p(\xi) \simeq -\frac{8}{\pi}\frac{1}{\xi_0^2}\xi - \frac{2}{\pi}\int_{-\alpha}^{\alpha}d\eta\,\frac{1}{4+(\xi-\eta)^2}k_p(\eta), \tag{49}$$

respectively.   The solution of (49) is of the form

$$k_p(\xi) = \frac{1}{\xi_0^2}\gamma(\xi).$$

Therefore the excitation energy ε_p is given by

$$\varepsilon_p \simeq h - \frac{2}{\xi_0^2} - \int_{-\alpha}^{\alpha}d\xi\,\frac{\xi}{(1+\xi^2)^2}k_p(\xi)$$

$$\simeq h - \frac{q^2}{4(1-2\rho)^2}\left[2 + \int_{-\alpha}^{\alpha}d\xi\,\frac{\xi}{(1+\xi^2)^2}\gamma(\xi)\right] \tag{50}$$

for small q.

(iv)   To see the energy of the particle-like branch at its end point $q=\pi(1-2\rho)$, we put $\xi_0 \to \alpha + 0$. In this limit $k_p(\xi) = k_H(\xi)$, which leads to

$$\varepsilon_p \to 0 \quad \text{for} \quad q \to \pi(1-2\rho) - 0.$$

In the same way we find that

$$\varepsilon_h \to 0 \quad \text{for} \quad q \to \pi(1-2\rho) + 0.$$

In addition to this it is easy to show that ε_p as well as ε_h is proportional to the deviation of q from the end point $\pi(1-2\rho)$.

(v)   As for the hole-like branch it is shown that the spectrum is symmetric with respect to the middle point $q=\pi(1-\rho)$. One can easily see this by replacing ξ_0 by $-\xi_0$ in (43), (44) and (46) and remembering that $f(\xi)$ is an even function of ξ. This symmetry leads to $\varepsilon_h=0$ at $q=\pi$.

(vi)   For numerical calculations of the spectrum the integral equations (20), (27), (33) and (43) have been solved by approximating them by 41 coupled linear equations. The solutions were used to determine the magnetic-field dependence of the spectrum. Figure 1 shows the α vs h and α vs ρ relations. The dispersion relation of the dC-P spectrum is shown in Fig. 2. A remarkable feature of the

spectrum is that it goes to zero at $q = \pi(1-2\rho) = 2\pi\sigma$ (σ: magnetization). This feature is common to the excitation spectrum of the 1D XY model in a magnetic field as will be discussed in the next section.
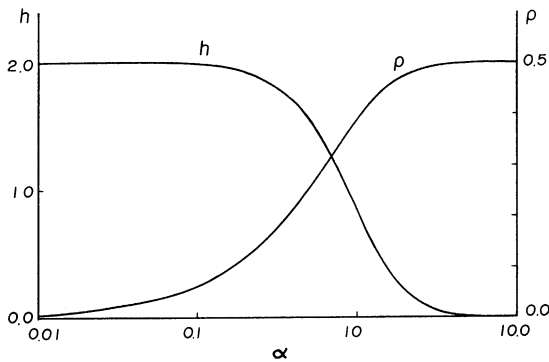

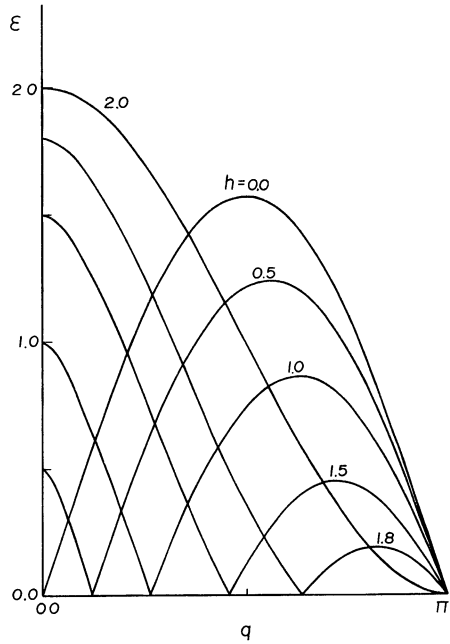Fig. 1. $h(\equiv g\mu_B H/2J)$ and ρ as a function of α.

Fig. 2. The dispersion relation of the one-spin-flop dC-P spectrum for some values of h.

§ 3. Discussion

(i) As we have mentioned in § 1, Pytte calculated the field dependence of the spin-wave spectrum of the system (1), using the Bulaevskii approximation:[5] The XY part of the isotropic exchange Hamiltonian is treated exactly with the Fermion representation, while the Ising part is taken into account only within the Hartree-Fock approximation. This theory predicts the excitation spectrum similar to that of the 1D XY model as expected. In Fig. 3 we reproduce for comparison Pytte's prediction[4] for the spin wave spectrum. As a matter of fact his spectrum consists of two branches for each q. The overall feature of the lower part of his spectrum (shown with solid lines in Fig. 3) is close to our result in Fig. 2.[*] Therefore the feature of our spectrum that it goes to zero at $q = 2\pi\sigma$ may be understood as a property common to the 1D XY model. Some differences between Figs. 2 and 3 are easily noticeable: according to (50) $\varepsilon_p(q) = h - cq^2$ for small q. The relation $\lim_{q\to 0}\varepsilon_p(q) = h$ should hold for the one-spin-flop excited state. The Pytte theory, however, does not satisfy this condition presumably due to his unequal

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[*] His spectrum also goes to zero at $q = 2\pi\sigma$, although the H dependence of σ in the Pytte theory is slightly different from Griffiths's exact result.

treatment of the XY and Z parts of the isotropic Hamiltonian.

(ii) Let us turn to the spin-wave spectrum in the classical (Anderson) theory. Here it is assumed that the sublattice magnetizations are perpendicular to the weak field and cant along the field axis with the increase of the field. By starting with this configuration in the ground state the classical spin wave can be easily calculated as[9]

$$\left(\frac{h\omega_\pm(q)}{2JzS}\right)^2 = (1 \pm \gamma_q)\left(1 \mp \left(1 - \frac{h^2}{2}\right)\gamma_q\right),$$

$$\left(-\frac{\pi}{2} \leq q \leq \frac{\pi}{2}\right) \qquad (51)$$

where $z = 2$, $S = 1/2$ and $\gamma_q = \cos q$ in the present case. Unfolding the spectrum into the original Brillouin zone as

$$\begin{cases} \omega = \omega_+ & \text{for} \quad -\pi/2 \leq q \leq \pi/2, \\ \omega = \omega_- & \text{for} \quad \pi/2 \leq q \leq \pi \end{cases}$$

$$\text{or} \quad -\pi \leq q \leq -\pi/2,$$
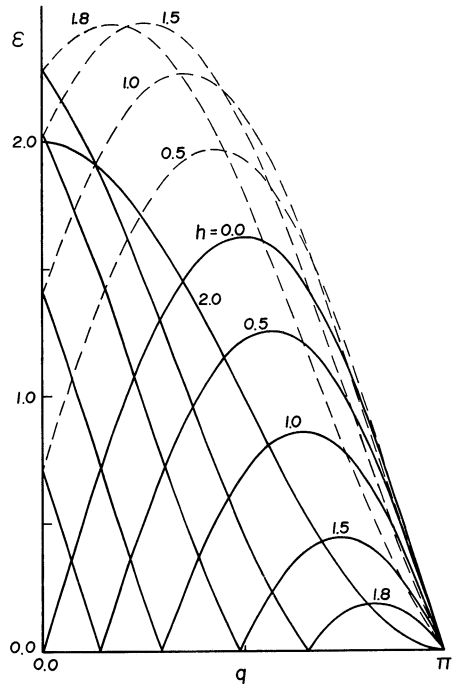
$$(52)$$

Fig. 3. The magnetic field dependence of the spin-wave spectrum calculated by Pytte.[4] His spectrum consists of two branches for each wave vector. The broken lines show the upper branch of the spectrum.

one may compare it with our result. Although the $q \to 0$ and $q \to \pm\pi$ limits of (52) are in agreement with ours, the q dependence in (52) is different from our spectrum. Especially the spectrum (52) does not go to zero between 0 and π.

(iii) In this paper we have calculated the one-spin flop dC-P spectrum in a magnetic field; however we have not yet examined whether the spin-wave excitation is dominated by this dC-P spectrum or not. In other words we have not evaluated the contribution of the dC-P spectrum to the intensity of magnetic excitations. This will be left for a future study. It is very likely that our dC-P spectrum is the lower bound of the spin excitation *continuum*: above the dC-P excitation energy there should exist continuously other types of excitations, which correspond to many-particle-hole simultaneous excitations.[*] If it is true, the wave vector $2\pi\sigma$, at which the spectrum goes to zero, might correspond to the wave vector of the spin-Peierls instability,[10),11)] as Pytte argues.[4]

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[*] In fact, in the case of the 1D XY model the operator S_j^+ (or S_j^-) is not equivalent to a single Fermion operator, but to a combination of odd number of Fermion operators.[6] Therefore the motion of S_j^+ is described by a combination of simultaneous many Fermion excitations.

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