CHAPTER III

CALCULATION OF SOME THERMODYNAMIC QUANTITIES OF 1D SPIN-1/2 XY MODEL USING STATIC SPIN-SPAN CORRELATION FUNCTION.

3.1 INTRODUCTION.

The essential quantity that enters most important physical properties is the spin-spin correlation function. The results of the calculations of finite temperature correlation functions have been applied to calculate the longitudinal susceptibility of isotropic XY model, specific heat and static structure factor of anisotropic XY system. The zero-field longitudinal susceptibility $\chi_z$ and the specific heat ($c$) of anisotropic XY chain have already been calculated by Katsura in a different way. Katsura considered a 1d spin-1/2 anisotropic Heisenberg Hamiltonian in presence of magnetic field,

$$H = -2J \sum_{i=1}^{N} (J_x S_i x S_{i+1} + J_y S_i y S_{i+1} + J_z S_i z S_{i+1}) - g \mu_B H \sum_{i=1}^{N} S_i z$$  \hspace{1cm} (1)$$

The Hamiltonian was diagonalized when $J_z=0$ ie for anisotropic XY model with the help of Jordan Wigner transformation and the partition function was derived. From the derivatives of this partition function the specific heat and the susceptibility were derived. Tonegawa calculated the static
structure factor for isotropic XY model. For zero temperature he made an analytic calculation, but for finite temperature he followed the formalism of Lieb, Schultz and Mattis\textsuperscript{18} to calculate the correlation functions. For anisotropic XY system no such calculations exist for static structure factor.

3.2 CALCULATION OF LONGITUDINAL SUSCEPTIBILITY ($\chi_z$) OF ISOTROPIC SPIN-1/2 XY MODEL.

Here we shall report the calculation of zero-field longitudinal susceptibility $\chi_z$. In the calculation of $\chi_z$ as given by Katsura\textsuperscript{19} there is a lowering of the susceptibility curve as $T \to 0$ which is not correct and it arises because of a numerical error in the calculation. Katsura published an erratum\textsuperscript{(67)} in which he pointed out this error and showed that $\chi_z |J|/Nm^2 (m=0.5\mu_B)$ should tend to a constant value $2/\pi$ as $T \to 0$ and the results of $\chi_z |J|/Nm^2$ are wrong for the part $0 < 2kT/|J| < 0.25$. The correct values are obtained in our present calculations\textsuperscript{(66)} where $\chi_z$ is calculated exactly using linear response theory. Katsura and Inawashiro\textsuperscript{68} solved the Hamiltonian (1) with $J_x=J_y$ by the linked-cluster expansion method and obtained results up to second order in the anisotropy parameter $J_z/J_x$. The zeroth-order result of this Hamiltonian corresponds to spin-1/2 XY model calculations and gives the correct values of $\chi_z$. We have, however, approached this in a different way to
solve for $\chi_z$ of 1D isotropic spin-1/2 XY model and obtained the correct results. In our present calculations the Hamiltonian is

$$\mathcal{H} = \mathcal{H}_0 + V$$

$$\mathcal{H}_0 = -2J \sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) \quad V = g \mu_B H \sum_{i=1}^{N} S_i^z$$

(2)

$$S_{N+1} = S_1$$

The Hamiltonian $\mathcal{H}_0$ has been diagonalised by Lieb et al$^{18}$ (1961). The zero-field finite temperature susceptibility is calculated using the linear response theory. In the theory, $V$ is treated as a perturbation over $\mathcal{H}_0$ and only the terms linear in $H$ in the expression for the magnetisation are retained.

The magnetization per spin at temperature $T$ is

$$M_z = (g \mu_B/N) \sum_i \frac{\text{Tr}[\exp(-\beta H)S_i^z]}{\text{Tr}[\exp(-\beta H)]}$$

(3)

To the first order in $V$, one obtains

$$\exp(-\beta H) = \exp(-\beta \mathcal{H}_0) \left[ 1 - \int_0^\beta \exp(\beta \mathcal{H}_0) V \exp(-\beta \mathcal{H}_0) dt \right]$$

(4)

Using this we get

$$\frac{\text{Tr}[\exp(-\beta H)S_i^z]}{\text{Tr}[\exp(-\beta H)]} = \frac{1}{\beta} \int_0^\beta \langle S_i^z \rangle \exp(\beta \mathcal{H}_0) dt$$

$$\langle S_i^z \rangle$$

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\[ V \exp(-\mathcal{H}_0) \langle \langle \exp(-\mathcal{H}_0)S_i^Z \rangle \rangle \]

where \[ \langle \langle A \rangle \rangle = \frac{\text{Tr} \left[ \exp(-\beta \mathcal{H}_0) A \right]}{\text{Tr} \left[ \exp(-\beta \mathcal{H}_0) \right]} \]

\[ M_z = \frac{\mu_B}{N} \sum_{i=1}^{N} \langle \langle S_i^Z(0) \rangle \rangle \mu_B H \int_0^\beta \text{dt} \left[ \langle \langle S_i^Z(t) \rangle \rangle \langle \langle S_i^Z(0) \rangle \rangle \langle \langle S_i^Z(t) S_i^Z(0) \rangle \rangle \right] \]

(7)

where, \[ S_i^Z(t) = \exp(\mathcal{H}_0) S_i^Z(0) \exp(-\mathcal{H}_0) \]

The zero field susceptibility

\[ \chi_z = \frac{\partial M_z}{\partial H} \bigg|_{H \rightarrow 0} = \frac{\mu_B^2}{N} \sum_{i=1}^{N} \int_0^\beta \text{dt} \langle \langle S_i^Z(t) S_i^Z(0) \rangle \rangle \langle \langle S_i^Z(t) \rangle \rangle \langle \langle S_i^Z(0) \rangle \rangle \]

\[ \langle \langle S_i^Z(t) \rangle \rangle \]

(8)

For 1d XY model spontaneous magnetization is zero, i.e., \[ \langle \langle S_i^Z \rangle \rangle = 0 \]

So

\[ \chi_z = \frac{\mu_B^2}{N} \sum_{i=1}^{N} \int_0^\beta \text{dt} \langle \langle S_i^Z(0) \rangle \rangle \langle \langle S_i^Z(t) \rangle \rangle \langle \langle S_i^Z(t) \rangle \rangle \]

(9)

Since \[ \sum_{i=1}^{N} S_i^Z \] commutes with \[ \mathcal{H}_0 \]

\[ \sum_{j} S_j^Z(t) = \sum_{j=1}^{N} \exp(\mathcal{H}_0) S_j^Z(0) \exp(-\mathcal{H}_0) = \sum_{j} S_j^Z(0) \]

(10)

Therefore, \[ \chi_z = \frac{\mu_B^2}{N} \sum_{i=1}^{N} \int_0^\beta \text{dt} \langle \langle S_i^Z S_i^Z \rangle \rangle \]

(11)
\[ \rho_r = \rho_{-r} \]

\[ \chi_z = g^2 \mu_B^2 / kT \left( \rho_0 + 2 \sum_{r=1}^{\infty} \rho_r^2 \right) \]  \hspace{1cm} (12)

The molar susceptibility is given by

\[ \chi_M = N g^2 \mu_B^2 / kT \left( \rho_0 + 2 \sum_{r=1}^{\infty} \rho_r^2 \right) \]  \hspace{1cm} (13)

At any temperature \( T \), \( \rho_r^z \) is calculated using Eqn(20) of chapter II. As \( r \) increases \( \rho_r^z \) decreases and \( \sum_r \rho_r^z \) converges to a limiting value after a certain number \( N \) of \( r \)-values have been included in the summation. To compare with existing results\(^{(19)}\) we compute \( \chi_M |J|/Nm^2 \), and so we are interested in the sum

\[ S(N) = 4 |J|/kT \left( 2 \sum_{r=1}^{N} \rho_r^z + \rho_0 \right) \]  \hspace{1cm} (14)

The convergence is obtained when \( S(N+1) - S(N) \sim 10^{-6} \). As \( T \) decreases \( N \) increases and we go to lower and lower temperature. In Table 2 we show how the numbers \( N \) of appreciable terms in the summation varies with temperature. In this way we are able to reproduce the results at low temperature in the region \( 0 < 2kT/|J| < 0.25 \) in which Katsura obtained the wrong result. It is evident from our calculation also that \( \chi_M |J|/Nm^2 \) approaches \( 2/\pi \) as \( T \rightarrow 0 \) which was also calculated by Niemeijer\(^{(20)}\). In Fig 13 our results are shown by full line curve which agrees with the result of Katsura except at the low
temperature region where the results of Katsura are shown by broken line curve. Our present calculation is very simple and the susceptibility can be derived over the whole temperature range from a single expression.

Table 2: Variation in the number of terms in the summation with temperature.

| N   | $2kT/|J|$ | $\chi_M|J|/Nm^2$ |
|-----|---------|-----------------|
| 11  | 1.0     | 0.7125          |
| 14  | 0.8     | 0.6924          |
| 17  | 0.6     | 0.6678          |
| 23  | 0.4     | 0.6486          |
| 45  | 0.2     | 0.6392          |
| 75  | 0.1     | 0.6372          |
| 95  | 0.08    | 0.6370          |
| 139 | 0.06    | 0.6368          |
| 165 | 0.04    | 0.6367          |
Fig 13. Longitudinal susceptibility ($\chi_{\parallel}$) of isotropic model.
3.3 CALCULATION OF SPECIFIC HEAT OF ANISOTROPIC XY CHAIN USING SPIN-SPIN CORRELATION FUNCTION.

The specific heat of anisotropic XY chain has been calculated by Katsura\textsuperscript{19} as early as in 1962. Katsura considered a 1D anisotropic Heisenberg model in presence of a magnetic field along $z$ direction.

The Hamiltonian was solved exactly when $J_z = 0$, i.e. for anisotropic XY system. Katsura calculated analytically the partition function and the internal energy. From the internal energy the specific heat was calculated as

\[
C/Nk = \frac{1}{\pi(2kT)^2} \int \omega \left( \frac{1}{2J_x} \frac{1}{2J_y} \frac{1}{2J_z} \cos 2\omega \right) \cos^2 \left( \frac{1}{2J_z} \frac{1}{2J_y} \frac{1}{2J_x} \cos 2\omega \right)^{1/2} / 2kT 
\]

(16)

Here $J_x, J_y$ corresponds to the isotropic XY model and either $J_z = 0$ or $J_0 = 0$ corresponds to the Ising model.

Now we will report an alternative way of calculating the specific heat\textsuperscript{57} of 1d XY model. The internal energy is related to the nearest neighbour spin correlation functions by the relation

\[
E = <H> = -2J \sum_{i=1}^{N} \left[ (1+\alpha) <S_i^x S_{i+1}^x> + (1-\alpha) <S_i^y S_{i+1}^y> \right] 
\]

(17)
Fig 14  Variation of energy with temperature.
Fig 15. Variation of specific heat with temperature.
Where the Hamiltonian $H$ is

$$
H = -2J \sum_{i=1}^{N} \left( (1+\alpha)S_i^x S_{i+1}^x + (1-\alpha)S_i^y S_{i+1}^y \right)
$$

(18)

The nearest neighbour spin correlation function at finite $T$ are calculated exactly as described in sec 2.3. Using these correlation functions the internal energy is obtained as a function of temperature for different anisotropy. The results are shown in Fig 14. For $\alpha = 0$ curve the energies agree with Katsura's result but for $\alpha = 1$ the energies agree if one scales the interaction parameter by a factor of 2 as evident from Eqns (15) & (17). In the Ising limit our Hamiltonian becomes $H = -4J \sum S_i^x S_{i+1}^x$ where in Katsura's calculation the corresponding part is $H = -2J \sum S_i^x S_{i+1}^x$.

The specific heat is calculated by numerically differentiating the internal energy with respect to temperature. The results for various anisotropies are shown in Fig 15. For $\alpha = 0$, our results agree with Katsura's results whereas the results obtained by quantum transfer matrix method differ at low temperatures. In quantum transfer matrix method, results obtained by the real space decomposition seem to be better than those obtained by checker board decomposition.

3.4 STATIC STRUCTURE FACTOR OF ANISOTROPIC XY MODEL.

The static structure factor or the wave number dependent static
spin-pair correlation function is defined as

\[ S_\alpha(k) = \sum_{n=-\infty}^{+\infty} \exp(ikn)p_n^\alpha, \quad \alpha=x,y,z \]  \hspace{1cm} (19)

Tonegawa\(^{47}\) calculated the \( x \)-component of structure factor \( S_x(k) \) for ferromagnetic isotropic XY system. They performed analytical calculation at \( T=0 \) and showed that \( S_x(k) \) diverges as \( k^{-1/2} \) as \( k \rightarrow 0 \). They performed numerical calculation for finite temperature and showed that \( S_x(k) \) has a maximum at \( k=0 \). As temperature increases the curve becomes broader and the maximum value decreases. This is due to the fact that \( T=0 \) is the critical temperature and in the critical region only long wave length modes of the correlation function is dominant, so only near \( k=0 \) the structure factor has appreciable values. The longitudinal component of static structure factor \( S_z(k) \) has been calculated by Katsura et al\(^{71}\) for isotropic XY system. \( S_z(k) \) does not depend on the sign of \( J \). In their calculation \( S_z(k) \) does not diverge at \( T=0 \). It has a maximum value at \( k=\pi \) and minimum (\( S_z(k)=0 \)) at \( k=0 \).

At \( T=0 \) the structure factor can be calculated analytically for anisotropic system. For this system long range order exists at \( T=0 \) in the \( x \)-direction, i.e., \( p_n^x \) = constant when \( n \) is large.

Therefore,

\[
S_x(k) = \int_{-\infty}^{+\infty} e^{ikn}p_n^x \, dn
\]

\[
\sim \text{const} \int_{0}^{\infty} \cos(kn) \, dn
\]  \hspace{1cm} (20)
ie, $S_x(k)$ does not exist for $k \neq 0$ and $S_x(k) \rightarrow \alpha$ at $k=0$.

Now

$$S_z(k) = \sum_{n=-\infty}^{+\infty} e^{ikn} \rho_n$$

(21)

$$S_z(0) = \sum_{n} \rho_n^z = 0 \quad \text{for } \alpha=0$$

$$= 0.25 \quad \text{for } \alpha=1.0$$

For $0 \leq \alpha \leq 1$ $S_z(0)$ lies between 0 to 0.25

$$S_z(\pi) = \sum_{n=-\infty}^{+\infty} (-1)^n \rho_n^z = 0.5 \quad \text{for } \alpha=0$$

(22)

$$=0.25 \quad \text{for } \alpha=1.0$$

For $0 \leq \alpha \leq 1$ $S_z(\pi)$ lies between 0.5 to 0.25.

For finite $T$ ($T = 1.4K$) we have calculated $S_x(k)$, $S_y(k)$ & $S_z(k)$ for different anisotropies. In Fig 16, Fig 17 & Fig 18 there are plotted $S_x(k)$, $S_y(k)$, $S_z(k)$ respectively against $k$. The same calculation is repeated for $T = 0.4K$ and are shown in Figs. 19, 20 and 21. We find that the structure factor becomes narrower as we go to lower temperatures.

In our calculation we have derived the finite temperature correlation function and then calculated the structure factor following the relation

$$S_{\alpha}(k) = \sum_{n=-\infty}^{\infty} e^{ikn} \rho_n^\alpha$$

(23)
Fig 16. Structure factor in x-direction when temperature is 1.4K.
Fig 17. Structure factor in $y$-direction when temperature is 1.4K.
Fig 18. Structure factor in z-direction when temperature is 1.4K.
Fig 19. Structure factor in x-direction when temperature is $0.4\,\text{K}$.

$T = 0.4\,\text{K}$

$\alpha = 0.8$
Fig 20. Structure factor in y-direction when temperature is 0.4K.
Fig 21. Structure factor in z-direction when temperature is 0.4 K.
\[ v_n = \sum_{n=-\infty}^{\infty} e^{i kn} \rho_n + \frac{\alpha}{\alpha} + \rho_0 \]

\[ = \sum_{n=-\infty}^{\infty} (\cos(kn) + i \sin(kn)) \rho_n + \sum_{n=1}^{\infty} (\cos(kn) + i \sin(kn)) \rho_n + \rho_0 \]

Now \( \rho_n^{\alpha} = \rho_n^{-\alpha} \),

So \( S_\alpha(k) = 2 \sum_{n=1}^{\infty} \cos(kn) \rho_n^{\alpha} + \rho_0^{\alpha} \) \hspace{1cm} (24)

\[ = \rho_0^{\alpha} + 2 \rho_1^{\alpha} \cos(k) + 2 \rho_2^{\alpha} \cos(2k) + \ldots . \]

We have calculated the convergent value of the series by direct summing the terms. Now from the figures it is evident that for \( \alpha=0 \), \( S_x(k) \) and \( S_y(k) \) are same. As \( \alpha \) increases \( S_y(k) \) decreases from the isotropic curve i.e. \( S_y(k) \) becomes flatter and \( S_x(k) \) becomes sharper than the isotropic curve. Thus in the Ising limit \( S_y(k) \) curve becomes a flat straight line and \( S_x(k) \) shows a peak which becomes a vertical line at \( T = 0 \). The \( S_z(k) \) curve has minimum at \( k=0 \) and maximum at \( k=\pi \). It becomes flatter as \( \alpha \) increases and becomes a straight line at \( \alpha=1.0 \) which means in the Ising limit only \( x \)-component of structure factor is dominant and in this limit the Hamiltonian has only \( x \) component of the spin. It is interesting to note that in the isotropic system correlation length in \( z \)-direction diverges at \( T=0 \) but susceptibility \( \chi_z \) and structure factor \( S_z(k) \) has no divergence at \( T=0 \).