Part one

Thermodynamics of non-interacting systems and ground states of interacting systems

1

Free energy and correlation functions of the XY model

1.1 The isotropic XY model

1.1.1 Introduction and historical overview

As the simplest case of a solvable model we consider the following spin 1/2 Hamiltonian,

$$\mathcal{H} = J \sum_{i=1}^{N} S_i^x S_{i+1}^x + S_i^y S_{i+1}^y - 2h \sum_{i=1}^{N} S_i^z, \quad S_{N+1}^\alpha \equiv S_1^\alpha, \tag{1.1}$$

$$[S_k^\alpha, S_l^\beta] = i\delta_{kl}\epsilon_{\alpha\beta\gamma}S_k^\gamma. \tag{1.2}$$

Each site has two states: an up-spin state and a down-spin state. S_i^x and S_i^y are represented by the Pauli matrices,

$$S_j^x = \frac{1}{2}\sigma_j^x, \quad S_j^y = \frac{1}{2}\sigma_j^y, \quad S_j^z = \frac{1}{2}\sigma_j^z,$$

$$\sigma_j^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_j^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_j^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.3}$$

For this Hamiltonian there are 2^N states, and it can be transformed as follows:

$$\mathcal{H} = \frac{J}{2} \sum_{i=1}^{N} S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ - 2h \sum_{i=1}^{N} S_i^z, S_k^\pm \equiv S_k^x \pm iS_k^y. \tag{1.4}$$

Lieb, Schultz and Mattis[61] and Katsura[47] investigated this model in detail. The operators $S_k^\pm$ satisfy the relations

$$\{S_i^+, S_i^-\} = 1, \quad [S_i^+, S_j^-] = 0 \quad \text{for} \quad i \neq j. \tag{1.5}$$

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The above commutation relations are neither fermionic nor bosonic. But if we introduce the operators

$$c_k = \prod_{i=1}^{k-1}(2S_i^+ S_i^- - 1)S_k^+, \quad c_k^\dagger = S_k^- \prod_{i=1}^{k-1}(2S_i^+ S_i^- - 1),$$

these satisfy the fermionic commutation relations

$$\{c_k^\dagger, c_l\} = \delta_{kl}, \quad \{c_k, c_l\} = \{c_k^\dagger, c_l^\dagger\} = 0. \tag{1.6}$$

Fortunately one can find the expression for spin operators using these fermionic operators

$$S_k^- = \prod_{i=1}^{k-1}(1 - 2c_i^\dagger c_i)c_k^\dagger, \quad S_k^+ = \prod_{i=1}^{k-1}(1 - 2c_i^\dagger c_i)c_k. \tag{1.7}$$

The Hamiltonian (1.1) is transformed as

$$\mathcal{H} = -\frac{J}{2}\sum_{i=1}^{N-1} c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1} + \frac{J}{2}\alpha(c_1^\dagger c_N + c_N^\dagger c_1) - hN + 2h\sum_{i=1}^{N} c_i^\dagger c_i, \tag{1.8}$$

where $\alpha \equiv \prod_{k=1}^{N}(1 - 2c_k^\dagger c_k)$. The total number of down-spins M is a constant of motion. The value of α is $(-1)^M$. We introduce the Fourier transformation of these fermionic operators:

$$c_q = \frac{1}{\sqrt{N}}\sum_{k=1}^{N}\exp(-iqk)c_k, \quad q = 2\pi n/N, \tag{1.9}$$

where n is integer (half-odd integer) for odd (even) M. These operators satisfy

$$\{c_q, c_p\} = \{c_q^\dagger, c_p^\dagger\} = 0, \quad \{c_q, c_p^\dagger\} = \delta_{pq}. \tag{1.10}$$

The Hamiltonian is the same as that of one-dimensional spinless fermions

$$\mathcal{H} = -hN + \sum_q (2h - J\cos q)c_q^\dagger c_q. \tag{1.11}$$

The lowest energy state at fixed M is

$$\prod_{l=1}^{M} c_{\pi(M+1-2l)/N}^\dagger |0\rangle, \tag{1.12}$$

and the total energy is

$$-h(N - 2M) - J\sum_{l=1}^{M}\cos(\pi(M + 1 - 2l)/N). \tag{1.13}$$

In this way the XY model is treated by the transformation of spin operators to fermion operators. (1.7) is called the Jordan–Wigner transformation.

1.1.2 Energy eigenvalues of the Hamiltonian and the partition function

General eigenstates for fixed M are

$$\prod_{j=1}^{M} c^\dagger (2\pi I_j/N)|0\rangle. \tag{1.14}$$

Here $\{I_1, I_2, ..., I_M\}$ is a set of different integers or half-odd integers. If two sets of integers are different, the two corresponding states are orthogonal. The total number of states with M down-spins and $N - M$ up-spins is given by the binomial coefficient

$$C_N^M = \frac{N!}{M!(N-M)!}. \tag{1.15}$$

The total number of states represented by (1.14) is

$$C_N^1 + C_N^2 + ... + C_N^N = 2^N. \tag{1.16}$$

Thus the states represented by (1.14) give a complete orthonormal set of eigenstates of the Hamiltonian (1.1).

The partition function of this system is

$$Z = z^{-N/2} \Big(\frac{1}{2} \Big[\prod_{l=1}^{N} \big(1 + ze^{\frac{J\cos(2\pi l/N)}{T}}\big) - \prod_{l=1}^{N} \big(1 - ze^{\frac{J\cos(2\pi l/N)}{T}}\big) \Big]$$
$$+ \frac{1}{2} \Big[\prod_{l=1}^{N} \big(1 + ze^{\frac{J\cos(\pi(2l-1)/N)}{T}}\big) + \prod_{l=1}^{N} \big(1 - ze^{\frac{J\cos(\pi(2l-1)/N)}{T}}\big) \Big] \Big), \tag{1.17}$$

where $z \equiv \exp(-2h/T)$. The first bracket gives the odd M states and the second gives the even M states. The second term in each bracket is much smaller than the first term, and so we can neglect them in the thermodynamic limit.

In the case of the lowest energy state, the energy per site in the large N, M limit is

$$e = -h + \frac{1}{2\pi} \int_{-\pi M/N}^{\pi M/N} (2h - J\cos q)dq$$
$$= -h(1 - 2M/N) + \Big(\frac{J\sin(\pi M/N)}{\pi} \Big). \tag{1.18}$$

The free energy per site in the thermodynamic limit is the same as for non-interacting fermions

$$f = -\frac{T}{N}\ln Z = -h - T\int_{-\pi}^{\pi}\ln[1+\exp(-(2h-J\cos q)/T)]\frac{\mathrm{d}q}{2\pi}. \qquad (1.19)$$

The entropy per site of this system is as follows,

$$s = -\frac{\partial f}{\partial T} = \int\frac{\mathrm{d}q}{2\pi}u\left(\frac{2h-J\cos q}{T}\right),$$

$$u(x) \equiv \ln(2\cosh x/2) - \frac{x}{2}\tanh x/2. \qquad (1.20)$$

The function $u(x)$ is a symmetric and rapidly decreasing function of x

$$u(x) = u(-x), \qquad \int_{-\infty}^{\infty}u(x)\mathrm{d}x = \frac{\pi^2}{3}. \qquad (1.21)$$

Thus the low-temperature entropy is

$$s \simeq \frac{1}{\pi}\frac{T}{J\cos^{-1}(2h/J)}\int_{-\infty}^{\infty}u(x)\mathrm{d}x = \frac{\pi T}{3J\cos^{-1}(2h/J)}. \qquad (1.22)$$

The specific heat per site is

$$C = T\frac{\partial s}{\partial T} = \frac{\pi T}{3J\cos^{-1}(2h/J)}. \qquad (1.23)$$

On the other hand the velocity of a low energy excitation is

$$v_s = J\cos^{-1}(2h/J).$$

Then the specific heat is written as

$$C = \frac{\pi T}{3v_s}. \qquad (1.24)$$

1.1.3 Correlation functions

The static correlation function $\langle S_l^z S_m^z\rangle$ is called the longitudinal correlation function and $\langle S_l^- S_m^+\rangle$ is the transverse correlation function. These can be calculated analytically[65]. In the fermion representation, the correlation functions are written as follows:

$$\langle S_l^z S_m^z\rangle = \langle(1-2c_l^\dagger c_l)(1-2c_m^\dagger c_m)\rangle/4 = \frac{1}{4} - \frac{M}{N} + \langle c_l^\dagger c_l c_m^\dagger c_m\rangle, \qquad (1.25)$$

$$\langle S_l^- S_m^+\rangle = \langle c_l^\dagger \prod_{k=l+1}^{m-1}(1-2c_k^\dagger c_k)c_m\rangle. \qquad (1.26)$$

It should be noted that the longitudinal correlation function is represented by averages of four fermion operators, but the transverse correlation function is represented by averages of many fermion operators. The value of $\langle c_l^\dagger c_l c_m^\dagger c_m \rangle$ is given by $\langle c_l^\dagger c_l \rangle \langle c_m^\dagger c_m \rangle - \langle c_l^\dagger c_m \rangle \langle c_m^\dagger c_l \rangle$. Here we have used Wick's theorem. Thus we have

$$\langle S_l^z S_m^z \rangle = \left(\frac{1}{2} - \frac{M}{N} \right)^2 - u_{lm} u_{ml}, \qquad (1.27)$$

$$u_{lm} \equiv \langle c_l^\dagger c_m \rangle. \qquad (1.28)$$

In principle we can decompose the thermal average of complicated operators of non-interacting fermions into products of averages of two fermion operators using Wick's theorem. Thus we can calculate (1.26) analytically. The highest order term is

$$(-2)^{m-l-1} \langle c_l^\dagger \prod_{k=l+1}^{m-1} (c_k^\dagger c_k) c_m \rangle.$$

This is decomposed as

$$2^{m-l-1} \det \begin{bmatrix} u_{l,l+1} & u_{l+1,l+1} & u_{l+2,l+1} & \cdots & u_{m-1,l+1} \\ u_{l,l+2} & u_{l+1,l+2} & u_{l+2,l+2} & \cdots & u_{m-1,l+2} \\ u_{l,l+3} & u_{l+1,l+3} & u_{l+2,l+3} & \cdots & u_{m-1,l+3} \\ . & . & . & \cdots & . \\ . & . & . & \cdots & . \\ u_{l,m} & u_{l+1,m} & u_{l+2,m} & \cdots & u_{m-1,m} \end{bmatrix}.$$

The other terms are also written as determinants of this kind. Summing up all terms we have the transverse correlation function,

$$\langle S_l^- S_m^+ \rangle = 2^{m-l-1} \times \det$$
$$\begin{bmatrix} u_{l,l+1} & u_{l+1,l+1} - \frac{1}{2} & u_{l+2,l+1} & . & u_{m-1,l+1} \\ u_{l,l+2} & u_{l+1,l+2} & u_{l+2,l+2} - \frac{1}{2} & . & u_{m-1,l+2} \\ u_{l,l+3} & u_{l+1,l+3} & u_{l+2,l+3} & . & u_{m-1,l+3} \\ . & . & . & . & . \\ u_{l,m-1} & u_{l+1,m-1} & u_{l+2,m-1} & . & u_{m-1,m-1} - \frac{1}{2} \\ u_{l,m} & u_{l+1,m} & u_{l+2,m} & . & u_{m-1,m} \end{bmatrix}.$$

In the limit $N \to \infty$ we have u_{lm} for the ground state at $N = 2M$

$$u_{lm} = \frac{1}{2\pi} \int_{-\pi/2}^{\pi/2} e^{ik(l-m)} dk = \begin{cases} \frac{1}{2} & \text{for } l = m, \\ \frac{\sin \pi(l-m)/2}{\pi(l-m)} & \text{for } l \neq m. \end{cases}$$

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Then we have the longitudinal correlation function

$$\langle S_l^z S_m^z \rangle = \begin{cases} \frac{1}{4} & \text{for } l = m, \\ -(1 - (-1)^{l-m})\frac{1}{\pi^2(l-m)^2} & \text{for } l \neq m. \end{cases} \qquad (1.29)$$

and a determinant expression of the transverse correlation function,

$$S_{xy}(m - l) = 2\langle S_l^- S_m^+ \rangle =$$

$$2^{m-l}\pi^{-(m-l)}\det \begin{bmatrix} 1 & 0 & 1 & 0 & -\frac{1}{3} & \cdots \\ 0 & 1 & 0 & 1 & 0 & \cdots \\ -\frac{1}{3} & 0 & 1 & 0 & 1 & \cdots \\ . & . & . & \cdots & . & \\ . & . & . & \cdots & . & \\ . & . & -\frac{1}{3} & 0 & 1 & 0 \\ . & . & 0 & -\frac{1}{3} & 0 & 1 \end{bmatrix}. \qquad (1.30)$$

The determinant is represented by A_n^2 for $l - m = 2n$ and $A_n A_{n-1}$ for $l - m = 2n - 1$, where A_n is the determinant of an $n \times n$ matrix with elements $x_{i,j} = (-1)^{i-j}/(2(i - j) + 1)$,

$$A_n \equiv \det \begin{bmatrix} 1 & 1 & -\frac{1}{3} & \cdots & \frac{(-1)^n}{2n-3} \\ -\frac{1}{3} & 1 & 1 & \cdots & \\ . & . & . & \cdots & . \\ . & . & . & \cdots & . \\ . & . & -\frac{1}{3} & 1 & 1 \\ \frac{(-1)^{n-1}}{2n-1} & . & . & -\frac{1}{3} & 1 \end{bmatrix}. \qquad (1.31)$$

One can eliminate $x_{1,j}, j \geq 2$ by putting $x'_{i,j} = x_{i,j} - x_{i,1}x_{1,j}$ without changing the value of the determinant. The new elements are

$$\frac{4(i-1)(j-1)(-1)^{i-j}}{(2i-1)(2j-3)(2(i-j)+1)}, \quad j \geq 2.$$

By this operation one gets the following recursion relation:

$$A_1 = 1, \quad A_n = \frac{((2n-2)!!)^2}{(2n-1)!!(2n-3)!!}A_{n-1}. \qquad (1.32)$$

Then we have

$$A_n = \prod_{j=1}^{n-1} \frac{(2n-2j)^{2j}}{(2n+1-2j)^{2j-1}}. \qquad (1.33)$$

If we define $B_n = (2/\pi)^n A_n$, the two-point function is given as

$$S_{xy}(2n) = B_n^2, \quad S_{xy}(2n-1) = B_n B_{n-1}.$$

B_n satisfies:

$$\frac{B_{n+1}}{B_n} = \frac{2}{\pi} \prod_{j=1}^{n} \left(1 - \left(\frac{1}{2j}\right)^2\right)^{-1}.$$

Using $2/\pi = \prod_{j=1}^{\infty}(1 - (2j)^{-2})$, we have:

$$\ln \frac{B_{n+1}}{B_n} = \sum_{j=n+1}^{\infty} \ln(1 - (2j)^{-2}) \simeq -\frac{1}{4n}. \qquad (1.34)$$

Then we can expect that B_n behaves as $n^{-1/4}$. The two-point function $S_{xy}(n)$ decays as $n^{-1/2}$. On the other hand, $S_{zz}(n)$ decays as n^{-2}. Thus the correlation exponents are different for S_{zz} and S_{xy}. We find that two-point functions decay algebraically and not exponentially at zero temperature. At finite temperature these decay exponentially.

1.2 The anisotropic XY model

We consider the anisotropic case of the XY model:

$$\mathscr{H} = \sum_{j=1}^{N} J_x S_j^x S_{j+1}^x + J_y S_j^y S_{j+1}^y - 2h \sum_{j=1}^{N} S_j^z. \qquad (1.35)$$

This is written in terms of $S^{\pm}$ operators as follows:

$$\mathscr{H} = \frac{1}{2} \sum_{j=1}^{N} J(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+) + J'(S_j^+ S_{j+1}^+ + S_j^- S_{j+1}^-)$$

$$-2h \sum_{j=1}^{N} S_j^z, \quad J \equiv \frac{J_x + J_y}{2}, \quad J' \equiv \frac{J_x - J_y}{2}. \qquad (1.36)$$

This Hamiltonian changes the number of down-spins by two. Thus space is divided by the parity of number of down-spins. By the Jordan–Wigner transformation (1.7) we have

$$\mathscr{H} = -\frac{J}{2} \left[-\alpha(c_1^\dagger c_N + c_N^\dagger c_1) + \sum_{j=1}^{N-1} c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}\right]$$

$$-\frac{J'}{2} \left[-\alpha(c_1^\dagger c_N^\dagger + c_N c_1) + \sum_{j=1}^{N-1} c_{j+1}^\dagger c_j^\dagger + c_j c_{j+1}\right]$$

$$-hN + 2h \sum_{j=1}^{N} c_j^\dagger c_j, \quad \alpha = \prod(1 - 2c_j^\dagger c_j). \qquad (1.37)$$

We can show that $\alpha^2 = 1$ and $[\mathscr{H}, \alpha] = 0$. The Hamiltonian and α are simultaneously diagonalized and the eigenvalue of α is ± 1. The Fourier transformation of these fermionic operators is

$$c_q = \frac{1}{\sqrt{N}} \frac{1-i}{\sqrt{2}} \sum_{k=1}^{N} \exp(-iqk)c_k, \quad q = 2\pi n/N, \tag{1.38}$$

where n is integer (half-odd integer) for $\alpha = -1(+1)$.

$$\mathscr{H} = -hN + \sum_{q}{}' (2h - J\cos q)(c_q^\dagger c_q + c_{-q}^\dagger c_{-q}) + J'\sin q(c_q^\dagger c_{-q}^\dagger + c_{-q}c_q). \tag{1.39}$$

Here $\sum_{q}'$ means the sum over $0 < q < \pi$.

1.2.1 The subspace $\alpha = 1$

In this Hamiltonian, particles with momentum q and $-q$ are coupled. We apply the following transformation for fermion operators c_q and c_{-q},

$$c_q = \cos\theta_q \eta_q + \sin\theta_q \eta_{-q}^\dagger, \quad c_{-q} = -\sin\theta_q \eta_q^\dagger + \cos\theta_q \eta_{-q},$$
$$\eta_q = \cos\theta_q c_q - \sin\theta_q c_{-q}^\dagger, \quad \eta_{-q} = +\sin\theta_q c_q^\dagger + \cos\theta_q c_{-q}. \tag{1.40}$$

$Nq/2\pi$ is half-odd integer. The Hamiltonian (1.36) is transformed as

$$\mathscr{H} = -hN + \sum_{q}{}' 2\sin^2\theta_q(2h - J\cos q) + 2\sin\theta_q\cos\theta_q J'\sin q$$

$$+[(2h - J\cos q)\cos 2\theta_q - J'\sin q \sin 2\theta_q](\eta_q^\dagger\eta_q + \eta_{-q}^\dagger\eta_{-q})$$

$$+[(2h - J\cos q)\sin 2\theta_q + J'\sin q \cos 2\theta_q](\eta_q^\dagger\eta_{-q}^\dagger + \eta_{-q}\eta_q). \tag{1.41}$$

The last term is removed if we put

$$\tan 2\theta_q = \frac{J'\sin q}{J\cos q - 2h}. \tag{1.42}$$

Thus the Hamiltonian becomes

$$\mathscr{H} = \sum_q \epsilon(q)(\eta_q^\dagger\eta_q - \frac{1}{2}),$$

$$\epsilon(q) = \sqrt{(J\cos q - 2h)^2 + (J'\sin q)^2}. \tag{1.43}$$

The lowest energy state $|\Psi\rangle$ must satisfy $\eta_q|\Psi\rangle = 0$. The following state satisfies this condition,

$$|\Psi\rangle = \prod_{q}{}' (\cos\theta_q + \sin\theta_q c_q^\dagger c_{-q}^\dagger)|0\rangle. \tag{1.44}$$

As we are considering the case $\alpha = 1$, the total number of quasi particles must be even. So the number of states which belong to this subspace is not 2^N but $\sum_j C_{2j}^N = 2^{N-1}$.

1.2.2 The subspace $\alpha = -1$

The number of particles must be odd in this subspace. Then the Hamiltonian is the same form as (1.43) but $qN/2\pi$ must be an integer. The lowest energy state in this subspace is

$$|\Psi\rangle = c_0^\dagger \prod_q{}' (\cos\theta_q + \sin\theta_q c_q^\dagger c_{-q}^\dagger)|0\rangle. \qquad (1.45)$$

The general states are given by an even number of excitations from this state. The number of states is also 2^{N-1}. These states are orthogonal to each other and therefore all these states together form a complete set of wave vectors.

1.2.3 The free energy

Using the results of 1.2.1 and 1.2.2, one obtains the partition function of the system,

$$Z = \exp\left(\frac{\sum_q \epsilon(q)}{2T}\right)\frac{1}{2}\left\{\prod_q(1 + e^{-\epsilon(q)/T}) + \prod_q(1 - e^{-\epsilon(q)/T})\right\}$$
$$+ \exp\left(\frac{\sum_{q'} \epsilon(q')}{2T}\right)\frac{1}{2}\left\{\prod_{q'}(1 + e^{-\epsilon(q')/T}) - \prod_{q'}(1 - e^{-\epsilon(q')/T})\right\}, \qquad (1.46)$$

where $qN/2\pi$ is a half-odd integer and $q'N/2\pi$ is an integer. In the thermodynamic limit the second term in $\{\ldots\}$ is much smaller than the first term and we obtain the free energy per site. The free energy is given by the logarithm of the partition function

$$f = -\frac{T}{N}\ln Z$$
$$= e_0 - \frac{T}{2\pi}\int_{-\pi}^{\pi}\ln(1 + \exp(-\sqrt{(J\cos q - 2h)^2 + (J'\sin q)^2}/T))dq.$$
$$(1.47)$$

Here e_0 is the ground state energy per site

$$e_0 = -\frac{1}{4\pi}\int_{-\pi}^{\pi}\sqrt{(J\cos q - 2h)^2 + (J'\sin q)^2}dq.$$

2

Systems with a delta-function potential

2.1 The boson problem

2.1.1 The $c = 0$ case

Here we consider the system

$$\mathcal{H} = -\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + 2c \sum_{i<j} \delta(x_i - x_j). \tag{2.1}$$

At first we consider the cases $c = 0$ and $c = \infty$. We assume periodic boundary conditions.

In second quantized form, the Hamiltonian (2.1) at $c = 0$ is written as

$$\mathcal{H} = \sum_k k^2 a_k^\dagger a_k, \quad k = 2\pi n/L,$$

$$[a_k, a_q^\dagger] = \delta_{k,q}, \quad [a_k, a_q] = [a_k^\dagger, a_q^\dagger] = 0. \tag{2.2}$$

The eigenstates and eigenvalues are given by

$$\prod_k (n_k!)^{-1/2} (a_k^\dagger)^{n_k} |0\rangle, \quad \sum_k k^2 n_k. \tag{2.3}$$

A set of integers $\{n_k\}$ gives an eigenstate. The ground state of this system is $n_0 = N$, $n_{k \neq 0} = 0$. The partition function of the grand canonical ensemble at chemical potential A is

$$\Xi = \prod_k \sum_{n_k = 0,1,2,\dots} \exp(-(k^2 - A)n_k/T) = \prod_k (1 - \exp[-(k^2 - A)/T])^{-1}. \tag{2.4}$$

The Gibbs free energy is given by

$$G = -T \ln \Xi = T \sum_k \ln(1 - \exp[-(k^2 - A)/T]). \tag{2.5}$$

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