Ising Model in Two Dimensions

Contents

Chapter 1

Introduction

In a landmark paper, Onsager [1] exactly calculated the free energy of the two-dimensional ferromagnetic Ising model in a zero mahnetic field on a reguler lattice. Since his original paper, a number of more transparent solutions to the problem have appeared. Here we present the solution given by Schultz et al. [2].

We also explain the low and high temperature expansions of the partition function, and prove the Kramers-Wannier duality.

Chapter 2

Ising Model in One Dimension

The Ising model of a ferromagnet or antiferromagnet on a lattice. It was first studied in 1925 by Lenz ans Ising, who showed that in one dimension the model does not have a phase transition for $T > 0$. They concluded (incorrectly) that this model does not exhibit a phase transition at non-zero temperature for $d > 1$, and so could not describe real magnetic systems.

2.1 Ising model

The degrees of freedom are classical spin variables S_i, residing on vertices of a $1d$ lattice, which take two values: up and down:

$$S_i = \pm 1.$$

The spins interact with an external magnetic field and with each other through exchange interactions J which couple two spins.

The form of the Hamiltonian is

$$H = -J \sum_{i=1}^{N-1} S_i S_{i+1} + h \sum_{i=1} S_i.$$

The partion function is given by

$$Z_N = \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} \exp \left\{ \beta J \sum_{i=1}^{N-1} S_i S_{i+1} + \beta h \sum_{i=1} S_i \right\}.$$

2.2 Transfer Matrix

The transfer matrix method reduces the problem of calculating the partition function to the problem of finding the eigenvalues of a certain matrix.

We consider periodic boudary conditions: $S_{N+1} = S_1$.

$$Z_N(h, K) = \sum_{S_1} \cdots \sum_{S_N} \left[e^{\frac{h}{2}(S_1+S_2)+KS_1S_2} \right] \cdot \left[e^{\frac{h}{2}(S_2+S_3)+KS_2S_3} \right] \cdots \left[e^{\frac{h}{2}(S_N+S_1)+KS_NS_1} \right]$$

We can think of each term as a matrix element of a matrix $\mathbf{V}$:

$$T_{S_1S_2} = e^{\frac{h}{2}(S_1+S_2)+KS_1S_2}$$

Observe that S_1 and S_2 are the labels of the matrix elements:

$$\mathbf{V} = \begin{pmatrix} V_{11} & V_{1-1} \\ V_{-11} & V_{-1-1} \end{pmatrix} = \begin{pmatrix} e^{h+K} & e^{-K} \\ e^{-K} & e^{-h+K} \end{pmatrix}$$

Then

$$Z_N(h, K) = \sum_{S_1} \cdots \sum_{S_N} V_{S_1S_2} V_{S_2S_3} V_{S_3S_4} \cdots V_{S_NS_1}.$$

Thus

$$Z_N(h, K) = \sum_{S_1} V^N_{S_1S_2} = \mathrm{Tr}(\mathbf{V}^N).$$

To compute $\mathrm{Tr}(\mathbf{V}^N)$ we first diagonalise $\mathbf{V}$, by multiplying with a matrix $\mathbf{S}$ whose columns are eigevectors of $\mathbf{V}$ and post-multiplying with a matrix $\mathbf{S}^{-1}$ whose rows are the transpose of eigevectors of $\mathbf{V}$, i.e. perform a similarity trasformation. Since $\mathbf{V}$ is real and symmetric $\mathbf{S}^T = \mathbf{S}^{-1}$ and the diagonalised forn of $\mathbf{V}$ is

$$\mathbf{V}' = \mathbf{S}^{-1}\mathbf{V}\mathbf{S}$$

where

$$\mathbf{V}' = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

where λ_1 and λ_2 are the eigenvalues of $\mathbf{V}$. ow using the cyclic property of the trace, implies that

$$\mathrm{Tr}(\mathbf{V}) = \mathrm{Tr}(\mathbf{V}')$$

to give

$$\mathrm{Tr}(\mathbf{V}^N) = \lambda_1^N + \lambda_2^N.$$

Now consider the case that $\lambda_1 \neq \lambda_2$ (the degenerate case will be discussed later). Assuming $\lambda_1 > \lambda_2$, we have

$$Z_N(h, K) = \lambda_1^N \left(1 + \left[\frac{\lambda_2}{\lambda_1}\right]^N\right)$$

and in the thermodyamic limit $N \to \infty$

$$Z_N(h, K) \approx \lambda_1^N \left(1 + \mathcal{O}(e^{-\alpha N})\right),$$

where $\alpha \equiv \ln(\lambda_1/\lambda_2)$ is a positive constant. So only the largest eigenvalue of the transfer matrix is important in the thermodyamic limit. The free energy is give by

$$-k_B T \lim_{N\to\infty} N^{-1} \ln Z = -T \ln k_B \lambda_1.$$

We can easily compute λ_1. The eigenvalues of $\mathbf{V}$ are given by

$$\det \begin{pmatrix} e^{h+K} - \lambda & e^{-K} \\ e^{-K} & e^{-h+K} - \lambda \end{pmatrix} = 0.$$

From which we have the characteristic polynomial

$$\lambda^2 - \lambda(e^h + e^{-h})e^K + e^{2K} - e^{-2K} = 0$$

or

$$\left(\lambda - \cosh h e^K\right)^2 - \cosh^2 h e^{2K} + e^{2K} - e^{-2K} = 0$$

or

$$\left(\lambda - \cosh h e^{K}\right)^2 - e^{2K}(\sinh^2 h + e^{-4K}) = 0$$

Solving, we obtain

$$\lambda_{1,2} = e^{K}\left[\cosh h \pm \sqrt{\sinh^2 h + e^{-4K}}\right]$$

and

$$\begin{aligned} N^{-1}F_N(h,K) &= -k_B T \ln\left\{e^{K}\left[\cosh h \pm \sqrt{\sinh^2 h + e^{-4K}}\right]\right\} \\ &= -J - k_B T \ln\left[\cosh h \pm \sqrt{\sinh^2 h + e^{-4K}}\right] \end{aligned}$$

since $K \equiv \beta J$. This is the general result for the free energy of the one dimensional Ising model in an external magnetic field.

Chapter 3

Ising Model in Two Dimensions

3.1 Transfer Matrix

2.1

We will apply the method of transfer matrix in two dimensions. We first formulate the one-dimensional problem in a slightly different way. Consider, again, the Hamiltonian

$$H = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} - h \sum_i \sigma_i \tag{3.1}$$

The partition function is

$$Z = \sum_{\{\sigma\}} \left(e^{\beta h \sigma_1} e^{K \sigma_1 \sigma_2}\right) \left(e^{\beta h \sigma_2} e^{K \sigma_2 \sigma_3}\right) \cdots \left(e^{\beta h \sigma_N} e^{K \sigma_N \sigma_1}\right) \tag{3.2}$$

Again we can think of each term as a matrix element of a matrix T

$$V_{S_1 S_2} = e^{\beta S_1} e^{K S_1 S_2}$$

Using S_1 and S_2 as labels of matrix elements, we have:

$$\mathbf{V} = \begin{pmatrix} V_{11} & V_{1-1} \\ V_{-11} & V_{-1-1} \end{pmatrix} = \begin{pmatrix} e^{\beta h} e^{K} & e^{\beta h} e^{-K} \\ e^{-\beta h} e^{-K} & e^{-\beta h} e^{K} \end{pmatrix}$$

Then

$$Z = \sum_{S_1} \cdots \sum_{S_N} V_{S_1 S_2} V_{S_2 S_3} \cdots V_{S_N S_1}.$$

Each matrix $\mathbf{V}$ can be written as the product

$$\mathbf{V} = \mathbf{V}_1 \mathbf{V}_2 = \begin{pmatrix} e^{\beta h} & 0 \\ 0 & e^{-\beta h} \end{pmatrix} \begin{pmatrix} e^{K} & e^{-K} \\ e^{-K} & e^{K} \end{pmatrix}$$

and

$$Z = \sum_{S_1} \sum_{\tilde{S}_1} \cdots \sum_{S_N} \sum_{\tilde{S}_N} (V_1)_{S_1 S_1} (V_2)_{\tilde{S}_1 S_2} V_{S_2 S_3} \cdots V_{S_N S_1}$$

We now introduce two orthonormal basis states $|+1\rangle$ and $|-1\rangle$ and Pauli operators, which in this basis have the representation

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{3.3}$$

with $\sigma_x = \sigma^+ + \sigma^-$ and $\sigma_y = -i(\sigma^+ - \sigma^-)$. The Boltzmann weight $\exp\{\beta h \sigma_i\}$ can be expressed as a diagonal matrix, $\mathbf{V}_1$, in this basis

$$\langle +1|\mathbf{V}_1|+1\rangle = e^{\beta h}, \quad \langle -1|\mathbf{V}_1|-1\rangle = e^{-\beta h}$$

or

$$\mathbf{V}_1 = \exp\{\beta h \sigma_z\}. \tag{3.4}$$

Similarly, we define the operator $\mathbf{V}_2$ corresponding to the nearest-neighbour coupling by its matrix elements in this basis:

$$\begin{aligned} \langle +1|\mathbf{V}_2|+1\rangle &= \langle -1|\mathbf{V}_2|-1\rangle = e^{K} \\ \langle +1|\mathbf{V}_2|-1\rangle &= \langle -1|\mathbf{V}_2|+1\rangle = e^{-K} \end{aligned}$$

Therefore

$$
\begin{aligned}
\mathbf{V}_2 = e^{K}\mathbb{1} + e^{-K}\sigma_x &= A(K)\exp\{K^*\sigma_x\} \\
&= A(K)\left(\sum_{n=0}^{\infty}\frac{(K^*)^{2n}}{(2n)!}\mathbb{1} + \sum_{n=0}^{\infty}\frac{(K^*)^{2n+1}}{(2n+1)!}\sigma_x\right) \\
&= A(K)\left(\cosh K^*\mathbb{1} + \sinh K^*\sigma_x\right)
\end{aligned} \tag{3.5}
$$

So the constants $A(K)$ and K^* are determined by

$$
\begin{aligned}
A\cosh K^* &= e^{K} \\
A\sinh K^* &= e^{-K}
\end{aligned} \tag{3.6}
$$

or $\tanh K^* = \exp\{-2K\}$, $A = \sqrt{2\sinh 2K}$. Using these results, we write the partition function as follows:

$$
\begin{aligned}
Z &= \sum_{\mu=+1,-1;\tilde{\mu}=+1,-1} \langle\mu_1|\mathbf{V}_1|\tilde{\mu}_1\rangle\langle\tilde{\mu}_1|\mathbf{V}_2|\mu_2\rangle\langle\mu_2|\mathbf{V}_1|\tilde{\mu}_2\rangle\langle\tilde{\mu}_2|\mathbf{V}_2|\mu_2\rangle\cdots\langle\mu_{2N}|\mathbf{V}_1|\tilde{\mu}_{2N}\rangle\langle\tilde{\mu}_{2N}|\mathbf{V}_2|\mu_1\rangle \\
&= \mathrm{Tr}\left(\mathbf{V}_1\mathbf{V}_2\right)^N \\
&= \mathrm{Tr}\left(\mathbf{V}_2^{1/2}\mathbf{V}_1\mathbf{V}_2^{1/2}\right)^N \\
&= \lambda_1^N + \lambda_2^N
\end{aligned} \tag{3.7}
$$

where λ_1 and λ_2 are the two eigenvalues of the Hermitian operator

$$
\mathbf{V} = \left(\mathbf{V}_2^{1/2}\mathbf{V}_1\mathbf{V}_2^{1/2}\right) = \sqrt{2\sinh 2K}\,e^{K^*\sigma_x/2}e^{\beta h\sigma_z}e^{K^*\sigma_x/2}. \tag{3.8}
$$

In arriving at this symmetric form of the transfer matrix $\mathbf{V}$ we have used the trace of the product of two matrices under cyclic permutation of the factors. Clearly, in the case $h = 0$, the two eigenvalues are given by $\lambda_1 = A\exp(K^*)$ and $\lambda_2 = A\exp(-K^*)$.

We note that in this procedure a one-dimensional problem in classical statistics has been transformed into a zero-dimensional (only one "site") quantum-mechanical ground-state problem (largest eigenvalue).

3.2 $2d$ Ising model as quantum mechanical problem

We now genralise this procedure to the two-dimensional Ising model and consider an $M \times M$ square lattice with periodic boundary conditions. The spin variables now have two indices corresponding to row and columns of the square latice respectively

$$\sigma_{r,c} = \pm 1, \qquad r, c = 1, \ldots, M.$$

where the label r refers to rows , c to columns.

The Hamiltonian

$$H = -J \sum_{r,c} \sigma_{r,c}\sigma_{r+1,c} - J \sum_{r,c} \sigma_{r,c}\sigma_{r,c+1} \tag{3.9}$$

with periodic boundary conditions $\sigma_{r+M,c} = \sigma_{r,c+M} = \sigma_{r,c}$.

Write H as

$$H = -J \sum_c \left(\sum_r \sigma_{r,c}\sigma_{r,c+1} \right) - J \sum_c \left(\sum_r \sigma_{r,c}\sigma_{r+1,c} \right).$$

The second term contains only interactions in column c and is, in this sense, analogous to to the magnetic term in (3.1). The first term is the coupling between neigbouring columns and will lead to a non-diagonal factor in the complete transfer matrix.

Note that

$$\begin{aligned}
Z &= \sum_{\sigma_{r,c}} e^{K \sum_{r=1}^{M} \sum_{c=1}^{M} (\sigma_{r,1}\sigma_{r+1,c} + K\sigma_{r,c}\sigma_{r,c+1})} \\
&= \sum_{\sigma_{r,c}} e^{K \sum_{r=1}^{M} \sigma_{r,1}\sigma_{r+1,1}} e^{K \sum_{r=1}^{M} \sigma_{r,1}\sigma_{r,2}} e^{K \sum_{r=1}^{M} \sigma_{r,2}\sigma_{r+1,2}} e^{K \sum_{r=1}^{M} \sigma_{r,2}\sigma_{r,3}} \times \\
&\qquad e^{K \sum_{r=1}^{M} \sigma_{r,3}\sigma_{r+1,3}} e^{K \sum_{r=1}^{M} \sigma_{r,3}\sigma_{r,4}} \ldots e^{K \sum_{r=1}^{M} \sigma_{r,M}\sigma_{r+1,M}} e^{K \sum_{r=1}^{M} \sigma_{r,M}\sigma_{M,1}} \\
&= \sum_{\sigma_{r,c}} e^{K \sum_{r=1}^{M} \sigma_{r,1}\sigma_{r+1,1}} e^{(M-2n_{1,2})K} e^{K \sum_{r=1}^{M} \sigma_{r,2}\sigma_{r+1,2}} e^{(M-2n_{2,3})K} \times \\
&\qquad e^{K \sum_{r=1}^{M} \sigma_{r,3}\sigma_{r+1,3}} e^{(M-2n_{3,4})K} \ldots e^{K \sum_{r=1}^{M} \sigma_{r,M}\sigma_{r+1,M}} e^{(M-2n_{M,1})K}.
\end{aligned} \tag{3.10}$$

where $n_{i,i+1}$ counts, as we move up from one row to the next starting at the row 1 and ending at row M, the number of times the orientation at the site on column i differs from the orientation on the nearest-neigbouring site to the right.

In analogy with the one-diemnsional case, we now introduce the 2^M basis states

$$|\mu\rangle \equiv |\mu_1, \mu_2, \ldots, \mu_M\rangle \equiv |\mu_1\rangle|\mu_2\rangle \cdots |\mu_M\rangle \tag{3.11}$$

$$
\begin{aligned}
\sigma_{jz}|\mu_1,\mu_2,\ldots,\mu_M\rangle &= \mu_j\,|\mu_1,\mu_2,\ldots,\mu_M\rangle \\
\sigma_j^{+}|\mu_1,\mu_2,\ldots,\mu_M\rangle &= \delta_{\mu_j,-1}|\mu_1,\mu_2,\ldots,\mu_j+2,\ldots\mu_M\rangle \\
\sigma_j^{-}|\mu_1,\mu_2,\ldots,\mu_M\rangle &= \delta_{\mu_j,1}|\mu_1,\mu_2,\ldots,\mu_j-2,\ldots\mu_M\rangle
\end{aligned} \tag{3.12}
$$

Moreover, we impose the commutation relations

$$
[\sigma_{j\alpha},\sigma_{m\beta}]=0 \qquad \text{for } j\neq m.
$$

For $j=m$ the usual Pauli matrix commutation relations apply,

$$
[\sigma_{j\alpha},\sigma_{j\beta}]=2i\epsilon_{\alpha\beta\gamma}\sigma_{j\gamma}.
$$

We think of the index μ_i as the orientation of the ith spin in a given column, with each column having its own ith spin. It is obvious that the Boltzmann factors $\exp\left\{K\sum_{r=1}^{M}\sigma_{r,c}\sigma_{r+1,c}\right\}$ arer given by the matrix elements of the operator $\mathbf{V}_1=\exp\left\{K\sum_{j=1}^{M}\sigma_{jz}\sigma_{j+1,z}\right\}$,

$$
\begin{aligned}
\langle\{\mu\}|\mathbf{V}_1|\{\mu'\}\rangle &= \langle\mu_1,\mu_2,\ldots,\mu_M|\prod_{j=1}^{M}\exp\left\{K\sum_{j=1}^{M}\sigma_{jz}\sigma_{j+1,z}\right\}|\mu_1',\mu_2',\ldots,\mu_M'\rangle \\
&= \exp\left\{K\sum_{r=1}^{M}\sigma_{r,c}\sigma_{r+1,c}\right\}
\end{aligned} \tag{3.13}
$$

Similarly, the matrix element

$$
\begin{aligned}
\langle\{\mu\}|\mathbf{V}_2|\{\mu'\}\rangle &= \langle\mu_1,\mu_2,\ldots,\mu_M|\prod_{j=1}^{M}\left(e^{K}\mathbb{1}+e^{-K}\sigma_{jx}\right)|\mu_1',\mu_2',\ldots,\mu_M'\rangle \\
&= \langle\mu_1,\mu_2,\ldots,\mu_M|\prod_{j=1}^{M}\left(e^{K}\mathbb{1}+e^{-K}(\sigma_j^{+}+\sigma_j^{-})\right)|\mu_1',\mu_2',\ldots,\mu_M'\rangle \\
&= \exp\{(M-2n)K\}
\end{aligned} \tag{3.14}
$$

where n is the number of the indices $\{\mu'\}$ that differ from the corresponding indices in $\{\mu\}$, as

$$
\langle\mu_j|\left(e^{K}\mathbb{1}+e^{-K}(\sigma_j^{+}+\sigma_j^{-})\right)|\mu_j'\rangle=\begin{cases} e^{K} & \text{if } \mu_j=\mu_j' \\ e^{-K} & \text{if } \mu_j\neq\mu_j'. \end{cases}
$$

$$
\begin{aligned}
Z &= \sum_{\substack{\{\mu^{(1)}\},\{\tilde{\mu}^{(1)}\},\{\tilde{\mu}^{(1)}\},\{\mu^{(2)}\},\ldots\\ \ldots,\{\tilde{\mu}^{(M)}\},\{\mu^{(M)}\}}} \langle\mu^{(1)}|\mathbf{V}_1|\tilde{\mu}^{(1)}\rangle\langle\tilde{\mu}^{(1)}|\mathbf{V}_2|\mu^{(2)}\rangle\langle\mu^{(2)}|\mathbf{V}_1|\tilde{\mu}^{(2)}\rangle\cdots\langle\tilde{\mu}^{(M)}|\mathbf{V}_2|\mu^{(1)}\rangle \\
&= \mathrm{Tr}\,(\mathbf{V}_1\mathbf{V}_2)^M \\
&= \mathrm{Tr}\left(\mathbf{V}_2^{1/2}\mathbf{V}_1\mathbf{V}_2^{1/2}\right)^M \qquad (3.15)
\end{aligned}
$$

where $|\mu^{(j)}\rangle$ is a basis state as in (3.11), and the over each $\{\mu^{(j)}\}$ is, over all 2^M basis states.

3.3 Transformation to an interacting fermion problem

$$
\begin{aligned}
\sigma_j^+ &= \exp\left\{\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m\right\} c_j^\dagger \\
\sigma_j^- &= c_j \exp\left\{-\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m\right\} = \exp\left\{\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m\right\} c_j \qquad (3.16)
\end{aligned}
$$

where the operators c, $c^\dagger$ obey the commutation relations

$$
\begin{aligned}
[c_j, c_m^\dagger]_+ &= c_j c_m^\dagger + c_m^\dagger c_j = \delta_{jm} \\
[c_j, c_m]_+ &= [c_j^\dagger, c_m^\dagger]_+ = 0.
\end{aligned}
$$

$$
\begin{aligned}
c_j c_m^\dagger c_m &= -c_m^\dagger c_j c_m + \delta_{jm} c_m \\
&= c_m^\dagger c_m c_j + \delta_{jm} c_m \\
&= c_m^\dagger c_m c_j (1-\delta_{jm}) + \delta_{jm} c_m
\end{aligned}
$$

This implies

$$
c_j \exp\left\{-\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m\right\} = \exp\left\{-\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m\right\} c_j.
$$

The operator $c_m^\dagger c_m$ is the fermion number operator for site m with integer eigenvalues 0 and 1 (we have used $e^{i\pi n} = e^{-i\pi n}$ in the last step of (3.16)).

We have

$$\begin{aligned} c_m^\dagger c_m c_j^\dagger &= -c_m^\dagger c_j^\dagger c_m + \delta_{jm} c_m^\dagger \\ &= c_m^\dagger c_m c_j^\dagger + \delta_{jm} c_m^\dagger \\ &= c_j^\dagger c_m^\dagger c_m (1-\delta_{jm}) + \delta_{jm} c_m \end{aligned}$$

Useful to note

$$c_j^\dagger c_j c_m^\dagger c_m = c_j^\dagger c_m^\dagger c_m c_j + \delta_{jm} c_j^\dagger c_m = c_m^\dagger c_m c_j^\dagger c_j - \delta_{mj} c_m^\dagger c_j + \delta_{jm} c_j^\dagger c_m$$

or

$$c_j^\dagger c_j c_m^\dagger c_m = c_m^\dagger c_m c_j^\dagger c_j .$$

We will now prove that the spin commutation relaions are preserved under this transformation.

$$\begin{aligned} c_j \exp\left\{-\pi i c_j^\dagger c_j\right\} &= c_j \sum_{n=0}^{\infty} \frac{(-\pi i)^n}{n!} (c_j^\dagger c_j)^n \\ &= \sum_{n=0}^{\infty} \frac{(\pi i)^n}{n!} c_j \\ &= e^{\pi i} c_j = -c_j \end{aligned}$$

$$\begin{aligned} & [\sigma_j^-, \sigma_j^+] \\ = \; & \left[c_j \exp\left\{-\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m\right\}, \exp\left\{\pi i \sum_{\ell=1}^{n-1} c_\ell^\dagger c_\ell\right\} c_n^\dagger \right] \\ = \; & c_j \exp\left\{-\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m\right\} \exp\left\{\pi i \sum_{\ell=1}^{n-1} c_\ell^\dagger c_\ell\right\} c_n^\dagger - \exp\left\{\pi i \sum_{\ell=1}^{n-1} c_\ell^\dagger c_\ell\right\} c_n^\dagger c_j \exp\left\{-\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m\right\} \\ = \; & c_j \exp\left\{\pi i \sum_{m=j+1}^{n-1} c_m^\dagger c_m\right\} e^{\pi i c_j^\dagger c_j} c_n^\dagger - c_n^\dagger \exp\left\{\pi i \sum_{\ell=1}^{n-1} c_\ell^\dagger c_\ell\right\} \exp\left\{-\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m\right\} c_j \\ = \; & \exp\left\{\pi i \sum_{m=j+1}^{n-1} c_m^\dagger c_m\right\} \left(c_j e^{\pi i c_j^\dagger c_j} c_n^\dagger - c_n^\dagger e^{\pi i c_j^\dagger c_j} c_j \right) \end{aligned}$$

Noting that $\exp\left\{\pi i c_j^\dagger c_j\right\} c_j = c_j$ and $c_j \exp\left\{\pi i c_j^\dagger c_j\right\} = -c_j$, we have $[\sigma_j^-, \sigma_j^+] = 0$ for $n \neq j$. We also immediately see that the on-site anticommutator

$$[\sigma_j^-, \sigma_j^+]_+ = [c_j^-, c_j^+]_+ = 1.$$

Using (3.16) we can write the operators $\mathbf{V}_1$ and $\mathbf{V}_2$ in terms of fermion operators. The operator $\mathbf{V}_2$ can immediately be written down

$$\mathbf{V}_2 = (2\sinh 2K)^{M/2} \exp\left\{2K^* \sum_{j=1}^{M} \left(c_j^\dagger c_j - \frac{1}{2}\right)\right\}. \tag{3.17}$$

Note that for $j \neq M$ the term

$$\begin{aligned}
&(\sigma_j^+ + \sigma_j^-)(\sigma_{j+1}^+ + \sigma_{j+1}^-) \\
&= \left(\exp\left\{\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m\right\} c_j^\dagger + \exp\left\{\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m\right\} c_j\right) \\
&\quad \times \left(\exp\left\{-\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m\right\} e^{\pi i c_j^\dagger c_j} c_{j+1}^\dagger + \exp\left\{-\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m\right\} e^{\pi i c_j^\dagger c_j} c_{j+1}\right) \\
&= c_j^\dagger e^{-\pi i c_j^\dagger c_j} c_{j+1}^\dagger + c_j^\dagger e^{-\pi i c_j^\dagger c_j} c_{j+1} + c_j e^{-\pi i c_j^\dagger c_j} c_{j+1}^\dagger + c_j e^{-\pi i c_j^\dagger c_j} c_{j+1} \\
&= c_j^\dagger c_{j+1}^\dagger + c_j^\dagger c_{j+1} - c_j c_{j+1}^\dagger - c_j c_{j+1} \\
&= c_j^\dagger c_{j+1}^\dagger + c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + c_{j+1} c_j
\end{aligned}$$

For the specific case $j = M$,

$$\begin{aligned}
&(\sigma_M^+ + \sigma_M^-)(\sigma_1^+ + \sigma_1^-) \\
&= \exp\left\{\pi i \sum_{j=1}^{M-1} c_j^\dagger c_j\right\} c_M^\dagger (c_1^\dagger + c_1) + \exp\left\{\pi i \sum_{j=1}^{M-1} c_j^\dagger c_j\right\} c_M (c_1^\dagger + c_1) \\
&= \exp\left\{\pi i \sum_{j=1}^{M} c_j^\dagger c_j\right\} \left[e^{\pi i c_M^\dagger c_M} (c_M^\dagger + c_M)(c_1^\dagger + c_1)\right] \\
&= (-1)^n (c_M - c_M^\dagger)(c_1^\dagger + c_1)
\end{aligned}$$

where $n = \sum_{j=1}^{M} c_j^\dagger c_j$ is the total fermion number operator.

$$\mathbf{V}_1 = \exp\left\{ K \sum_{j=1}^{M-1} (c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1}) + K(-1)^n (c_M - c_M^\dagger)(c_1^\dagger + c_1) \right\} \tag{3.18}$$

The operator n commutes with $\mathbf{V}_2$ but not with $\mathbf{V}_1$. However, $(-1)^n$ commutes with both $\mathbf{V}_1$, and $\mathbf{V}_2$ as the various terms in $\mathbf{V}_1$ change the total fermion number by 0 or ± 2. That is,

$$[\mathbf{V}_1, \exp\left\{ \pi i \sum_{j=1}^{M} c_j^\dagger c_j \right\}] = 0 \qquad [\mathbf{V}_2, \exp\left\{ \pi i \sum_{j=1}^{M} c_j^\dagger c_j \right\}] = 0$$

As $\mathbf{V}_1$ changes the total fermion number by 0 or ± 2 it will map a state with an even total number of fermions to another state with an even total number of fermions. Similarly, it will map a state with a odd total number of fermions to another state with an odd total number of fermions. Thus if we consider separately the subspaces of even and odd total number of fermions, we may write $\mathbf{V}_1$ in the simple universal way, that is

$$\mathbf{V}_1 = \exp\left\{ K \sum_{j=1}^{M} (c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1}) \right\} \tag{3.19}$$

due to the ability to impose the differing boundary conditions

$$\begin{aligned} c_{M+1} &\equiv -c_1, \quad c_{M+1}^\dagger \equiv -c_1^\dagger \quad \text{for } n \text{ even} \\ c_{M+1} &\equiv c_1, \quad c_{M+1}^\dagger \equiv c_1^\dagger \quad \text{for } n \text{ odd} \end{aligned} \tag{3.20}$$

for the even and odd case. This is easily verified,

$$\sum_{j=1}^{M} (c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1}) = \sum_{j=1}^{M-1} (c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1}) + (c_M^\dagger - c_M)(c_{M+1}^\dagger + c_{M+1})$$
$$= \sum_{j=1}^{M-1} (c_j^\dagger - c_j)(c_{j+1}^\dagger + c_{j+1}) + (c_M - c_M^\dagger)(-1)^n (c_1^\dagger + c_1)$$

which is the same as the exponent of (3.18). With the choice of boundary conditions (3.20) on the fermion creation and annihilation operators, we have recovered translational invariance following from

$$\mathbf{V}_1 = \exp\left\{ K \sum_{j=1}^{M} (c^\dagger_{j+k} - c_{j+k})(c^\dagger_{j+1+k} + c_{j+1+k}) \right\}.$$

and that we know that $\mathbf{V}_2$ is translationally invariant. With translational invariance recovered we now carry out the canonical transformation

$$\begin{aligned} a_q &= \frac{1}{\sqrt{M}} \sum_{j=1}^{M} c_j e^{-iqj} \\ a^\dagger_q &= \frac{1}{\sqrt{M}} \sum_{j=1}^{M} c^\dagger_j e^{iqj} \end{aligned} \tag{3.21}$$

with inverse

$$\begin{aligned} c_j &= \frac{1}{\sqrt{M}} \sum_{q} a_q e^{iqj} \\ c^\dagger_j &= \frac{1}{\sqrt{M}} \sum_{q} a^\dagger_q e^{-iqj} \end{aligned} \tag{3.22}$$

To reproduce the boundary conditions (3.20), we take $q = \ell\pi/M$ with

$$\begin{aligned} \ell &= \pm 1, \pm 3, \ldots, \pm(M-1) \quad \text{for } n \text{ even} \\ \ell &= 0, \pm 2, \pm 4, \ldots, \pm(M-2), M \quad \text{for } n \text{ odd} \end{aligned}$$

and where we have assumed, without loss of generality, that M is even. It is easy to check that the operators a_q, $a^\dagger_q$ obey the fermion commutation relations, that is $[a_q, a^\dagger_{q'}] = \delta_{q,q'}$ and $[a_q, a_{q'}] = [a^\dagger_q, a^\dagger_{q'}] = 0$ for all q and q'.

Substituting into (3.17) and (3.19), we find for n **even**,

$$\begin{aligned} \mathbf{V}_2 &= (2\sinh 2K)^{M/2} \exp\left\{ 2K^* \sum_{q>0} \left(a^\dagger_q a_q + a^\dagger_{-q} a_{-q} - 1 \right) \right\} \\ &= (2\sinh 2K)^{M/2} \prod_{q>0} \mathbf{V}_{2q} \end{aligned} \tag{3.23}$$

and

$$
\begin{aligned}
\mathbf{V}_1 &= \exp\left\{2K\sum_{q>0}\left[\cos q\left(a_q^\dagger a_q + a_{-q}^\dagger a_{-q}\right) - i\sin q\left(a_q^\dagger a_{-q}^\dagger + a_q a_{-q}\right)\right]\right\} \\
&= \prod_{q>0}\mathbf{V}_{1q} \qquad (3.24)
\end{aligned}
$$

where, in (3.23) and (3.24), we have combied the terms corresponding to q and $-q$, and writing the resultining operators as products, using the fact that bilinear operators with different wave vectors commute. This is a great simplification since the eigenvalues of the transfer matrix can now be written as a productof eigenvalues of, as we shall see, at most 4×4 matrices.

For the case of **odd** n we also need the operators $\mathbf{V}_{1q}$ and $\mathbf{V}_{2q}$ for $q = \pi$ and $q = 0$. These are given by

$$
\begin{aligned}
\mathbf{V}_{10} &= \exp\left\{2Ka_0^\dagger a_0\right\} \qquad & \mathbf{V}_{20} &= \exp\left\{2K^*(a_0^\dagger a_0 - \frac{1}{2})\right\} \\
\mathbf{V}_{1\pi} &= \exp\left\{2Ka_\pi^\dagger a_\pi\right\} \qquad & \mathbf{V}_{2\pi} &= \exp\left\{2K^*(a_\pi^\dagger a_\pi - \frac{1}{2})\right\} \qquad (3.25)
\end{aligned}
$$

which are already in diagonal form and commute with each other.

3.4 Calculation of Eigenvalues

We proceed to calculate the eigenvalues of the operator

$$
\mathbf{V}_q = \mathbf{V}_{2q}^{1/2}\mathbf{V}_{1q}\mathbf{V}_{2q}^{1/2}
$$

for $q \neq 0$ and $q \neq \pi$. Since we are dealing with fermions, for each individual q, we have only four possible states:

$$
|0\rangle,\ a_q^\dagger|0\rangle,\ a_{-q}^\dagger|0\rangle,\ \text{and}\ a_q^\dagger a_{-q}^\dagger|0\rangle
$$

where $|0\rangle$ is the zero particle state defined by

$$
a_q|0\rangle = a_{-q}|0\rangle = 0.
$$

These states are already eigenstates of $\mathbf{V}_2$ because

$$\begin{aligned}
\left(a_q^\dagger a_q + a_{-q}^\dagger a_{-q} - 1\right)|0\rangle &= -1\cdot|0\rangle \\
\left(a_q^\dagger a_q + a_{-q}^\dagger a_{-q} - 1\right)a_q^\dagger|0\rangle &= 0\cdot a_q^\dagger|0\rangle \\
\left(a_q^\dagger a_q + a_{-q}^\dagger a_{-q} - 1\right)a_q^\dagger|0\rangle &= 0\cdot a_{-q}^\dagger|0\rangle \\
\left(a_q^\dagger a_q + a_{-q}^\dagger a_{-q} - 1\right)a_q^\dagger a_{-q}^\dagger|0\rangle &= +1\cdot a_q^\dagger a_{-q}^\dagger|0\rangle
\end{aligned}$$

implies

$$\begin{aligned}
\mathbf{V}_{2q}|0\rangle &= \exp\left\{-2K^*\right\}|0\rangle \\
\mathbf{V}_{2q}a_q^\dagger|0\rangle &= a_q^\dagger|0\rangle \\
\mathbf{V}_{2q}a_{-q}^\dagger|0\rangle &= a_{-q}^\dagger|0\rangle \\
\mathbf{V}_{2q}a_q^\dagger a_{-q}^\dagger|0\rangle &= \exp\left\{2K^*\right\}a_q^\dagger a_{-q}^\dagger|0\rangle,
\end{aligned}$$

and since the operator $\mathbf{V}_1$ has non-zero off-diagonal matrix elements only between states that differ by two in fermion number, the problem reduces to finding the eigenvalues of $\mathbf{V}_q$ in the basis $|0\rangle$ and $|2\rangle = q_q^\dagger a_{-q}^\dagger|0\rangle$.

We have

$$\begin{aligned}
(a_q^\dagger a_q + a_{-q}^\dagger a_{-q})a_{\pm q}^\dagger|0\rangle &= (a_q^\dagger(1 - a_q^\dagger a_q) + a_{-q}^\dagger a_q^\dagger a_{-q})|0\rangle \\
&= a_{\pm q}^\dagger|0\rangle
\end{aligned}$$

and

$$(a_q^\dagger a_{-q}^\dagger + a_q a_{-q})a_{\pm q}^\dagger|0\rangle = 0$$

so that

$$\mathbf{V}_{1q}a_{\pm q}^\dagger|0\rangle = \exp\left\{2K\cos q\right\}a_{\pm q}^\dagger|0\rangle. \tag{3.26}$$

We note

$$\begin{aligned}\mathbf{V}_{2q}^{1/2}|0\rangle &= \exp\{-K^*\}|0\rangle \\ \mathbf{V}_{2q}^{1/2}|2\rangle &= \exp\{K^*\}|2\rangle \end{aligned} \tag{3.27}$$

By denoting the states $|1\rangle = a_q^\dagger|0\rangle$ and $|\overline{1}\rangle = a_{-q}^\dagger|0\rangle$ we can summarise the situation:

$$\begin{pmatrix} \langle 0|\mathbf{V}_{2q}^{1/2}|0\rangle & \langle 0|\mathbf{V}_{2q}^{1/2}|2\rangle & \langle 0|\mathbf{V}_{2q}^{1/2}|1\rangle & \langle 0|\mathbf{V}_{2q}^{1/2}|\overline{1}\rangle \\ \langle 2|\mathbf{V}_{2q}^{1/2}|0\rangle & \langle 2|\mathbf{V}_{2q}^{1/2}|2\rangle & \langle 2|\mathbf{V}_{2q}^{1/2}|1\rangle & \langle 2|\mathbf{V}_{2q}^{1/2}|\overline{1}\rangle \\ \langle 1|\mathbf{V}_{2q}^{1/2}|0\rangle & \langle 1|\mathbf{V}_{2q}^{1/2}|2\rangle & \langle 1|\mathbf{V}_{2q}^{1/2}|1\rangle & \langle 1|\mathbf{V}_{2q}^{1/2}|\overline{1}\rangle \\ \langle \overline{1}|\mathbf{V}_{2q}^{1/2}|0\rangle & \langle \overline{1}|\mathbf{V}_{2q}^{1/2}|2\rangle & \langle \overline{1}|\mathbf{V}_{2q}^{1/2}|1\rangle & \langle \overline{1}|\mathbf{V}_{2q}^{1/2}|\overline{1}\rangle \end{pmatrix} = \begin{pmatrix} \exp\{-K^*\} & 0 & 0 & 0 \\ 0 & \exp\{K^*\} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$\begin{pmatrix} \langle 0|\mathbf{V}_{1q}|0\rangle & \langle 0|\mathbf{V}_{1q}|2\rangle & \langle 0|\mathbf{V}_{1q}|1\rangle & \langle 0|\mathbf{V}_{1q}|\overline{1}\rangle \\ \langle 2|\mathbf{V}_{1q}|0\rangle & \langle 2|\mathbf{V}_{1q}|2\rangle & \langle 2|\mathbf{V}_{1q}|1\rangle & \langle 2|\mathbf{V}_{1q}|\overline{1}\rangle \\ \langle 1|\mathbf{V}_{1q}|0\rangle & \langle 1|\mathbf{V}_{1q}|2\rangle & \langle 1|\mathbf{V}_{1q}|1\rangle & \langle 1|\mathbf{V}_{1q}|\overline{1}\rangle \\ \langle \overline{1}|\mathbf{V}_{1q}|0\rangle & \langle \overline{1}|\mathbf{V}_{1q}|2\rangle & \langle \overline{1}|\mathbf{V}_{1q}|1\rangle & \langle \overline{1}|\mathbf{V}_{1q}|\overline{1}\rangle \end{pmatrix} = \begin{pmatrix} \alpha & \gamma & 0 & 0 \\ \beta & \delta & 0 & 0 \\ 0 & 0 & \exp\{2K\cos q\} & 0 \\ 0 & 0 & 0 & \exp\{2K\cos q\} \end{pmatrix}.$$

To obtain the matrix elements of $\mathbf{V}_{1q}$ in the basis $|0\rangle$ and $|2\rangle$, we let

$$\mathbf{V}_{1q}|0\rangle = \alpha(K)|0\rangle + \beta(K)|2\rangle.$$

Differentiating this expression with respect to K, we obtain

$$\begin{aligned} & \frac{\partial\alpha}{\partial K}(K)|0\rangle + \frac{\partial\beta}{\partial K}(K)|2\rangle \\ & \quad 2\left[\cos q\left(a_q^\dagger a_q + a_{-q}^\dagger a_{-q}\right) - i\sin q\left(a_q^\dagger a_{-q}^\dagger + a_q a_{-q}\right)\right]\mathbf{V}_{1q}|0\rangle \\ = {} & 2\left[\cos q\left(a_q^\dagger a_q + a_{-q}^\dagger a_{-q}\right) - i\sin q\left(a_q^\dagger a_{-q}^\dagger + a_q a_{-q}\right)\right](\alpha(K)|0\rangle + \beta(K)|2\rangle) \\ = {} & 2i\beta\sin q|0\rangle + [4\beta\cos q - 2i\alpha\sin q]|2\rangle \end{aligned} \tag{3.28}$$

or

$$\begin{aligned} \frac{\partial\alpha}{\partial K}(K) &= 2i\beta(K)\sin q \\ \frac{\partial\beta}{\partial K}(K) &= 4\beta(K)\cos q - 2i\alpha(K)\sin q. \end{aligned} \tag{3.29}$$

We solve these equations subject to the boundary confitions $\alpha(0) = 1$, $\beta(0) = 0$. The result is

$$\begin{aligned} \langle 0|\mathbf{V}_{1q}|0\rangle &= \alpha(K) = e^{2K\cos q}\left(\cosh 2K - \sinh 2K \cos q\right) \\ \langle 2|\mathbf{V}_{1q}|0\rangle &= \beta(K) = -ie^{2K\cos q}\sinh 2K \sin q \end{aligned} \tag{3.30}$$

By the same method we can finf the matrix elements $\langle 2|\mathbf{V}_{1q}|2\rangle$ and $\langle 0|\mathbf{V}_{1q}|2\rangle$. We let

$$\mathbf{V}_{1q}|2\rangle = \gamma(K)|0\rangle + \delta(K)|2\rangle.$$

Differentiating this expression with respect to K, we obtain

$$\begin{aligned} \frac{\partial\gamma}{\partial K}(K) &= 2i\delta(K)\sin q \\ \frac{\partial\delta}{\partial K}(K) &= 4\delta(K)\cos q - 2i\gamma(K)\sin q \end{aligned}$$

which are the same form as before, but this time we solve these equations subject to the boundary confitions $\gamma(0) = 0$, $\delta(0) = 1$. The result is

$$\begin{aligned} \langle 0|\mathbf{V}_{1q}|2\rangle &= \gamma(K) = ie^{2K\cos q}\sinh 2K \sin q = \langle 2|\mathbf{V}_{1q}|0\rangle^* \\ \langle 2|\mathbf{V}_{1q}|2\rangle &= \delta(K) = e^{2K\cos q}\left(\cosh 2K + \sinh 2K \cos q\right). \end{aligned} \tag{3.31}$$

We obtain the matrix

$$\mathbf{V}_{1q} = e^{2K\cos q}\begin{pmatrix} \cosh 2K - \sinh 2K\cos q & i\sinh 2K \sin q & 0 & 0 \\ -i\sinh 2K\sin q & \cosh 2K + \sinh 2K \cos q & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{3.32}$$

and

$$\mathbf{V}_q = \begin{pmatrix} \exp\{-K^*\} & 0 & 0 & 0 \\ 0 & \exp\{K^*\} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \left(\mathbf{V}_{1q}\right) \begin{pmatrix} \exp\{-K^*\} & 0 & 0 & 0 \\ 0 & \exp\{K^*\} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3.33}$$

The eigenvalues of this matrix are easily determined. Since we wish, eventually, to take the logarithm of the largest eigenvalue of the complete transfer matrix in order to calculate the free energy, we write the eigenvalues in the form

$$\lambda_q^{\pm} = \exp\left\{2K\cos q \pm \epsilon(q)\right\} \tag{3.34}$$

after some algebra, we obtain the equation

$$\cosh\epsilon(q) = \cosh 2K\cosh 2K^* + \cos q\sinh 2K\sinh 2K^*. \tag{3.35}$$

for $\epsilon(q)$. By convention we choose $\epsilon(q) \geq 0$. The minimum of RHS of (3.35) occurs when $q \rightarrow \pi$ and that, for all q.

$$\epsilon(q) > \epsilon_{min} = \lim_{q\rightarrow\pi}\epsilon(q) = 2|K - K^*| \tag{3.36}$$

where we have used the hyperbolic trig identity: $\cosh 2K\cosh 2K^* - \sinh 2K\sinh 2K^* = \cosh(2K - 2K^*)$ in (3.35). Also, note that

$$\lim_{q\rightarrow 0}\epsilon(q) = 2(K + K^*) \tag{3.37}$$

where we have used the the hyperbolic trig identity: $\cosh 2K\cosh 2K^* {+} \sinh 2K\sinh 2K^* = \cosh(2K + 2K^*)$ in (3.35).

n **even**

First we consider the subspace in which all states cantain an even number of fermions. In this case the allowed wave vectors do not include $q = 0$ or $q = \pi$, and comparing (3.34) and (3.26), we see that the largest eigenvalue of $\mathbf{V}_q$ for each q is λ_q^+. Recall from (3.23) that $(2\sinh 2K)^{M/2}\prod_{q>0}\mathbf{V}_{2q}$. Thus the largest eigenvalue in this subspace, Λ_{even}, is given by

$$\begin{aligned}\Lambda_{even} &= (2\sinh 2K)^{M/2}\prod_{q=0}\lambda_q^+ \\ &= (2\sinh 2K)^{M/2}\exp\left\{\sum_{q>0}2K\cos q + \epsilon(q)\right\} \\ &= (2\sinh 2K)^{M/2}\exp\left\{\frac{1}{2}\sum_q\epsilon(q)\right\}\end{aligned} \tag{3.38}$$

where, in the last step, we have used $\sum_q \cos q = 0$ and have also extended the summation over the entire range $-\pi < q < \pi$.

n **odd**

We now turn to the other subspace that which is more subtle. For $q \neq 0$ and $q \neq \pi$ the maximum possible eigenvalue is λ_q^+. As the operator $(-1)^n$ commutes with the operators $\prod_q \mathbf{V}_q$, the corresponding eignenstates are also eigenstates of $(-1)^n$. Moreover, since $\prod_q \mathbf{V}_q$ maps states onto states where $(-1)^n = -1$, these eigenstates are all states with $(-1)^n = -1$. To make the overall state have $(-1)^n = -1$, we occupy either the $q = 0$ state or the $q = \pi$ state while leaveing the other state empty. Which state should we choose? To answer this, we have already seen from (3.36) and (3.37) tha the maximum contribution is for the case $q \to 0$.

$$\Lambda_{odd} = (2\sinh 2K)^{M/2} \exp\left\{2K + \frac{1}{2}\sum_{q\neq 0,\pi} \epsilon(q)\right\}. \tag{3.39}$$

In the thermodynamical limit, $M \to \infty$, Λ_{even} and Λ_{even} are degenerate

Since the wave vectors in the two subspaces are not identical, a direct compariso between the two largest eigenvales is somewhat complicated. However, we note that

$$\begin{aligned} \frac{1}{2}\lim_{q\to 0}\epsilon(q) + \frac{1}{2}\lim_{q\to\pi}\epsilon(q) &= |K - K^*| + (K + K^*) \\ &= 2K \qquad \text{for } K > K^* \\ &= 2K^* \qquad \text{for } K^* > K^{\cdot} \end{aligned} \tag{3.40}$$

Thus if $K > K^*$, it is quite plausable, and can be shown rigorously in the thermodynamic limit $M \to \infty$, that Λ_{odd} and Λ_{even} are degenrate. Unless such degeneracy exists, the order parameter $m_0(T)$ will be strictly zero. This degeneracy, at a finite teperature marks the spontaneous magnetisation in the system. The critical temperature is given by $K = K^*$ the identity (follows from $\tanh K^* = \exp\{-2K\}$)

$$\sinh 2K \sinh 2K^* = 1 \tag{3.41}$$

or

$$\sinh 2\beta J \sinh 2\beta J^* = 1 \tag{3.42}$$

Kramer-Wannier duality

The relation (3.42) is known as the Kramer-Wannier duality and is very important. It relates free energy at low temperature to that at high temperature. Note, if J is large, then J^* is small. Essentially relabelling J as J^* one can map physics below the transition temperature to that above. We go into this in full detail in section 3.6.

3.5 Thermodynamical functions

Using (3.41) and $\cosh 2K^* = \coth 2K$, which follows from (3.6), we have

$$\cosh\left[\epsilon(q)\right] = \cosh 2K \coth 2K + \cos q. \tag{3.43}$$

Consider the funnction

$$f(x) = \frac{1}{2\pi}\int_0^{2\pi} d\phi \ln(\cosh x + \cos\phi). \tag{3.44}$$

Differentiating both sides with respect to x and evaluating th eresulting integral by contour integration, we find

$$\frac{df(x)}{dx} = \mathrm{sng}(x) \qquad \text{or} \qquad f(x) = |x|. \tag{3.45}$$

Takig $x = \epsilon(q)$ we obtain the integral representation

$$\epsilon(q) = \frac{1}{\pi}\int_0^{\pi} d\phi \ln(2\cosh 2K \coth 2K + 2\cos q + 2\cos\phi), \tag{3.46}$$

(remember we choose the convetion $\epsilon(q) \geq 0$).

We define

$$I = \frac{1}{2\pi}\int_0^{\pi} dq\epsilon(q) = \frac{1}{2\pi^2}\int_0^{\pi} dq \int_0^{\pi} d\phi \ln(2\cosh 2K \coth 2K + 2\cos q + 2\cos\phi) \tag{3.47}$$

Using the trigonometric identity

$$\cos q + \cos\phi = 2\cos\frac{q+\phi}{2}\cos\frac{q-\phi}{2}$$

and changing variables of integration to

$$\omega_1 = \frac{q-\phi}{2}, \qquad \omega_2 = \frac{q+\phi}{2}$$

we have

$$I = \frac{1}{\pi^2}\int_0^{\pi} d\omega_2 \int_0^{\pi/2} d\omega_1 \ln(2\cosh 2K \coth 2K + 4\cos\omega_1 \cos\omega_2) \tag{3.48}$$

The integration over ω_2 is almost in the form (3.44) and we can put it into this form by writing

$$\begin{aligned}
I &= \frac{1}{\pi^2}\int_0^{\pi} d\omega_2 \int_0^{\pi/2} d\omega_1 \ln(2\cos\omega_1) + \frac{1}{\pi^2}\int_0^{\pi} d\omega_2 \int_0^{\pi/2} d\omega_1 \ln\left(\frac{\cosh 2K \coth 2K}{\cos\omega_1} + 2\cos\omega_2\right) \\
&= \frac{1}{\pi^2}\int_0^{\pi} d\omega_2 \int_0^{\pi/2} d\omega_1 \ln(2\cos\omega_1) + \\
&\quad + \frac{1}{\pi^2}\int_0^{\pi} d\omega_2 \int_0^{\pi/2} d\omega_1 \ln\left(2\cosh\left[\cosh^{-1}\frac{\cosh 2K \coth 2K}{2\cos\omega_1}\right] + 2\cos\omega_2\right) \\
&= \frac{1}{\pi}\int_0^{\pi/2} d\omega_1 \ln(2\cos\omega_1) + \frac{1}{\pi}\int_0^{\pi/2} d\omega_1 \cosh^{-1}\frac{\cosh 2K \coth 2K}{2\cos\omega_1}
\end{aligned} \tag{3.49}$$

The first term is zero as we show below. We have $\cosh^{-1} x = \ln\left[x + \sqrt{x^2-1}\right]$ and hence

$$\begin{aligned}
I &= \frac{1}{\pi}\int_0^{\pi/2} d\omega_1 \ln(2\cos\omega_1) + \frac{1}{\pi}\int_0^{\pi/2} d\omega_1 \ln\left\{\frac{\cosh 2K \coth 2K}{2\cos\omega_1} + \sqrt{\left(\frac{\cosh 2K \coth 2K}{2\cos\omega_1}\right)^2 - 1}\right\} \\
&= \frac{1}{2}\ln\left(2\cosh 2K \coth 2K\right) + \frac{1}{\pi}\int_0^{\pi/2} d\omega_1 \ln\left\{\frac{1+\sqrt{1-\left(\frac{2\sinh 2K}{\cosh^2 2K}\right)^2 \cos^2\omega_1}}{2}\right\} \\
&= \frac{1}{2}\ln\left(2\cosh 2K \coth 2K\right) + \frac{1}{\pi}\int_0^{\pi/2?} d\theta \ln\left\{\frac{1+\sqrt{1-q^2(K)\sin^2\theta}}{2}\right\}
\end{aligned} \tag{3.50}$$

where

$$q(K) = \frac{2\sinh 2K}{\cosh^2 2K}. \tag{3.51}$$

So finally we arrive at

$$\beta g(0,T) = -\ln(2\cosh 2K) - \frac{1}{\pi}\int_0^{\pi/2} d\theta \ln\left\{\frac{1+\sqrt{1-q^2\sin^2\theta}}{2}\right\} \tag{3.52}$$

for the free energy per spin.

$$\begin{aligned}
\frac{dq(K)}{dK} &= \frac{4\cosh 2K \cdot \cosh^2 2K - 2\sinh 2K \cdot 4\cosh 2K \sinh 2K}{\cosh^4 2K} \\
&= \frac{4\cosh^2 2K - 8\sinh^2 2K}{\cosh^3 2K} \\
&= \frac{4\cosh^2 2K - 4\sinh^2 2K - 4\sinh^2 2K}{\cosh^3 2K} \\
&= \frac{4 - 4\sinh^2 2K}{\cosh^3 2K}
\end{aligned} \tag{3.53}$$

There is maximum at $\sinh 2K = 1$ $(K \geq 0)$ where q takes the values 1.

Internal energy per spin

The internal energy per spin is defined as:

$$\frac{\langle H \rangle}{N} = \frac{1}{N}\frac{\sum_{\{s_i\}} H \exp\{-\beta H\}}{Z[\beta]}$$

As $Z[\beta] = \sum_{\{s_i\}} \exp\{-\beta H\}$ the internal energy per spin is given by

$$-\frac{\partial}{\partial \beta} \ln Z[\beta]$$

Recall that $K = \beta J$. The internal energy per spin is given by

$$
\begin{aligned}
& u(T) \\
= \; & \frac{d}{d\beta}[\beta g(T)] \\
= \; & \frac{dK}{d\beta}\frac{d}{dK}[\beta g(T)] \\
= \; & J\frac{d}{dK}\left[-\ln(2\cosh 2K) - \frac{1}{\pi}\int_0^{\pi/2} d\theta \ln\left\{\frac{1+\sqrt{1-q^2\sin^2\theta}}{2}\right\}\right] \\
= \; & J\frac{d}{dK}\left[-\frac{\ln 2}{2} - \ln(\cosh 2K) - \frac{1}{\pi}\int_0^{\pi/2} d\theta \ln\left\{1+\sqrt{1-q^2\sin^2\theta}\right\}\right]
\end{aligned}
\tag{3.54}
$$

The details of this calculation are given in section 3.7. We find

$$
u(T) = -J\coth 2K\left[1 + \frac{2}{\pi}(2\tanh^2 2K - 1)K_1(q)\right]
$$

where

$$
K_1(q) = \frac{1}{\pi}\int_0^{\pi/2}\frac{d\phi}{\sqrt{1-q^2\sin^2\phi}}
$$

is the elliptic integral of the first kind. As $q \to 1$, the term $(2\tanh^2 2K - 1) \to 0$, and the internal energy is continuous at the transition.

The specific heat capacity per spin

The specific heat capacity in terms of the partion function is:

$$
\begin{aligned}
c(T) &= \frac{\partial\langle E\rangle}{\partial T} \\
&= \frac{\partial\beta}{\partial T}\frac{\partial\langle E\rangle}{\partial\beta} \\
&= -\frac{1}{k_B T^2}\frac{\partial\langle E\rangle}{\partial\beta} \\
&= -k_B\beta^2\frac{\partial\langle E\rangle}{\partial\beta} \\
&= k_B\beta^2\frac{\partial^2\ln Z}{\partial\beta^2}.
\end{aligned}
$$

We define

$$E_1(q) \quad = \quad \int_0^{\pi/2} dx \sqrt{1 - q^2 \sin^2 x}.$$

In section 3.7 we show that

$$\frac{dK_1(q)}{dq} = \frac{E_1(q)}{q(1-q^2)} - \frac{K_1(q)}{q}. \tag{3.55}$$

which implies

$$\frac{dK_1(q)}{dK} = \coth 2K \left[\frac{2\cosh^2 2K}{1 - \sinh^2 2K} E_1(q) + 2(2\tanh^2 2K - 1)K_1(q) \right] \tag{3.56}$$

The specific heat,

$$\frac{1}{k_B} c(T) = -\beta^2 \frac{\partial^2 \beta g(T)}{\partial \beta^2}.$$

This follows from

$$\frac{1}{k_B} c(T) = \frac{1}{k_B} \frac{\partial}{\partial T} u(T) = \frac{1}{k_B} \frac{\partial \beta}{\partial T} \frac{\partial}{\partial \beta} u(T) = -\frac{1}{k_B} \frac{1}{k_B T^2} \frac{\partial}{\partial \beta} u(T) = -\beta^2 \frac{\partial}{\partial \beta} u(T).$$

$$\frac{1}{k_B} c(T) = -\beta^2 \frac{\partial^2 \beta g(T)}{\partial \beta^2}.$$

Using the aove we can calculation an aexpression for the specific heat capacity. The calculation is done in section 3.7. The result is

$$\begin{aligned} & -\frac{1}{k_B} c(T) = -\beta^2 \frac{\partial}{\partial \beta} u(T) \\ = \quad & \frac{4}{\pi} (K \cosh^2 2K)^2 \left\{ K_1(q) - E_1(q) + (1 - \tanh^2 2K) \left[\frac{\pi}{2} + (2\tanh^2 2K - 1) K_1(q) \right] \right\} \end{aligned} \tag{3.57}$$

Recall

$$\beta = \frac{1}{k_B T} \qquad K = \beta J$$

and

$$\sinh \frac{2J}{k_B T_c} = 1.$$

The Elliptic function of the first kind has the asymptotic behaviour:

$$K_1(q) \sim -\frac{1}{2} \ln |1 - q| \quad \text{as } q \to 1^-$$

Say C is defined by $\sinh C = 1$, then we have the expansions:

$$\begin{aligned}
\sinh(C + y) &= \sinh C + y \cosh C + \frac{y^2}{2!} \sinh C + \cdots = 1 + \sqrt{2} y + \frac{y^2}{2} + \cdots \\
\cosh(C + y) &= \cosh C + y \sinh C + \frac{y^2}{2!} \cosh C + \cdots = \sqrt{2} + y + \frac{1}{\sqrt{2}} y^2 + \cdots
\end{aligned}$$

so that

$$\begin{aligned}
q(C + y) &= \frac{2 \sinh(C + y)}{\cosh^2(C + y)} \\
&= \frac{2(1 + \sqrt{2} y + y^2 + \cdots)}{(\sqrt{2} + y + \frac{1}{\sqrt{2}} y^2 + \cdots)^2} = \frac{1 + \sqrt{2} y + \cdots}{1 + \sqrt{2} y + \cdots} \\
&= (1 + \sqrt{2} y + \cdots)(1 - \sqrt{2} y + \cdots) \\
&= 1 - 2y^2 + \cdots
\end{aligned}$$

Using this we approximate $q(K)$ for temperatures, T, near to the critical temperature, T_c,

$$q(K) = q \left(\frac{2J}{k_B T_c} \frac{1}{1 + \frac{T - T_c}{T_c}} \right) \approx q \left(\frac{2J}{k_B T_c} \left(1 - \frac{T - T_c}{T_c} \right) \right) \approx 1 - 2 \left(\frac{2J}{k_B T_c} \right)^2 \left(1 - \frac{T}{T_c} \right)^2$$

where we assumed that $T > T_c$.

$$q(K) = q\left(\frac{2J}{k_B T_c}\frac{1}{1-\dfrac{T_c - T}{T_c}}\right) \approx q\left(\frac{2J}{k_B T_c}\left(1+\frac{T_c - T}{T_c}\right)\right) \approx 1 - 2\left(\frac{2J}{k_B T_c}\right)\left(1-\frac{T}{T_c}\right)^2$$

where we assumed that $T < T_c$. Using this in the asymptotic expression for $K_1(q)$ we have

$$K_1(q) \sim -\frac{1}{2}\ln|1-q| \sim -\ln\left|1-\frac{T}{T_c}\right|$$

and we have for the specific heat

$$\frac{1}{k_B}c(T) \approx -\frac{2}{\pi}\left(\frac{2J}{k_B T_C}\right)^2 \ln\left|1-\frac{T}{T_c}\right| + const$$

Spontaneous magnetisation

The spontaneous magnetisation is given by

$$\begin{aligned} m_0(T) &= -\lim_{h\to 0}\frac{\partial}{\partial h}g(h,T) \\ &= \left[1-\frac{(1-\tanh^2 K)^4}{16\tanh^4 K}\right]^{1/8} \qquad T < T_c \\ &= 0 \qquad\qquad\qquad\qquad\qquad T > T_c \end{aligned} \tag{3.58}$$

As $T \to T_c$ from below, the limiting form of the spontaneous magnetisation is given by

$$m_0(T) \approx \left[\frac{T_c - T}{T_c}\right]^{1/8} \equiv \left[\frac{T_c - T}{T_c}\right]^{\beta}.$$

We have

$$
\begin{aligned}
\frac{(1-\tanh^2 K)^4}{16\tanh^4 K} &= \frac{1}{16\cosh^8 K \tanh^4 K} \\
&= \frac{1}{16\cosh^4 K \sinh^4 K} \\
&= \frac{1}{(2\cosh K \sinh K)^4} \\
&= \frac{1}{\sinh^4 2K}.
\end{aligned}
$$

So that

$$
m_0(T) = \left[1 - (\sinh 2K)^{-4}\right]^{1/8} \qquad T < T_c
$$

Recall that $\sinh \dfrac{2J}{k_B T_c} = 1$. Let C denote the actual number that satisfies $\sinh C = 1$ ($C = \ln(1+\sqrt{2}) \approx 0.8814$) and that we have,

$$
\sinh(C + y) = 1 + \sqrt{2}y + \cdots
$$

For y small we have

$$
1 - (\sinh 2K)^{-4} \approx 1 - (1 + \sqrt{2}y)^{-4} \approx 4\sqrt{2}y.
$$

We make the expansion

$$
2K = \frac{2J}{k_B T} = \frac{2J}{k_B T_c} \frac{1}{1 - \dfrac{T_c - T}{T_c}} \approx \frac{2J}{k_B T_c}\left(1 + \frac{T_c - T}{T_c}\right) = \frac{2J}{k_B T_c} + y
$$

where

$$
y := \frac{2J}{k_B T_c}\frac{T_c - T}{T_c} = \ln(1+\sqrt{2})\frac{T_c - T}{T_c}
$$

Using this we finally obtain

$$
\begin{aligned}
m_0(T) &\approx \left[4\sqrt{2}\ln(1+\sqrt{2})\frac{T_c - T}{T_c}\right]^{1/8} \\
&\approx 1.2224\left[\frac{T_c - T}{T_c}\right]^{1/8} \\
&\approx \left[\frac{T_c - T}{T_c}\right]^{1/8}.
\end{aligned}
$$

Zero-field susceptibility

The asymptotic form as $T \to T_c$ of the zero-field susceptibility is also known [4]:

$$
\chi(0,T) = \lim_{h\to 0}\frac{\partial m(h,T)}{\partial h} \sim |T - T_c|^{-7/4} = |T - T_c|^{-\gamma}. \tag{3.59}
$$

3.6 Kramers-Wannier Duality

3.6.1 Low temperature expansion

The ground states are obvious. One ground state is all the spin are up, the other ground state is when all the spins are down.

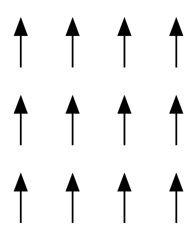


Figure 3.1: Ground state where all spin are up.

Both ground states have energy $E = E_0 = -2NJ$. The interactin with the spin to the neighbouring spin to the right and the neighbouring spin below cotributes the energy: $-2J$. We find the total energy found by adding up all such contributions for the N spins of the ssystem.

The first excited states arise from flipping a single spin. Each spin has $q = 4$ nearest neighbours, denoted by red lines in the example below, each of which contributes an energy cost of $2J$. The energy of the first excited state is therefore $E_1 = E_0 + 8J$.

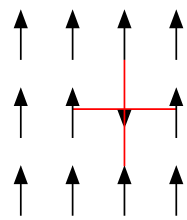
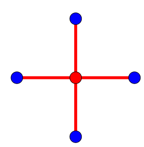


Figure 3.2: Ground state where all spin are up.

There are, of course, N different spins that we can flip and, correspondingly, the first energy level has a dengeneracy of N.

At this point we introduce a diagrammatic method to list the different states. We draw only the bonds which connect two spins with opposite orientation and, as in fig 3.3, denote these by red lines. We further draw the flipped spins as red dots, the unflipped spins as blue dots. The energy of the state is determined simply by the number of red lines in the diagram.

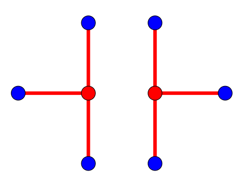


$E_1 = E_0 + 8J$

Degeneracy $= N$

Figure 3.3:

The next lowest state has six red bonds. It take te form given in fig (3.4)



$E_2 = E_0 + 12J$

Degeneracy $= \frac{1}{2}N(N-5)$

Figure 3.4:

where the extra factor of 2 in the degeneracy comes from the two possible orientatios (vertical and horizontal) of the graph.

We now move to states which sit at the third excited level. These have 8 red lines. The simplest cofiguratio consists of two, disconected, flipped spins depicted in fig 3.5.

The factor of N in the degeneracy comes from placing the first graph; the factor $N-5$ comes about from the fact that the flipped spin of the second graph can sit aywhere apart from at the five vertices used in the first graph. Finally, th efactor of $1/2$ comes from the interchange of the two graphs.

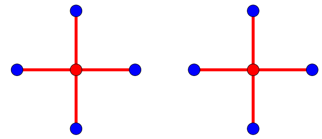


Figure 3.5:

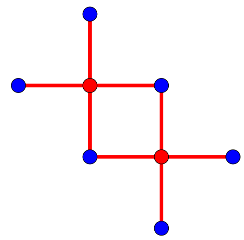


Figure 3.6:

This includes graphs as depicted in figure 3.6

There are three further graphs with the same energy E_3. These are fig 3.7

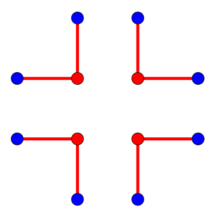


Figure 3.7:

and figure (3.8)

where the degeneracy comes from the two orientations (vertical and horizontal). And finally figure (3.9)

where the degeneracy comes from the four orientations (rotating the graph by 90^0).

Adding all the graphs above togather gives us an expansion of the partion function in powers of $e^{-\beta J} \ll 1$. This results in

$$Z = 2e^{2N\beta J}\left(1 + Ne^{-8\beta J} + 2Ne^{-12\beta J} + \frac{1}{2}\left(N^2 + 9N\right)e^{-16\beta J} + \cdots\right) \qquad (3.60)$$

where the factor of 2 originates from the two ground states of the system. At this point we make a note of what happens when we take the ln of the partion function,

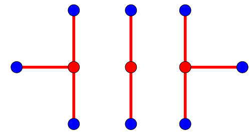


Figure 3.8:

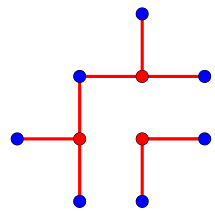


Figure 3.9:

$$
\begin{aligned}
\ln Z &= \ln 2 + 2N\beta J + \ln\left(1 + N(e^{-8\beta J} + 2e^{-12\beta J} + \frac{9}{2}e^{-16\beta J}) + \frac{1}{2}N^2 e^{-16\beta J} + \cdots\right) \\
&= \ln 2 + 2N\beta J + N(e^{-8\beta J} + 2e^{-12\beta J} + \frac{9}{2}e^{-16\beta J}) + \frac{1}{2}N^2 e^{-16\beta J} \\
&\quad -\frac{1}{2}N^2(e^{-8\beta J} + 2e^{-12\beta J} + \frac{9}{2}e^{-16\beta J})^2 \\
&= \ln 2 + 2N\beta J + Ne^{-8\beta J} + 2Ne^{-12\beta J} + \frac{9}{2}Ne^{-16\beta J} + \mathcal{O}(e^{-20\beta J}) \qquad (3.61)
\end{aligned}
$$

where we have used $\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \cdots$. The thing to notice is that the N^2 term in the partition function (3.60) has cancelled out and $\log Z$ is proportional to N, which is to be expected since the free energy ofthe system is extensive. Looking back, we see that the N^2 term was associated to the disconnected diagrams in figure 3.5. As it turns out the partition function can be written as the exponential of the sum of connected diagrams.

3.6.2 High temperature expansion

We now turn to the 2d Ising model in the opposite limit of high temperature. Here we expect the partition function to be dominated by the completely random, disordered configurations of maximum entropy. Our goal is to find a way to expand the partition function in $\beta J \ll 1$.

We write the partition function as

$$Z = \sum_{\{s_i\}} \exp\left(\beta J \sum_{\langle ij \rangle} s_i s_j\right) = \sum_{\{s_i\}} \prod_{\langle ij \rangle} e^{\beta J s_i s_j}.$$

There is a useful way to rewrite $e^{\beta J s_i s_j}$ which relies on the fact that the product $s_i s_j$ only takes $\pm$:

$$\begin{aligned} e^{\beta J s_i s_j} &= \cosh \beta J + s_i s_j \sinh \beta J \\ &= \cosh \beta J (1 + s_i s_j \tanh \beta J). \end{aligned}$$

Using this, the partition function becomes

$$\begin{aligned} Z &= \sum_{\{s_i\}} \prod_{\langle ij \rangle} \cosh \beta J + s_i s_j \sinh \beta J \\ &= (\cosh \beta J)^{qN/2} \sum_{\{s_i\}} \prod_{\langle ij \rangle} (1 + s_i s_j \tanh \beta J). \end{aligned} \quad (3.62)$$

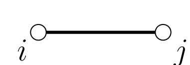
where the number of nearest neighbours is $q = 4$ for the $2d$ square lattice.

At high temperatures $\beta J \ll 1$ which, of course, means that $\tanh \beta J = \dfrac{e^{bJ} - e^{-bJ}}{e^{bJ} + e^{-bJ}} \ll 1$. The partition function is now naturally a product of powers of $\tanh \beta J$. We will represent the expansion graphically.

The leading order term has no factors of $\tanh \beta J$ and is simply

$$Z \approx (\cosh \beta J)^{2N} \sum_{\{s_i\}} 1 = 2^N (\cosh \beta J)^{2N}$$

Let's now turn to the leading correction. Expanding the partition function (3.62), each power of $\tanh \beta J$ is associated with a nearest order pair $\langle ij \rangle$. We represent this



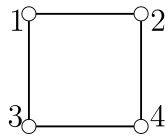
$= s_i s_j \tanh \beta J$

Figure 3.10:

Each factor of $\tanh \beta J$ comes with a sum over all spins s_i and s_j. They simply sum to zero,

$$\sum_{s_i,s_j} = +1 - 1 - 1 + 1 = 0.$$

The only way to avoid such sums to resulting in zero is to make sure that we are summing over an even number of spins on each site, since then we get factor of $s_i^2 = 1$ and no cancellations. Graphically, this means that every site must have an even number of lines attached to it. The first correction is then of the form



$$= (\tanh \beta J)^4 \textstyle\sum_{\{s_i\}} s_1 s_2 \; s_2 s_3 \; s_3 s_4 \; s_4 s_1$$
$$= 2^4 (\tanh \beta J)^4 \textstyle\sum'_{\{s_i\}} 1$$

Figure 3.11:

where $\sum'_{\{s_i\}} 1$ denotes the sum over spins that are not s_1, s_2, s_3, or s_4 and is equal to 2^{N-4}. There are N such terms since the upper left corner of the square can be on any one of the N lattice sites. (Assuming periodic boundary conditions for the lattice). So including the leading term and the first correction, we have

$$Z = 2^N (\cosh \beta J)^4 \left(1 + (\tanh \beta J)^4 + \cdots\right)$$

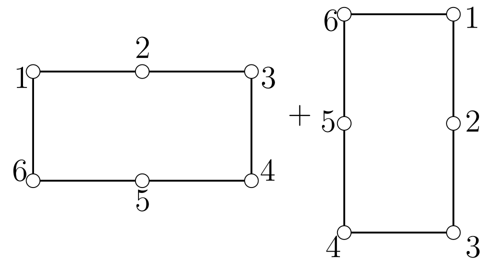
The next terms arise from graphs of length 6 and the only possibilities are rectangles, oriented as either landscape or portrait. The contribution from both rectangles is,

$$N (\tanh \beta J)^4 \sum_{\{s_i\}} s_1 s_2 \; s_2 s_3 \; s_3 s_4 \; s_4 s_5 \; s_5 s_6 \; s_6 s_1$$
$$= N 2^6 (\tanh \beta J)^4 \sum_{\{s_i\}}{}' 1$$
$$= N 2^6 (\tanh \beta J)^4 2^{N-6}$$

where the N arises from the fact that each of them can sit on one of N sites. These contribution are depicted in fig 3.12

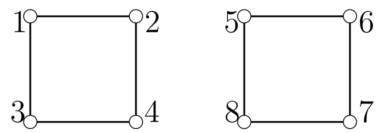
Now let's look at graphs of length 8. We have four different types of graphs. Firstly, there are the trivial, disconnected pair of squares

We consider the case where the two squares overlap at one site separately later, these correspond to four positionings of the second square. Explicitly, the calculation corresponding to figure 3.13 is,



$$= 2N \cdot 2^6 (\tanh \beta J)^4 2^{N-6}$$

Figure 3.12:



$$= \tfrac{1}{2} N(N-9) 2^4 2^4 (\tanh \beta J)^8 2^{N-8}$$

Figure 3.13:

$$\begin{aligned} &\frac{1}{2} N(N-9)(\tanh \beta J)^8 \sum_{\{s_1,\ldots,s_4\}} s_1 s_2\ s_2 s_3\ s_3 s_4\ s_4 s_1 \sum_{\{s_5,\ldots,s_8\}} s_5 s_6\ s_6 s_7\ s_7 s_8\ s_8 s_1 {\sum_{\{s_i\}}}' 1 \\ &= 2^N \frac{1}{2} N(N-9)(\tanh \beta J)^8 \end{aligned} \tag{3.63}$$

Here the first factor of N is the possible positions of the first square; the factor of $N-9$ arises because the possible location of the upper left corner of the second square can't be on the top left vertex of the first square because that cant occur, but nor can it be in the four positions indicated in figures 3.14 (a), 3.14 (b), 3.14 (c), or 3.14 (d) because they involve three lines comming off a site and therefore vanish when we sum over spins, and we are considering the cases where the two squares overlap at a single site later. Finally, the factor of 1/2 comes from the fact that the two squares are identical.

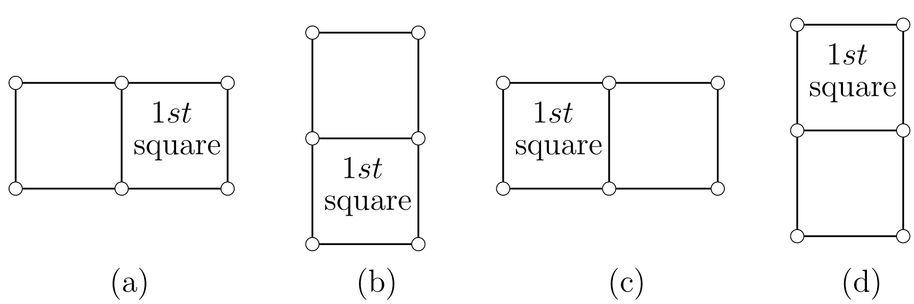
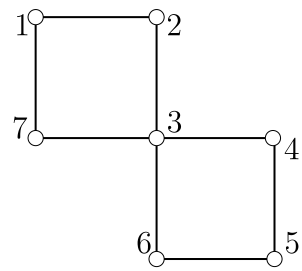


Figure 3.14:

Explicitly, the calculation corresponding to fig 3.15 is,



$= \frac{1}{2}N2^7(\tanh\beta J)^8 2^{N-7}$

Figure 3.15:

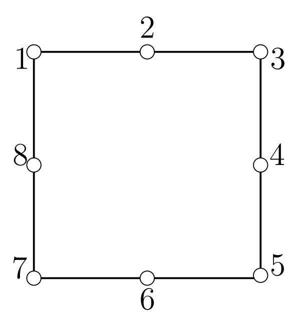
$$
\begin{aligned}
&2N(\tanh\beta J)^8 \sum_{\{s_1,\ldots,s_7\}} s_1s_2\ s_2s_3\ s_3s_4\ s_4s_5\ s_5s_6\ s_6s_7\ s_7s_4\ s_4s_3 {\sum_{\{s_i\}}}' 1 \\
&= 2N(\tanh\beta J)^8 \sum_{\{s_1,\ldots,s_7\}} s_1^2s_2^2s_3^4s^5s^2s_7^2 \cdot 2^{N-7} \\
&= 2\cdot 2^N N(\tanh\beta J)^8
\end{aligned}
\tag{3.64}
$$

Here the first factor of N is the possible positions of the first square. We need only consider the case where the top left corner of the second square attached to the bottom right corner of the first square, and the graph rotated by 90^0.

Adding the contributions from (3.63) and (3.64) gives

$$2^N\frac{1}{2}N(N-9)(\tanh\beta J)^8 + 2\cdot 2^N N(\tanh\beta J)^8 = 2^N\frac{1}{2}N(N-5)(\tanh\beta J)^8$$

The other graphs of length 8 are a large square, a rectagle and a corner. The large square gives a contribution depicted in fig 3.16



$= N2^8(\tanh\beta J)^8 2^{N-8}$

Figure 3.16:

There are two orientations for the rectangle.

Finally, the corner graph (figure 3.18) has four orientations giving $4N2^N\,(\tanh\beta J)^8$.

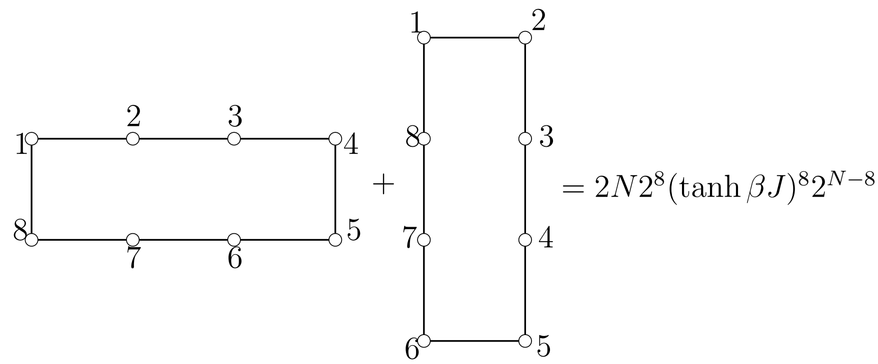


Figure 3.17:

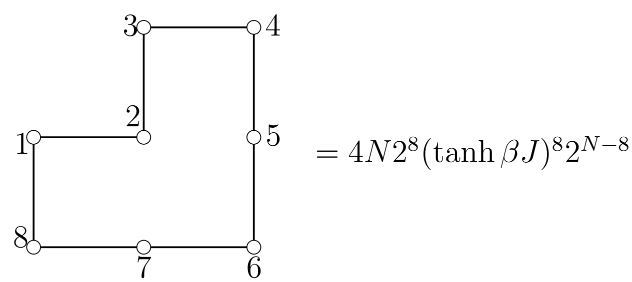


Figure 3.18:

Adding all contributions together gives the first few terms in the high temperature expansion of the partition function

$$Z = 2^N (\cosh \beta J)^{2N} \left(1 + (N \tanh \beta J)^4 + 2N (\tanh \beta J)^6 + \frac{1}{2} \left(N^2 + 9N \right) (\tanh \beta J)^8 + \dots \right)$$

Taking the ln of the partition function results in

$$\ln Z = N \ln 2 + 2N \cosh \beta J + N (\tanh \beta J)^4 + 2N (\tanh \beta J)^6 + \frac{9}{2} N (\tanh \beta J)^8 + \mathcal{O}(\tanh^{10} \beta J)$$

3.6.3 Kramers-Wannier Duality

In the previous sections we computed the partition function perturbatively in two extreme regimesof low temperature ad high temoerature. The physics in the low temperature and high temperature is, of course, very different. At low temperatures, the partition function is dominated by the lowest energy states; at high temperatures it is dominated by maximally disordered states. Yet comparing the partition functions at low temperature and high temperature reveals an extraordinary fact: the expansions are the same! More concretely, the two series agree if we exchange

$$\exp\{-2\beta J\} \leftrightarrow \tanh\beta J. \tag{3.65}$$

Of course, we have only checked the agreement to the first few orders in perturbation theory. Below we shall prove that this continues to all orders in perturbation theory. The symmetry of the partition function under the interchange (3.65) is knownas Kramers-Wannier duality. Before we prove this duality, we will first just assume that it is true and extract some consequences.

We can express the statement of the duality more clearly. The Ising model at temperature β is related to the same model at temperature β^*; defined as

$$\exp\{-2\beta^* J\} \leftrightarrow \tanh\beta J. \tag{3.66}$$

This way of writing things hides the symmetry of the transformation. A little algebra shows that this is equivalent to

$$\sinh 2\beta^* J = \frac{1}{\sinh 2\beta J}.$$

Notice that this is a high temperature/low temperature duality. When βJ is large, $\beta^* J$ is small. Kramers-Wannier duality is the statement that, when $B = 0$, the partition functions of the Ising model at two temperatures are related by

$$\begin{aligned} Z[\beta] &= \frac{2^N(\cosh\beta J)^{2N}}{2\exp\{2N\beta^* J\}} Z[\beta^*] \\ &= 2^{N-1}\left(\cosh\beta J \sinh\beta J\right)^N Z[\beta^*]. \end{aligned} \tag{3.67}$$

This means that if you know the thermodynamics of the Ising model at one temperature, then you also know the thermodynamics at the other temperature. Notice however, that it does not say that all the physics of the two models is equivalent. In particular, when one system is in the ordered phase, the other typically lies in the disordered phase.

The key idea is that various graphs in the two expansions are related. For example, the two "corner" diagrams in figure 3.19.

The two graphs are dual. The red lines in the first graph itersect the black lines in the second as can been seen by placing them on top of each other, depicted in fig 3.20

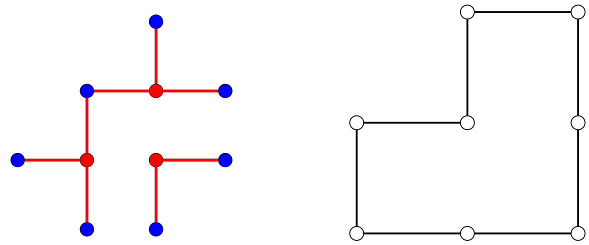


Figure 3.19:

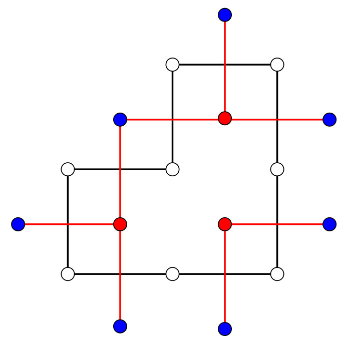


Figure 3.20:

The same relationship between graphs occurs more generally; the graphs appearing in the low temperature expansion are in one-to-one correspondence with dual graphs of the high temperature expansion. We will show how this occurs and how one may map the partition functions onto each other.

We start by writing the partition function (3.62) tailored for the high temperature expansion and presenting it in a slightly different way,

$$\begin{aligned} Z[\beta] &= \sum_{\{s_i\}} \prod_{\langle ij \rangle} \Big(\cosh \beta J + s_i s_j \sinh \beta J \Big) \\ &= \sum_{\{s_i\}} \prod_{\langle ij \rangle} \sum_{k_{ij}=0,1} C_{k_{ij}}[\beta J] (s_i s_j)^{k_{ij}} \end{aligned} \tag{3.68}$$

where we have introduced the variable k_{ij} associated to each nearest neighbour pair that takes values 0 and 1, together with the functions,

$$C_0[\beta J] = \cosh \beta J \qquad \text{and} \qquad C_1[\beta J] = \sinh \beta J.$$

The variables in the original Ising model were spins on the lattice sites. The observation that the graphs which appear in the two expansions are dual suggests that it might be advantageous to focus attetion on the links between lattice sites. Clearly, we have one link for every nearest neighbour pair. If we label the links by l, we can rewrite the partition function as

$$\begin{aligned} Z &= \sum_{\{s_i\}} \sum_{\{k_l=0,1\}} \prod_l C_{k_l}[\beta J](s_i s_j)^{k_l} \\ &= \sum_{\{k_l=0,1\}} \sum_{\{s_i\}} \prod_l C_{k_l}[\beta J](s_i s_j)^{k_l} \\ &= \sum_{\{k_l=0,1\}} \prod_l \sum_{\{s_i\}} C_{k_l}[\beta J](s_i s_j)^{k_l}. \end{aligned}$$

Notice that the label k_{ij} has now become a variable that lives on the links l rather than on the original lattice sites i.

At this stage, we do the sum over the spins s_i. We have seen that if a given spin, say s_i, appears in a term an odd number of times, then that term will vanish when we sum over the spin. Alternatively, if the spin s_i appears an even number of times, then the sum will give 2. We will say that a given link l is turned on in configurations with $k_l = 1$ and turned off when $k_l = 0$. In this language, a term in the sum over spin s_i contributes only if an even number of links attached to site i are turned on. The partition function then becomes

$$Z = 2^N \sum_{\{k_l=0,1\}} \prod_l C_{k_l}[\beta J] \Big|_{Constrained} . \tag{3.69}$$

Rather than summing over spins on lattice sites, we are now summing over the new variables k_l living on links. The "Constrained" label on the sum is there to remind us that we don't sum over all k_l configurations; only those for which an even number of links are turned on for every lattice site. This is makes things awkward. It's telling us that the k_l are not really independent variables. There are some constraints that must be imposed.

Fortunately, for the $2d$ square lattice, there is a simple way to solve the constraint. We introduce yet more variables, $\tilde{s}_i$ which, like the original spin variables, take values ± 1. However, the $\tilde{s}_i$ do not live on the original lattice sites. Instead, they live on the vertices of the dual lattice. For the $2d$ square lattice, the dual vertices are draw in the figure 3.21. The original lattice sites are in white; the dual lattice sites in black.

The link variables k_l are related to the two nearest spin variables $\tilde{s}_i$ as follows:

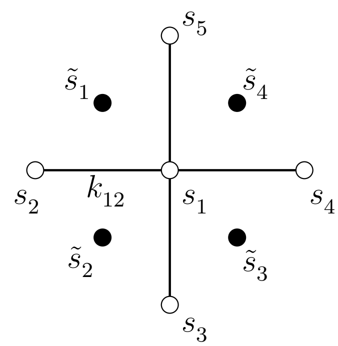


Figure 3.21:

$$
\begin{aligned}
k_{12} &= \frac{1}{2}(1-\tilde{s}_1\tilde{s}_2)\\
k_{13} &= \frac{1}{2}(1-\tilde{s}_2\tilde{s}_3)\\
k_{14} &= \frac{1}{2}(1-\tilde{s}_3\tilde{s}_4)\\
k_{15} &= \frac{1}{2}(1-\tilde{s}_4\tilde{s}_4)
\end{aligned}
$$

Thus we have replaced four variables k_l taking values $0, 1$ with four variables $\tilde{s}_i$ taking values ± 1.

$$
\begin{aligned}
k_{12}+k_{13}+k_{14}+k_{15} &= 2-\frac{1}{2}(1-\tilde{s}_1\tilde{s}_2+\tilde{s}_2\tilde{s}_3+\tilde{s}_3\tilde{s}_4)+\tilde{s}_4\tilde{s}_4)\\
&= \frac{1}{2}(\tilde{s}_1+\tilde{s}_3)(\tilde{s}_2+\tilde{s}_4)\\
&= 0, 2, 4
\end{aligned}
$$

In other words, the number of links that are turned on must be even. But that is exactly what we want. Writing the k_l in terms of the auxiliary spins $\tilde{s}_i$ automatically solves the constraint that is imposed on the sum in (3.69). Moreover, it is simple to check that for every configuration $\{k_l\}$ obeying the constraint, there are two configurations of $\{\tilde{s}_i\}$ (flipp all the "spins" $\tilde{s}_i$). This means that we can replace the constrained sum over $\{k_l\}$ with an unconstrained sum over $\{\tilde{s}_i\}$, and by including an additional factor of $1/2$,

$$
Z = \frac{1}{2}2^N \sum_{\{\tilde{s}_i\}} \prod_{\langle ij\rangle} C_{\frac{1}{2}-\tilde{s}_i\tilde{s}_j}[\beta J]. \tag{3.70}
$$

Finally, can obtain a simple expression for C_0 and C_1 in terms of $\tilde{s}_i$. We write

$$
\begin{aligned}
C_k[\beta K] &= \cosh\beta J \exp\left(k \ln\tanh\beta K\right) \\
&= \left(\sinh\beta J\cosh\beta K\right)^{1/2}\exp\left(-\frac{1}{2}\tilde{s}_i\tilde{s}_j \ln\tanh\beta J\right)
\end{aligned}
$$

Sunstituting this into (3.70) gives

$$
\begin{aligned}
Z[\beta] &= 2^{N-1}\sum_{\{\tilde{s}_i\}}\prod_{\langle ij\rangle}\left(\sinh\beta J\cosh\beta K\right)^{1/2}\exp\left(-\frac{1}{2}\tilde{s}_i\tilde{s}_j \ln\tanh\beta J\right) \\
&= 2^{N-1}\left(\sinh\beta J\cosh\beta K\right)^{N}\sum_{\{\tilde{s}_i\}}\exp\left(-\frac{1}{2}\ln\tanh\beta J\sum_{\langle ij\rangle}\tilde{s}_i\tilde{s}_j\right)
\end{aligned}
$$

But this final form of the partition function in terms of the dual spins $\tilde{s}_i$ has exactly the same functional form as the original partition function in terms of the spins s_i. More precisely, we can write

$$
Z[\beta] = 2^{N-1}\left(\sinh 2\beta J\right) Z[\beta^*]
$$

where

$$
\exp\left(-2\beta^* J\right) = \tanh\beta J.
$$

This completes the proof of the Krammer-Wannier duality for the $2d$ Ising model on a square lattice.

3.7 Calculational details

2.1 Other commutators

2.2 Completeness relations for finite Fourier transformations

Even case:

The q takes the values

$$
\pm\frac{\pi}{M}, \pm\frac{3\pi}{M}, \ldots, \pm\frac{(M-1)\pi}{M} \quad \text{for } n \text{ even.}
$$

For $j = j'$,

$$\begin{aligned}\frac{1}{M}\sum_q e^{iq(j-j')} &= \frac{1}{M}\sum_q 1 \\ &= 1.\end{aligned}$$

For $j \neq j'$,

$$\begin{aligned}\frac{1}{M}\sum_q e^{iq(j-j')} &= \frac{1}{M}\left(e^{-i\frac{\pi J}{M}} + e^{-i\frac{3\pi J}{M}} + \cdots + e^{-i\frac{(M-1)\pi J}{M}}\right) + \left(e^{i\frac{\pi J}{M}} + e^{i\frac{3\pi J}{M}} + \cdots + e^{i\frac{(M-1)\pi J}{M}}\right) \\ &= \frac{1}{M}e^{-i\frac{\pi n}{M}}\frac{1-e^{-i\frac{\pi J}{M}M}}{1-e^{-i\frac{2\pi J}{M}}} + e^{i\frac{\pi J}{M}}\frac{1}{M}\frac{1-e^{i\frac{2\pi J}{M}M}}{1-e^{i\frac{2\pi n}{M}}} \\ &= -\frac{1}{M}e^{i\frac{\pi n}{M}}\frac{1-e^{-i\pi J}}{1-e^{i\frac{2\pi J}{M}}} + e^{i\frac{\pi J}{M}}\frac{1}{M}\frac{1-e^{i\pi J}}{1-e^{i\frac{2\pi J}{M}}} \\ &= 0\end{aligned}$$

as $J \equiv j - j' = \pm 1, \pm 2, \ldots, \pm(M-1)$.

For $q = q'$,

$$\begin{aligned}\frac{1}{M}\sum_{j=1}^{M} e^{ij(q-q')} &= \frac{1}{M}\sum_q 1 \\ &= 1.\end{aligned}$$

For $q \neq q'$.

$$\begin{aligned}\frac{1}{M}\sum_{j=1}^{M} e^{ij(q-q')} &= \frac{1}{M}\sum_{j=1}^{M} e^{i\frac{\pi Q}{M}j} \\ &= \frac{1}{M}e^{i\frac{n\pi}{M}}\frac{1-e^{i\frac{\pi Q}{M}M}}{1-e^{i\frac{\pi Q}{M}}} \\ &= 0\end{aligned}$$

as $Q \equiv q - q' = \pm 2, \pm 4, \ldots, \pm 2(M-1)$.

Odd case:

The q takes the values

$$0, \pm\frac{2\pi}{M}, \pm\frac{4\pi}{M}, \dots, \pm\frac{(M-2)\pi}{M}, \pi \quad \text{for } n \text{ odd.}$$

For $j = j'$,

$$\begin{aligned}\frac{1}{M}\sum_q e^{iq(j-j')} &= \frac{1}{M}\sum_q 1 \\ &= 1.\end{aligned}$$

For $j \neq j'$,

$$\begin{aligned}&\frac{1}{M}\sum_q e^{iq(j-j')} \\ =\ & \frac{1}{M}\left(e^{-i\frac{2\pi J}{M}} + e^{-i\frac{4\pi J}{M}} + \cdots + e^{-i\frac{2\pi J}{M}\frac{M-2}{2}}\right) + \frac{1}{M}\left(1 + e^{i\frac{2\pi J}{M}} + e^{i\frac{4\pi J}{M}} + \cdots + e^{i\frac{2\pi J}{M}\frac{M-2}{2}} + e^{i\pi J}\right) \\ =\ & \frac{1}{M}\left(e^{-i\frac{2\pi J}{M}} + e^{-i\frac{4\pi J}{M}} + \cdots + e^{-i\frac{2\pi J}{M}\frac{M-2}{2}} + e^{-i\pi J}\right) + \frac{1}{M}\left(1 + e^{i\frac{2\pi J}{M}} + e^{i\frac{4\pi J}{M}} + \cdots + e^{i\frac{2\pi J}{M}\frac{M-2}{2}}\right) \\ =\ & \frac{1}{M}e^{-i\frac{2\pi J}{M}}\frac{1-e^{-i\frac{2\pi J}{M}\frac{M}{2}}}{1-e^{-i\frac{2\pi J}{M}}} + \frac{1}{M}\frac{1-e^{i\frac{2\pi J}{M}\frac{M}{2}}}{1-e^{i\frac{2\pi n}{M}}} \\ =\ & -\frac{1}{M}\frac{1-e^{-i\pi J}}{1-e^{i\frac{2\pi J}{M}}} + \frac{1}{M}\frac{1-e^{i\pi J}}{1-e^{i\frac{2\pi J}{M}}} \\ =\ & 0\end{aligned}$$

as $J = \pm 1, \pm 2, \dots, \pm(M-1)$.

For $q = q'$,

$$\begin{aligned}\frac{1}{M}\sum_{j=1}^{M} e^{ij(q-q')} &= \frac{1}{M}\sum_q 1 \\ &= 1.\end{aligned}$$

For $q \neq q'$.

$$\begin{aligned}
\frac{1}{M}\sum_{j=1}^{M} e^{ij(q-q')} &= \frac{1}{M}\sum_{j=1}^{M} e^{i\frac{\pi Q}{M}j} \\
&= \frac{1}{M} e^{i\frac{\pi Q}{M}} \frac{1-e^{i\frac{\pi Q}{M}M}}{1-e^{i\frac{\pi Q}{M}}} \\
&= 0
\end{aligned}$$

as $Q = \pm 2, \pm 4, \ldots, \pm(2M-2)$.

2.3 Inverse transformation of (3.21)

$$\begin{aligned}
\frac{1}{\sqrt{M}}\sum_{j=1}^{M} c_j e^{-iqj} &= \frac{1}{\sqrt{M}}\sum_{j=1}^{M}\left(\sum_{q'} \frac{1}{\sqrt{M}} a_{q'} e^{iq'j}\right) e^{-iqj} \\
&= \sum_{q'} a_{q'} \cdot \frac{1}{M}\sum_{j=1}^{M} e^{i(q'-q)j} \\
&= \sum_{q'} a_{q'} \delta_{q,q'} \\
&= a_q
\end{aligned}$$

$$\begin{aligned}
\frac{1}{\sqrt{M}}\sum_{q} a_q e^{iqj} &= \frac{1}{\sqrt{M}}\sum_{q}\left(\sum_{j'=1}^{M} \frac{1}{\sqrt{M}} c_{j'} e^{-iqj'}\right) e^{iqj} \\
&= \sum_{j'=1}^{M} c_{j'} \cdot \frac{1}{M}\sum_{q} e^{iq(j'-j')} \\
&= \sum_{j'} c_{j'} \delta_{j,j'} \\
&= c_j \qquad (3.71)
\end{aligned}$$

2.4 The operators a_q, $a_q^\dagger$ obey fermion commutation relations

$$
\begin{aligned}
[a_q, a_{q'}^\dagger]_+ &= [\frac{1}{\sqrt{M}}\sum_{j=1}^{M} c_j e^{-iqj}, \frac{1}{\sqrt{M}}\sum_{j'=1}^{M} c_j^\dagger e^{iq'k}]_+ \\
&= \frac{1}{M}\sum_{j=1}^{M}\sum_{j'=1}^{M}[c_j, c_{j'}^\dagger]_+ e^{i(q'j'-qj)} \\
&= \frac{1}{M}\sum_{j=1}^{M}\sum_{j'=1}^{M}\delta_{j,j'} e^{i(q'j'-qj)} \\
&= \frac{1}{M}\sum_{j=1}^{M} e^{ij(q'-q)} \\
&= \delta_{q,q'}
\end{aligned}
$$

$$
\begin{aligned}
[a_q, a_{q'}]_+ &= \frac{1}{M}\sum_{j=1}^{M}\sum_{j'=1}^{M}[c_j, c_{j'}]_+ e^{-i(q'j'+qj)} \\
&= 0
\end{aligned}
$$

$$
\begin{aligned}
[a_q^\dagger, a_{q'}^\dagger]_+ &= \frac{1}{M}\sum_{j=1}^{M}\sum_{j'=1}^{M}[c_j^\dagger, c_{j'}^\dagger]_+ e^{i(q'j'+qj)} \\
&= 0
\end{aligned}
$$

3.7.1 V_2 in $q-$space for n even and n odd

n even

For n even we have

$$\begin{aligned}
\sum_{j=1}^{M} c_j^\dagger c_j &= \frac{1}{M}\sum_{j=1}^{M}\sum_q\sum_{q'} a_q^\dagger e^{-iqj} a_{q'} e^{iq'j} \\
&= \sum_q\sum_{q'} a_q^\dagger a_{q'} \frac{1}{M}\sum_{j=1}^{M} e^{i(q'-q)j} \\
&= \sum_q\sum_{q'} a_q^\dagger a_{q'} \delta_{q,q'} \\
&= \sum_q a_q^\dagger a_q \\
&= \sum_{q>0} (a_q^\dagger a_q + a_{-q}^\dagger a_{-q}).
\end{aligned}$$

Note there are $M/2$ terms in the sum $\sum_{q>0}$, so that

$$\begin{aligned}
\mathbf{V}_2 &= (2\sinh 2K)^{M/2} \exp\left\{ 2K^* \sum_{j=1}^{M} \left(c_j^\dagger c_j - \frac{1}{2} \right) \right\} \\
&= (2\sinh 2K)^{M/2} \exp\left\{ 2K^* \sum_{q>0} \left(a_q^\dagger a_q + a_{-q}^\dagger a_{-q} - 1 \right) \right\}.
\end{aligned}$$

Recall ()

$$\mathbf{V}_1 = \exp\left\{ K \sum_{j=1}^{M} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}^\dagger - c_j c_{j+1}) \right\}$$

We have

$$\begin{aligned}
\sum_{j=1}^{M} c_j^\dagger c_{j+1} &= \frac{1}{M}\sum_{j=1}^{M}\sum_q\sum_{q'} a_q^\dagger e^{-iqj} a_{q'} e^{iq'(j+1)} \\
&= \sum_q\sum_{q'} e^{iq'} a_q^\dagger a_{q'} \frac{1}{M}\sum_{j=1}^{M} e^{i(q'-q)j} \\
&= \sum_q\sum_{q'} e^{iq'} a_q^\dagger a_{q'} \delta_{q,q'} \\
&= \sum_q e^{iq} a_q^\dagger a_q \\
&= \sum_{q>0} (e^{iq} a_q^\dagger a_q + e^{-iq} a_{-q}^\dagger a_{-q}).
\end{aligned}$$

and

$$
\begin{aligned}
\sum_{j=1}^{M} c_{j+1}^{\dagger} c_j &= \frac{1}{M} \sum_{j=1}^{M} \sum_{q} \sum_{q'} a_q^{\dagger} e^{-iq(j+1)} a_{q'}^{\dagger} e^{iq'j} \\
&= \sum_{q} e^{-iq} a_q^{\dagger} a_q \\
&= \sum_{q>0} (e^{-iq} a_q^{\dagger} a_q + e^{iq} a_{-q}^{\dagger} a_{-q})
\end{aligned}
$$

and

$$
\begin{aligned}
\sum_{j=1}^{M} c_j^{\dagger} c_{j+1}^{\dagger} &= \frac{1}{M} \sum_{j=1}^{M} \sum_{q} \sum_{q'} a_q^{\dagger} e^{-iqj} a_{q'}^{\dagger} e^{-iq'(j+1)} \\
&= \sum_{q} \sum_{q'} e^{-iq'} a_q^{\dagger} a_{q'}^{\dagger} \delta_{q,-q'} \\
&= \sum_{q} e^{iq} a_q^{\dagger} a_{-q}^{\dagger} \\
&= \sum_{q>0} (e^{iq} a_q^{\dagger} a_{-q}^{\dagger} + e^{-iq} a_{-q}^{\dagger} a_q^{\dagger}) \\
&= \sum_{q>0} (e^{iq} a_q^{\dagger} a_{-q}^{\dagger} - e^{-iq} a_q^{\dagger} a_{-q}^{\dagger}) \\
&= 2i \sum_{q>0} \sin q a_q^{\dagger} a_{-q}^{\dagger}
\end{aligned}
$$

and

$$
\begin{aligned}
-\sum_{j=1}^{M} c_j c_{j+1} &= -\frac{1}{M} \sum_{j=1}^{M} \sum_{q} \sum_{q'} a_q e^{iqj} a_{q'} e^{iq'(j+1)} \\
&= -\sum_{q} \sum_{q'} e^{iq'} a_q a_{q'} \delta_{q,-q'} \\
&= -\sum_{q} e^{iq} a_q a_{-q} \\
&= -\sum_{q>0} (e^{-iq} a_q a_{-q} + e^{iq} a_{-q} a_q) \\
&= 2i \sum_{q>0} \sin q a_q a_{-q}
\end{aligned}
$$

So

$$
\begin{aligned}
&\sum_{j=1}^{M}(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}^\dagger - c_j c_{j+1}) \\
&\quad = \sum_{q>0}(e^{iq} a_q^\dagger a_q + e^{-iq} a_{-q}^\dagger a_{-q}) + \sum_{q>0}(e^{-iq} a_q^\dagger a_q + e^{iq} a_{-q}^\dagger a_{-q}) \\
&\quad + \sum_{q>0} 2i \sin q a_q^\dagger a_{-q}^\dagger + \sum_{q>0} 2i \sin q a_q a_{-q} \\
&\quad = \sum_{q>0}[2\cos q(a_q^\dagger a_q + a_{-q}^\dagger a_{-q}) - 2i \sin q(a_q^\dagger a_{-q}^\dagger + a_q a_{-q})]
\end{aligned}
$$

and

$$
\mathbf{V}_1 = \exp\left\{2K \sum_{q>0}[\cos q(a_q^\dagger a_q + a_{-q}^\dagger a_{-q}) - 2i \sin q(a_q^\dagger a_{-q}^\dagger + a_q a_{-q})]\right\}.
$$

n **odd**

For n even we have

$$
\begin{aligned}
\sum_{j=1}^{M} c_j^\dagger c_j &= \sum_q a_q^\dagger a_q \\
&= \sum_{0<q<\pi} (a_q^\dagger a_q + a_{-q}^\dagger a_{-q}) + a_0^\dagger a_0 + a_\pi^\dagger a_\pi.
\end{aligned}
$$

Note there are $(M-2)/2$ terms in the sum $\sum_{0<q<\pi}$, so that

$$
\begin{aligned}
\mathbf{V}_2 &= (2\sinh 2K)^{M/2} \exp\left\{2K^* \sum_{j=1}^{M} \left(c_j^\dagger c_j - \frac{1}{2}\right)\right\} \\
&= (2\sinh 2K)^{M/2} \exp\left\{2K^* \sum_{0<q<\pi} \left(a_q^\dagger a_q + a_{-q}^\dagger a_{-q} - 1\right)\right\} \mathbf{V}_{20} \mathbf{V}_{2\pi}
\end{aligned}
$$

where

$$
\mathbf{V}_{20} = \exp\left\{2K^*(a_0^\dagger a_0 - \frac{1}{2})\right\}, \qquad \mathbf{V}_{2\pi} = \exp\left\{2K^*(a_\pi^\dagger a_\pi - \frac{1}{2})\right\}
$$

Recall ()

$$\mathbf{V}_1 = \exp\left\{K\sum_{j=1}^{M}(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}^\dagger - c_j c_{j+1})\right\}$$

We have

$$\begin{aligned}\sum_{j=1}^{M} c_j^\dagger c_{j+1} &= \sum_q e^{iq} a_q^\dagger a_q \\ &= \sum_{0<q<\pi} (e^{iq} a_q^\dagger a_q + e^{-iq} a_{-q}^\dagger a_{-q}) + a_0^\dagger a_0 - a_\pi^\dagger a_\pi.\end{aligned}$$

and

$$\begin{aligned}\sum_{j=1}^{M} c_{j+1}^\dagger c_j &= \sum_q e^{-iq} a_q^\dagger a_q \\ &= \sum_{0<q<\pi} (e^{-iq} a_q^\dagger a_q + e^{iq} a_{-q}^\dagger a_{-q}) + a_0^\dagger a_0 - a_\pi^\dagger a_\pi.\end{aligned}$$

and

$$\begin{aligned}\sum_{j=1}^{M} c_j^\dagger c_{j+1}^\dagger &= \sum_q e^{iq} a_q^\dagger a_{-q}^\dagger \\ &= \sum_{0<q<\pi} (e^{iq} a_q^\dagger a_{-q}^\dagger + e^{-iq} a_{-q}^\dagger a_q^\dagger) + a_0^\dagger a_0 - a_\pi^\dagger a_\pi \qquad (a_{-\pi} = a_\pi) \\ &= \sum_{0<q<\pi} (e^{iq} a_q^\dagger a_{-q}^\dagger - e^{-iq} a_q^\dagger a_{-q}^\dagger) + a_0^\dagger a_0 - a_\pi^\dagger a_\pi \\ &= 2i \sum_{0<q<\pi} \sin q\, a_q^\dagger a_{-q}^\dagger + a_0^\dagger a_0 - a_\pi^\dagger a_\pi.\end{aligned}$$

and

$$
\begin{aligned}
-\sum_{j=1}^{M} c_j c_{j+1} &= -\frac{1}{M}\sum_{j=1}^{M}\sum_{q}\sum_{q'} a_q e^{iqj} a_{q'} e^{iq'(j+1)} \\
&= -\sum_{q}\sum_{q'} e^{iq'} a_q a_{q'} \delta_{q,-q'} \\
&= -\sum_{q} e^{iq} a_q a_{-q} \\
&= -\sum_{0<q<\pi} (e^{-iq} a_q a_{-q} + e^{iq} a_{-q} a_q) - a_0^\dagger a_0 + a_\pi^\dagger a_\pi \\
&= 2i\sum_{q>0} \sin q a_q a_{-q} - a_0^\dagger a_0 + a_\pi^\dagger a_\pi
\end{aligned}
$$

$$
\begin{aligned}
&\sum_{j=1}^{M} (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}^\dagger - c_j c_{j+1}) \\
&\quad = \sum_{0<q<\pi} (e^{iq} a_q^\dagger a_q + e^{-iq} a_{-q}^\dagger a_{-q}) + a_0^\dagger a_0 - a_\pi^\dagger a_\pi + \sum_{q>0} (e^{-iq} a_q^\dagger a_q + e^{iq} a_{-q}^\dagger a_{-q}) + a_0^\dagger a_0 - a_\pi^\dagger a_\pi \\
&\quad + \sum_{0<q<\pi} 2i \sin q a_q^\dagger a_{-q}^\dagger - a_0^\dagger a_0 + a_\pi^\dagger a_\pi + \sum_{q>0} 2i \sin q a_q a_{-q} + a_0^\dagger a_0 - a_\pi^\dagger a_\pi \\
&\quad = \sum_{0<q<\pi} [2\cos q (a_q^\dagger a_q + a_{-q}^\dagger a_{-q}) - 2i \sin q (a_q^\dagger a_{-q}^\dagger + a_q a_{-q})] + 2a_0^\dagger a_0 - 2a_\pi^\dagger a_\pi
\end{aligned}
$$

and

$$
\mathbf{V}_1 = \exp\left\{ 2K \sum_{q>0} [\cos q (a_q^\dagger a_q + a_{-q}^\dagger a_{-q}) - 2i \sin q (a_q^\dagger a_{-q}^\dagger + a_q a_{-q})] \right\} \mathbf{V}_{10} \mathbf{V}_{1\pi}
$$

where

$$
\mathbf{V}_{10} = \exp\left\{ 2K a_0^\dagger a_0 \right\}, \qquad \mathbf{V}_{1\pi} = \exp\left\{ -2K a_\pi^\dagger a_\pi \right\}.
$$

3.7.2 Differential equation for $\mathbf{V}_{1q}|0\rangle = \alpha(K)|0\rangle + \beta(K)|2\rangle$

We have

$$
\begin{aligned}
(a_q^\dagger a_q + a_{-q}^\dagger a_{-q})|0\rangle &= (a_q^\dagger a_q + a_{-q}^\dagger a_{-q})|0\rangle \\
&= 0
\end{aligned}
$$

and

$$\begin{aligned}
(a_q^\dagger a_q + a_{-q}^\dagger a_{-q})|2\rangle &= (a_q^\dagger a_q + a_{-q}^\dagger a_{-q}) a_q^\dagger a_{-q}^\dagger |0\rangle \\
&= (a_q^\dagger (1 - a_q^\dagger a_q) + a_q^\dagger a_{-q}^\dagger a_{-q}) a_{-q}^\dagger |0\rangle \\
&= (a_q^\dagger a_{-q}^\dagger + a_q^\dagger a_{-q}^\dagger)|0\rangle \\
&= 2|2\rangle
\end{aligned}$$

and

$$\begin{aligned}
(a_q^\dagger a_{-q}^\dagger + a_q a_{-q})|0\rangle &= (a_q^\dagger a_{-q}^\dagger + a_q a_{-q})|0\rangle \\
&= |2\rangle.
\end{aligned}$$

and

$$\begin{aligned}
(a_q^\dagger a_{-q}^\dagger + a_q a_{-q})|2\rangle &= (a_q^\dagger a_{-q}^\dagger + a_q a_{-q}) a_q^\dagger a_{-q}^\dagger |0\rangle \\
&= a_q a_{-q} a_q^\dagger a_{-q}^\dagger |0\rangle \\
&= -a_q a_q^\dagger a_{-q} a_{-q}^\dagger |0\rangle \\
&= -(1 - a_q^\dagger a_q)(1 - a_{-q}^\dagger a_{-q})|0\rangle \\
&= -|0\rangle.
\end{aligned}$$

So that

$$\begin{aligned}
&2\left[\cos q \left\{a_q^\dagger a_q + a_{-q}^\dagger a_{-q}\right\} - i \sin q \left\{a_q^\dagger a_{-q}^\dagger + a_q a_{-q}\right\}\right](\alpha|0\rangle + \beta|2\rangle) \\
&= 2i\beta \sin q|0\rangle + \left[4\beta \cos q - 2i\alpha \sin q\right]|2\rangle
\end{aligned}$$

3.7.3 Solving differential equations

(i)

$$\begin{aligned}
\frac{\partial \alpha}{\partial K}(K) &= 2i\beta(K) \sin q \\
\frac{\partial \beta}{\partial K}(K) &= 4\beta(K) \cos q - 2i\alpha(K) \sin q.
\end{aligned}$$

We solve these equations subject to the boundary confitions $\alpha(0) = 1$, $\beta(0) = 0$.

$$\frac{\partial}{\partial K}\begin{pmatrix}\alpha(K)\\ \beta(K)\end{pmatrix} = \begin{pmatrix}0 & 2i\sin q\\ -2i\sin q & 4\cos q\end{pmatrix}\begin{pmatrix}\alpha(K)\\ \beta(K)\end{pmatrix}$$

The solution is

$$\begin{pmatrix}\alpha(K)\\ \beta(K)\end{pmatrix} = e^{AK}\begin{pmatrix}1\\ 0\end{pmatrix}$$

where

$$A = \begin{pmatrix}0 & 2i\sin q\\ -2i\sin q & 4\cos q\end{pmatrix}$$

The eigenvalues satisfy

$$\det\begin{pmatrix}-\lambda & 2i\sin q\\ -2i\sin q & 4\cos q-\lambda\end{pmatrix} = 0$$

or

$$\lambda^2 - 4\lambda\cos q - 4\sin^2 q = 0.$$

So that

$$\lambda = 2\cos q \pm 2. \tag{3.72}$$

As the eigenvalues are real and distinct e^{AK} is then given by the expression

$$e^{AK} = e^{\lambda_1 K}\mathbb{1} + \frac{e^{\lambda_2 K} - e^{\lambda_1 K}}{\lambda_2 - \lambda_1}(A - \lambda_1\mathbb{1}).$$

Substituting in the eigenvalues (3.72) into this expression and at the same time acting upon the expression with $\begin{pmatrix}1\\ 0\end{pmatrix}$ yields,

$$
\begin{aligned}
&\begin{pmatrix}\alpha(K)\\ \beta(K)\end{pmatrix}\\
= \;& e^{AK}\begin{pmatrix}1\\0\end{pmatrix}\\
= \;& \left[\begin{pmatrix}e^{2K\cos q+2K} & 0\\ 0 & e^{2K\cos q+2K}\end{pmatrix} + \frac{e^{2K\cos q+2K}-e^{2K\cos q-2K}}{4}\begin{pmatrix}-2\cos q-2 & 2i\sin q\\ -2i\sin q & 2\cos q-2\end{pmatrix}\right]\begin{pmatrix}1\\0\end{pmatrix}\\
= \;& e^{2K\cos q}\left[\begin{pmatrix}e^{2K} & 0\\ 0 & e^{2K}\end{pmatrix} + \sinh 2K\begin{pmatrix}-\cos q-1 & i\sin q\\ -i\sin q & \cos q-1\end{pmatrix}\right]\begin{pmatrix}1\\0\end{pmatrix}\\
= \;& e^{2K\cos q}\left[\begin{pmatrix}e^{2K}\\ 0\end{pmatrix} + \sinh 2K\begin{pmatrix}-\cos q-1\\ -i\sin q\end{pmatrix}\right]\\
= \;& e^{2K\cos q}\begin{pmatrix}\cosh 2K-\sinh 2K\cos q\\ -i\sinh 2K\sin q\end{pmatrix}
\end{aligned}
$$

From which we read off the formula for $\alpha(K)$ and $\beta(K)$.

(ii)

We need to solve

$$
\begin{aligned}
\frac{\partial\gamma}{\partial K}(K) &= 2i\delta(K)\sin q\\
\frac{\partial\delta}{\partial K}(K) &= 4\delta(K)\cos q-2i\gamma(K)\sin q.
\end{aligned}
$$

with the boudary conditions $\gamma(0)=0$ and $\delta(0)=1$.

$$
\begin{aligned}
&\begin{pmatrix}\gamma(K)\\ \delta(K)\end{pmatrix}\\
= \;& e^{AK}\begin{pmatrix}0\\1\end{pmatrix}\\
= \;& e^{2K\cos q}\left[\begin{pmatrix}e^{2K} & 0\\ 0 & e^{2K}\end{pmatrix} + \sinh 2K\begin{pmatrix}-\cos q-1 & i\sin q\\ -i\sin q & \cos q-1\end{pmatrix}\right]\begin{pmatrix}0\\1\end{pmatrix}\\
= \;& e^{2K\cos q}\left[\begin{pmatrix}0\\ e^{2K}\end{pmatrix} + \sinh 2K\begin{pmatrix}i\sin q\\ \cos q-1\end{pmatrix}\right]\\
= \;& e^{2K\cos q}\begin{pmatrix}i\sinh 2K\sin q\\ \cosh 2K+\sinh 2K\cos q\end{pmatrix}
\end{aligned}
$$

3.7.4 Calculating the eigenvalues of $\mathbf{V}_q$ for n even $(0 < q < \pi)$

Given

$$\mathbf{V}_{1q} = e^{2K\cos q} \begin{pmatrix} \cosh 2K - \sinh 2K \cos q & i \sinh 2K \sin q & 0 & 0 \\ -i \sinh 2K \sin q & \cosh 2K + \sinh 2K \cos q & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$\mathbf{V}_q = \begin{pmatrix} \exp\{-K^*\} & 0 & 0 & 0 \\ 0 & \exp\{K^*\} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \left(\mathbf{V}_{1q}\right) \begin{pmatrix} \exp\{-K^*\} & 0 & 0 & 0 \\ 0 & \exp\{K^*\} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

we calculate the eigenvalues.

We have that

$$\det \left[\begin{pmatrix} e^{-K^*} & 0 & 0 & 0 \\ 0 & e^{K^*} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \left(\mathbf{V}_{1q}\right) \begin{pmatrix} e^{-K^*} & 0 & 0 & 0 \\ 0 & e^{K^*} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} \lambda & 0 & 0 & 0 \\ 0 & \lambda & 0 & 0 \\ 0 & 0 & \lambda & 0 \\ 0 & 0 & 0 & \lambda \end{pmatrix} \right] = 0$$

So two of the eigenvalues are $e^{2K\cos q}$. The other two eigenvalues are give by the quadratic equation

$$\det \left[\begin{pmatrix} \exp\{-K^*\} & 0 \\ 0 & \exp\{K^*\} \end{pmatrix} \left(\mathbf{V}_{1q}\right) \begin{pmatrix} \exp\{-K^*\} & 0 \\ 0 & \exp\{K^*\} \end{pmatrix} - \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix} \right] = 0 \quad (3.73)$$

where λ is the eigenvalue. The equation $\det A = 0$ is equivalent to the equation $\det(BAB) = 0$ when $\det B \neq 0$. Using this fact we can write (3.73) as

$$\det \left[\left(\mathbf{V}_{1q}\right) - \begin{pmatrix} \exp\{K^*\} & 0 \\ 0 & \exp\{-K^*\} \end{pmatrix} \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix} \begin{pmatrix} \exp\{K^*\} & 0 \\ 0 & \exp\{-K^*\} \end{pmatrix} \right] = 0$$

or

$$\det \left[\left(\mathbf{V}_{1q}\right) - \begin{pmatrix} \lambda \exp\{2K^*\} & 0 \\ 0 & \lambda \exp\{-2K^*\} \end{pmatrix} \right] = 0.$$

Substituting the explicit expression for $\mathbf{V}_{1q}$ given above and the assumed form for the eigevalues $\lambda_q^{\pm} = \exp\{2K\cos q \pm \epsilon(q)\}$, we have

$$\det\left[\begin{pmatrix}\cosh 2K - \sinh 2K\cos q & i\sinh 2K\sin q \\ -i\sinh 2K\sin q & \cosh 2K + \sinh 2K\cos q\end{pmatrix} - \begin{pmatrix}\exp\{2K^* \pm \epsilon(q)\} & 0 \\ 0 & \exp\{-2K^* \pm \epsilon(q)\}\end{pmatrix}\right] = 0$$

or

$$\det\begin{pmatrix}\cosh 2K - \sinh 2K\cos q - e^{\{2K^*\pm\epsilon(q)\}} & i\sinh 2K\sin q \\ -i\sinh 2K\sin q & \cosh 2K + \sinh 2K\cos q - e^{\{-2K^*\pm\epsilon(q)\}}\end{pmatrix} = 0.$$

Expanding the determinant gives

$$\cosh^2 2K - \sinh^2 2K\cos^2 q - \sinh^2 2K\sin^2 q - e^{\{2K^*\pm\epsilon(q)\}}(\cosh 2K + \sinh 2K\cos q) \\ -e^{\{-2K^*\pm\epsilon(q)\}}(\cosh 2K - \sinh 2K\cos q) + e^{\pm 2\epsilon(q)} = 0$$

which upon using the identity $\cosh^2 2K - \sinh^2 2K\cos^2 q - \sinh^2 2K\sin^2 q = 1$ and simplifing we finally obtain

$$\begin{aligned}\cosh\epsilon(q) &= 2e^{2K^*}(\cosh 2K + \sinh 2K\cos q) + 2e^{-2K^*}(\cosh 2K - \sinh 2K\cos q) \\ &= \cosh 2K\cosh 2K^* + \cos q\sinh 2K\sinh 2K^*.\end{aligned}$$

3.7.5 Calculating the eigenvalues of $\mathbf{V}_q$ for n odd

To make the overall state have $(-1)^n = -1$ for n odd

We occupy the $q = 0$ state but leave the $q = \pi$ staes empty.

$$\mathbf{V}_1 = \exp\left\{2K\sum_{q>0}[\cos q(a_q^\dagger a_q + a_{-q}^\dagger a_{-q}) - 2i\sin q(a_q^\dagger a_{-q}^\dagger + a_q a_{-q})]\right\}\mathbf{V}_{10}\mathbf{V}_{1\pi}$$

where

$$\mathbf{V}_{10} = \exp\left\{2Ka_0^\dagger a_0\right\}, \qquad \mathbf{V}_{1\pi} = \exp\left\{-2Ka_\pi^\dagger a_\pi\right\}$$

and

$$\mathbf{V}_{20} = \exp\left\{2K^*(a_0^\dagger a_0 - \frac{1}{2})\right\}, \qquad \mathbf{V}_{2\pi} = \exp\left\{2K^*(a_\pi^\dagger a_\pi - \frac{1}{2})\right\}$$

$$\begin{aligned}\mathbf{V}_0 &= \mathbf{V}_{20}^{1/2}\mathbf{V}_{10}\mathbf{V}_{20}^{1/2} \\ &= \exp\left\{K + 2(K+K^*)(a_0^\dagger a_0 - \frac{1}{2})\right\}\end{aligned}$$

$$\begin{aligned}\mathbf{V}_\pi &= \mathbf{V}_{2\pi}^{1/2}\mathbf{V}_{1\pi}\mathbf{V}_{2\pi}^{1/2} \\ &= \exp\left\{-K - 2(K-K^*)(a_\pi^\dagger a_\pi - \frac{1}{2})\right\}\end{aligned}$$

We consider the stattes $|0\rangle$, $a_0^\dagger|0\rangle$

$$\begin{aligned}\mathbf{V}_0|0\rangle &= \exp\left\{-K^*\right\}|0\rangle \\ \mathbf{V}_0 a_0^\dagger|0\rangle &= \exp\left\{(2K+K^*)\right\}a_0^\dagger|0\rangle\end{aligned}$$

$$\begin{pmatrix}\langle 0|\mathbf{V}_0|0\rangle & \langle 0|\mathbf{V}_0|1\rangle \\ \langle 1|\mathbf{V}_0|0\rangle & \langle 1|\mathbf{V}_0|1\rangle\end{pmatrix} = \begin{pmatrix}\exp\left\{-K^*\right\} & 0 \\ 0 & \exp\left\{2K+K^*\right\}\end{pmatrix}$$

Therefore, the eigenvalues are $\exp\left\{-K^*\right\}$ and $\exp\left\{2K+K^*\right\}$. Their product is

$$\exp\left\{2K\right\}.$$

3.7.6 Relations involving K and K^*

(i)

Recall

$$A\cosh K^* = e^K, \qquad A\sinh K^* = e^{-K}.$$

Thus

$$A^2 = A^2\cosh^2 K^* - A^2\sinh^2 K^* = e^{2K} - e^{-2K} = 2\sinh 2K$$

and so

$$\sinh 2K \sinh 2K^* = A\cosh K^* A\sinh K^* = 1.$$

(ii)

We prove

$$\cosh 2K^* = \coth 2K$$

$$\begin{aligned}
\cosh 2K^* &= \cosh^2 K^* + \sinh^2 K^* \\
&= \frac{e^{2K} + e^{-2K}}{A^2} \\
&= \frac{2\cosh 2K}{2\sinh 2K} \\
&= \coth 2K.
\end{aligned}$$

3.7.7 Differentiating the thermodynamical function $f(x)$

Recall the function

$$f(x) = \int_0^{2\pi} d\phi \ln(\cosh x + \cos\phi).$$

Differentiating both sides with respect to x gives

$$\frac{df(x)}{dx} = \int_0^{2\pi} d\phi \frac{\sinh x}{\cosh x + \cos\phi}.$$

and evaluating the resulting integral by contour integration. We make the substitution $z = e^{i\phi}$. Then

$$\cos\phi = \frac{1}{2}\left(z + \frac{1}{z}\right), \qquad d\phi = \frac{dz}{iz}.$$

Takig C to be, the unit we obtain

$$\begin{aligned}
\frac{df(x)}{dx} &= \int_0^{2\pi} d\phi \frac{\sinh x}{\cosh x + \cos\phi} \\
&= \oint_C \frac{\sinh x}{\cosh x + \frac{1}{2}\left(z + \frac{1}{z}\right)} \frac{dz}{iz} \\
&= -i \oint_C \frac{2\sinh x}{z^2 + 2z\cosh x + 1} dz \\
&= -i \oint_C \frac{2\sinh x}{(z + e^{-x})(z + e^{x})} dz
\end{aligned}$$

For $x > 1$ the pole is at $-e^{-x}$ and

$$\frac{df(x>0)}{dx} = \lim_{z \to -e^{-x}} \frac{2\sinh x}{-e^{-x} + e^{x}} = +1.$$

For $x < 1$ the pole is at $-e^{x}$ and

$$\frac{df(x<0)}{dx} = \lim_{z \to -e^{x}} \frac{2\sinh x}{z + e - x} = -1.$$

Therefore $\dfrac{df(x)}{dx} = \mathrm{sgn}(x)$, and $f(x) = |x|$.

3.7.8 Change of variables

Recal

$$I = \frac{1}{2\pi}\int_0^{\pi} dq \epsilon(q) = \frac{1}{2\pi^2}\int_0^{\pi} dq \int_0^{\pi} d\phi \ln(2\cosh 2K \coth 2K + 2\cos q + 2\cos\phi)$$

We used the trigonometric identity

$$\cos q + \cos\phi = 2\cos\frac{q+\phi}{2}\cos\frac{q-\phi}{2}$$

and changig variables of integration to

$$\omega_1 = \frac{q-\phi}{2}, \qquad \omega_2 = \frac{q+\phi}{2}.$$

We have

$$\begin{aligned} q=0,\phi=0 &\Rightarrow \omega_1=0,\omega_2=0 \\ q=0,\phi=\pi &\Rightarrow \omega_1=-\frac{\pi}{2},\omega_2=\frac{\pi}{2} \\ q=\pi,\phi=\pi &\Rightarrow \omega_1=0,\omega_2=\pi \\ q=\pi,\phi=0 &\Rightarrow \omega_1=\frac{\pi}{2},\omega_2=\frac{\pi}{2} \end{aligned} \tag{3.74}$$

Let us the Jacobian for the transformation,

$$\begin{aligned} J &= \left| \begin{pmatrix} \frac{\partial q}{\partial \omega_1} & \frac{\partial q}{\partial \omega_2} \\ \frac{\partial \phi}{\partial \omega_1} & \frac{\partial \phi}{\partial \omega_2} \end{pmatrix} \right| \\ &= \left| \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \right| \\ &= 2. \end{aligned}$$

The region of itegration in the $\omega_1\omega_2$-plane with corners at $(0,0)$, $(-\frac{\pi}{2},\frac{\pi}{2})$, $(0,\pi)$, and $(\frac{\pi}{2},\frac{\pi}{2})$. Thus

$$\begin{aligned} I &= \frac{1}{\pi^2}\left(\int_{-\pi/2}^{0} d\omega_1 \int_{-\omega_1}^{\pi/2+\omega_1} d\omega_2 + \int_0^{\pi/2} d\omega_1 \int_{\omega_1}^{\pi-\omega_1} d\omega_2\right) \ln(2\cosh 2K \coth 2K + 4\cos\omega_1\cos\omega_2) \\ &= \int_0^{\pi/2} d\omega_1 \int_{\omega_1}^{\pi-\omega_1} d\omega_2 \ln(2\cosh 2K \coth 2K + 4\cos\omega_1\cos\omega_2). \end{aligned} \tag{3.75}$$

This integral can be split ito two parts, $I = I_1 + I_2$, where

$$I_1 = \int_0^{\pi/2} d\omega_1 \int_{\omega_1}^{\pi/2} d\omega_2 \ln(2\cosh 2K \coth 2K + 4\cos\omega_1\cos\omega_2) \tag{3.76}$$

$$I_2 = \int_0^{\pi/2} d\omega_1 \int_{\pi/2}^{\pi-\omega_1} d\omega_2 \ln(2\cosh 2K \coth 2K + 4\cos\omega_1\cos\omega_2) \tag{3.77}$$

By performing the change of coordinates $(\omega_1, \omega_2) \mapsto (\omega_2, \omega_1)$ in the integral (3.76) we find that

$$I_1 = \int_0^{\pi/2} d\omega_1 \int_0^{\omega_1} d\omega_2 \ln(2\cosh 2K \coth 2K + 4\cos\omega_1 \cos\omega_2).$$

Combining this with (3.76) gives

$$I_1 = \frac{1}{2} \int_0^{\pi/2} d\omega_1 \int_0^{\pi/2} d\omega_2 \ln(2\cosh 2K \coth 2K + 4\cos\omega_1 \cos\omega_2). \tag{3.78}$$

By performing the change of coordinates $(\omega_1, \omega_2) \mapsto (\pi - \omega_2, \pi - \omega_1)$ in the integral (3.77) we find that

$$I_2 = \int_0^{\pi/2} d\omega_1 \int_{\pi-\omega_1}^{\pi} d\omega_2 \ln(2\cosh 2K \coth 2K + 4\cos\omega_1 \cos\omega_2) \tag{3.79}$$

Combining this with (3.77) gives

$$I_2 = \frac{1}{2} \int_0^{\pi/2} d\omega_1 \int_{\pi/2}^{\pi} d\omega_2 \ln(2\cosh 2K \coth 2K + 4\cos\omega_1 \cos\omega_2) \tag{3.80}$$

Combining (3.78) and (3.80) we finally have

$$I = \frac{1}{\pi^2} \int_0^{\pi} d\omega_2 \int_0^{\pi/2} d\omega_1 \ln(2\cosh 2K \coth 2K + 4\cos\omega_1 \cos\omega_2) \tag{3.81}$$

Internal energy per spin

Recall that $K = \beta J$. The internal energy per spin is given by

$$
\begin{aligned}
& u(T) \\
= \; & \frac{d}{d\beta}[\beta g(T)] \\
= \; & \frac{dK}{d\beta}\frac{d}{dK}[\beta g(T)] \\
= \; & J\frac{d}{dK}\left[-\ln(2\cosh 2K) - \frac{1}{\pi}\int_0^{\pi/2} d\theta \ln\left\{\frac{1+\sqrt{1-q^2\sin^2\theta}}{2}\right\}\right] \\
= \; & J\frac{d}{dK}\left[-\frac{\ln 2}{2} - \ln(\cosh 2K) - \frac{1}{\pi}\int_0^{\pi/2} d\theta \ln\left\{1+\sqrt{1-q^2\sin^2\theta}\right\}\right] \\
= \; & J\frac{d}{dK}\left[-\frac{1}{\pi}\int_0^{\pi/2} d\theta \left(2\ln(\cosh 2K) + \ln\left\{1+\sqrt{1-q^2\sin^2\theta}\right\}\right)\right] \\
= \; & -J\coth 2K\frac{1}{\pi}\int_0^{\pi/2} d\theta \left[4\frac{\sinh^2 2K}{\cosh^2 2K} + \frac{1}{\coth 2K}\left(\frac{\frac{d}{dK}\left(1+\sqrt{1-q^2\sin^2\theta}\right)}{1+\sqrt{1-q^2\sin^2\theta}}\right)\right] \\
= \; & -J\coth 2K\frac{1}{\pi}\int_0^{\pi/2} d\theta \left[4\tanh 2K - \frac{\frac{1}{q}\frac{dq}{dK}}{\coth 2K}\left(\frac{q^2\sin^2\theta}{\sqrt{1-q^2\sin^2\theta}}\right)\left(\frac{1}{1+\sqrt{1-q^2\sin^2\theta}}\right)\right] \\
= \; & -J\coth 2K\frac{1}{\pi}\int_0^{\pi/2} d\theta \left[4\tanh 2K - 2\frac{1-\sinh^2 2K}{\cosh^2 2K}\frac{q^2\sin^2\theta}{\sqrt{1-q^2\sin^2\theta}}\frac{1}{1+\sqrt{1-q^2\sin^2\theta}}\right] \\
= \; & -J\coth 2K\frac{1}{\pi}\int_0^{\pi/2} d\theta \left[4\tanh^2 2K + 2(2\tanh^2 2K - 1)\frac{q^2\sin^2\theta}{\sqrt{1-q^2\sin^2\theta}}\frac{1}{1+\sqrt{1-q^2\sin^2\theta}}\right] \\
= \; & -J\coth 2K\left[1 + 2(2\tanh^2 2K - 1)\frac{1}{\pi}\int_0^{\pi/2} d\theta \left(1 + \frac{q^2\sin^2\theta}{\sqrt{1-q^2\sin^2\theta}}\frac{1}{1+\sqrt{1-q^2\sin^2\theta}}\right)\right] \\
= \; & -J\coth 2K\left[1 + 2(2\tanh^2 2K - 1)\frac{1}{\pi}\int_0^{\pi/2} d\theta \frac{\sqrt{1-q^2\sin^2\theta}+1}{\sqrt{1-q^2\sin^2\theta}}\frac{1}{1+\sqrt{1-q^2\sin^2\theta}}\right] \\
= \; & -J\coth 2K\left[1 + 2(2\tanh^2 2K - 1)\frac{1}{\pi}\int_0^{\pi/2} d\theta \frac{1}{\sqrt{1-q^2\sin^2\theta}}\right]
\end{aligned}
\tag{3.82}
$$

Specific heat integral

We have the definitions

$$
\begin{aligned}
K_1(q) &= \int_0^{\pi/2} dx \frac{1}{\sqrt{1-q^2\sin^2 x}} \\
E_1(q) &= \int_0^{\pi/2} dx \sqrt{1-q^2\sin^2 x}.
\end{aligned}
$$

We wish to show

$$
\frac{dK_1(q)}{dq} = \frac{E_1(q)}{q(1-q^2)} - \frac{K_1(q)}{q}. \tag{3.83}
$$

Define

$$
\begin{aligned}
F(\phi, q) &= \int_0^{\phi} dx \frac{1}{\sqrt{1-q^2\sin^2 x}} \\
E(\phi, q) &= \int_0^{\phi} dx \sqrt{1-q^2\sin^2 x}.
\end{aligned}
$$

First

$$
\begin{aligned}
\frac{\partial}{\partial x}\left(\frac{q^2\sin x\cos x}{\sqrt{1-q^2\sin^2 x}}\right) &= \frac{q^2(\cos^2 x-\sin^2 x)(1-q^2\sin^2 x)}{(1-q^2\sin^2 x)^{3/2}} + \frac{q^2\sin^2 x\cos^2 x}{(1-q^2\sin^2 x)^{3/2}} \\
&= \frac{q^2\cos^2 x - q^2\sin^2 x + q^4\sin^2 x}{(1-q^2\sin^2 x+q^4\sin^4 x)^{3/2}}. \qquad (3.84)
\end{aligned}
$$

Next

$$
\begin{aligned}
& -q(1-q^2)\frac{\partial F(\phi,q)}{\partial q} - (1-q^2)F(\phi,q) + E(\phi,q) \\
= \; & -(1-q^2)\int_0^\phi dx \frac{q^2\sin^2 x}{(1-q^2\sin^2 x)^{3/2}} + \int_0^\phi dx\sqrt{1-q^2\sin^2 x} - (1-q^2)\int_0^\phi dx \frac{1}{\sqrt{1-q^2\sin^2 x}} \\
= \; & \int_0^\phi dx \frac{(q^2-1)q^2\sin^2 x + (1-q^2\sin^2 x)^2 + (q^2-1)(1-q^2\sin^2 x)}{(1-q^2\sin^2 x)^{3/2}} \\
= \; & \int_0^\phi dx \frac{(1-q^2\sin^2 x)^2 + q^2 - 1}{(1-q^2\sin^2 x)^{3/2}} \\
= \; & \int_0^\phi dx \frac{-2q^2\sin^2 x + q^4\sin^4 x + q^2}{(1-q^2\sin^2 x)^{3/2}} \\
= \; & \int_0^\phi dx \frac{-2q^2\sin^2 x + q^4\sin^4 x + q^2}{(1-q^2\sin^2 x)^{3/2}} \\
= \; & \int_0^\phi dx \frac{-q^2\sin^2 x + \cos^2 x + q^4\sin^4 x}{(1-q^2\sin^2 x)^{3/2}}. \qquad (3.85)
\end{aligned}
$$

Integrating from 0 to ϕ (3.84) and comparing (3.85) we have

$$
\left(\frac{q^2\sin\phi\cos\phi}{\sqrt{1-q^2\sin^2\phi}}\right) = -q(1-q^2)\frac{\partial F(\phi,q)}{\partial q} - (1-q^2)F(\phi,q) + E(\phi,q)
$$

or

$$
\frac{\partial F(\phi,q)}{\partial q} = \frac{1}{1-q^2}\left[\frac{E(\phi,q)-(1-q^2)F(\phi,q)}{q} - \left(\frac{q\sin\phi\cos\phi}{\sqrt{1-q^2\sin^2\phi}}\right)\right].
$$

Putting $\phi = \pi/2$ we obtain (3.83).

We now substitute in the explicit expression for q into (3.83),

$$
q(K) = \frac{2\sinh 2K}{\cosh^2 2K}
$$

implying

$$
q(1-q^2) = \frac{2\sinh 2K}{\cosh^2 2K}\left(1 - \frac{4\sinh^2 2K}{\cosh^4 2K}\right) = \frac{2\sinh 2K(1-\sinh^2 2K)^2}{\cosh^6 2K}
$$

so

$$
\begin{aligned}
\frac{dK_1(q)}{dq} &= \frac{E_1(q)}{q(1-q^2)} - \frac{K_1(q)}{q} \\
&= \frac{\cosh^6 2K}{2\sinh 2K(1-\sinh^2 2K)^2} E_1(q) - \frac{\cosh^2 2K}{2\sinh 2K} K_1(q)
\end{aligned} \tag{3.86}
$$

$$
\begin{aligned}
\frac{dK_1(q)}{dK} &= \frac{dq}{dK}\frac{dK_1(q)}{dq} \\
&= \frac{4(1-\sinh^2 2K)}{\cosh^3 2K}\left[\frac{\cosh^6 2K}{2\sinh 2K(1-\sinh^2 2K)^2}E_1(q) - \frac{\cosh^2 2K}{2\sinh 2K}K_1(q)\right] \\
&= \frac{2\cosh^3 2K}{\sinh 2K(1-\sinh^2 2K)}E_1(q) - \frac{2(2-\cosh^2 2K)}{\cosh 2K\sinh 2K}K_1(q) \\
&= \frac{2\coth 2K\cosh^2 2K}{1-\sinh^2 2K}E_1(q) + 4\coth 2K(\tanh^2 2K - 1)K_1(q) + 2\coth 2K K_1(q) \\
&= \coth 2K\left[\frac{2\cosh^2 2K}{1-\sinh^2 2K}E_1(q) + 2(2\tanh^2 2K - 1)K_1(q)\right]
\end{aligned} \tag{3.87}
$$

Calculation of the specific heat capacity

$$
\begin{aligned}
&-\frac{1}{k_B}c(T) = -\beta^2\frac{\partial}{\partial\beta}u(T)\\
= \;& \beta^2 J\frac{d}{dK}\left(-J\coth 2K\left[1+\frac{2}{\pi}(2\tanh^2 2K-1)K_1(q)\right]\right)\\
= \;& \beta^2 J^2\frac{d}{dK}\coth 2K\left[1+\frac{2}{\pi}(2\tanh^2 2K-1)K_1(q)\right]\\
&+\beta^2J^2\coth 2K\left[\frac{8}{\pi}K_1(q)\tanh 2K\frac{d}{dK}\tanh 2K\right]+\beta^2J^2\coth 2K\left[\frac{2}{\pi}(2\tanh^2 2K-1)\frac{dK_1(q)}{dK}\right]\\
= \;& 2\beta^2J^2(\coth^2 2K-1)\left[1+\frac{2}{\pi}(2\tanh^2 2K-1)K_1(q)\right]\\
&\beta^2J^2\coth 2K\left[\frac{16}{\pi}\tanh 2K(1-\tanh^2 2K)K_1(q)\right]\\
&\beta^2J^2\coth 2K\left[\frac{2}{\pi}(2\tanh^2 2K-1)\coth 2K\left(\frac{2\cosh^2 2K}{1-\sinh^2 2K}E_1(q)+2(2\tanh^2 2K-1)K_1(q)\right)\right]\\
= \;& -2\beta^2J^2(1-\coth^2 2K)\\
&+\frac{4}{\pi}\beta^2J^2(\coth^2 2K-1)(2\tanh^2 2K-1)K_1(q)\\
&+\frac{4}{\pi}(\beta J\coth 2K)^2(1-\tanh^2 2K)4\tanh^2 2KK_1(q)+\frac{4}{\pi}(\beta J\coth 2K)^2(2\tanh^2 2K-1)^2K_1(q)\\
&+\frac{4}{\pi}(\beta J\coth 2K)^2\frac{(2\tanh^2 2K-1)\cosh^2 2K}{1-\sinh^2 2K}E_1(q)\\
= \;& -\frac{4}{\pi}(K\coth 2K)^2(\tanh^2 2K-1)\frac{\pi}{2}\\
&+\frac{4}{\pi}(K\coth 2K)^2(1-\tanh^2 2K)(2\tanh^2 2K-1)K_1(q)\\
&+\frac{4}{\pi}(K\cosh 2K)^2K_1(q)-\frac{4}{\pi}(K\cosh 2K)^2E_1(q)\\
= \;& \frac{4}{\pi}(K\cosh^2 2K)^2\left\{K_1(q)-E_1(q)+(1-\tanh^2 2K)\left[\frac{\pi}{2}+(2\tanh^2 2K-1)K_1(q)\right]\right\}
\end{aligned}
\tag{3.88}
$$

Asymptotic expression for the Elliptic integral of the first kind

The complete Elliptic integral of the first kind

$$K_1(q) = \int_0^{\pi/2} dx\frac{1}{\sqrt{1-q^2\sin^2 x}} = \int_0^1 \frac{dt}{\sqrt{1-t^2}\sqrt{1-q^2t^2}}$$

where the second integral representation follows from the first by making the substitution $t=\sin x$. We prove that as $q\to 1^-$,

$$K_1(q) \sim -\frac{1}{2}\ln|1-q| \tag{3.89}$$

by proving that as $q \to 1^-$,

$$\int_0^1 \frac{dt}{\sqrt{1-t^2}\sqrt{1-q^2t^2}} \sim -\frac{1}{2}\ln|1-q|.$$

We do this by splitting the integral as

$$\int_0^1 \frac{dt}{\sqrt{1-t^2}\sqrt{1-q^2t^2}} = \int_0^q \frac{dt}{\sqrt{1-t^2}\sqrt{1-q^2t^2}} + \int_q^1 \frac{dt}{\sqrt{1-t^2}\sqrt{1-q^2t^2}}. \tag{3.90}$$

and showing that

$$\int_0^q \frac{dt}{\sqrt{1-t^2}\sqrt{1-q^2t^2}} = -\frac{1}{2}\ln|1-q| + \mathcal{O}(1), \qquad \int_q^1 \frac{dt}{\sqrt{1-t^2}\sqrt{1-q^2t^2}} = \mathcal{O}(1) \tag{3.91}$$

We will make use of the fact that for $0 \le q < 1$ and $0 \le t \le q$ we have the following inequality

$$q < \frac{\sqrt{1-t^2}}{\sqrt{1-q^2t^2}} < 1. \tag{3.92}$$

which we proceed to prove. For $0 \le q < 1$ it is obvious that we have for $0 \le t \le q$ that

$$\frac{\sqrt{1-t^2}}{\sqrt{1-q^2t^2}} < 1.$$

We now prove the second part of (3.92). To that end we define $h(y) = (1-y^2)-q^2(1-q^2y^2)$. Its derivative is zero at $y = 0$ and is strictly negative for $y > 0$. This combined with $h(0) = 1-q^2 > 0$ and $h(q) = (1-q^2)^2 > 0$ for $0 \le q < 1$ implies that

$$(1-y^2) > q^2(1-q^2y^2)$$

or

$$q < \frac{\sqrt{1-y^2}}{\sqrt{1-q^2y^2}}.$$

We turn to proving the first part of (3.91). We have

$$\begin{aligned}
&\int_0^q \frac{dt}{\sqrt{1-t^2}\sqrt{1-q^2t^2}} \\
= \;& \int_0^q \frac{dt}{1-t^2}\frac{\sqrt{1-t^2}}{\sqrt{1-q^2t^2}} \\
= \;& \frac{1}{2}\int_0^q \frac{dt}{1-t}\frac{\sqrt{1-t^2}}{\sqrt{1-q^2t^2}} + \int_0^q \left(\frac{1}{(1-t)(1+t)} - \frac{1}{2(1-t)}\right)\frac{\sqrt{1-t^2}}{\sqrt{1-q^2t^2}}dt \\
= \;& \frac{1}{2}\int_0^q \frac{dt}{1-t}\frac{\sqrt{1-t^2}}{\sqrt{1-q^2t^2}} + \frac{1}{2}\int_0^q \frac{dt}{1+t}\frac{\sqrt{1-t^2}}{\sqrt{1-q^2t^2}} \\
= \;& \frac{1}{2}\int_0^q \frac{dt}{1-t}\frac{\sqrt{1-t^2}}{\sqrt{1-q^2t^2}} + \mathcal{O}(1).
\end{aligned}$$

as the second integral of the 4th line clearly remains finite as $q \to 1^-$. Then

$$\begin{aligned}
&\frac{1}{2}\int_0^q \frac{dt}{1-t}\frac{\sqrt{1-t^2}}{\sqrt{1-q^2t^2}} + \mathcal{O}(1) \\
= \;& \frac{1}{2}\int_0^q \frac{dt}{1-t} - \frac{1}{2}\int_0^k \frac{1-q}{1-t}dt + \frac{1}{2}\int_0^q \frac{dt}{1-t}\left(\frac{\sqrt{1-t^2}}{\sqrt{1-q^2t^2}} - q\right) + \mathcal{O}(1) \qquad (3.93)
\end{aligned}$$

Obviously

$$\int_0^q \frac{1-q}{1-t}dt = -(1-q)\ln(1-q)$$

and remains finite as $q \to 1^-$ (in fact it tends to zero as $q \to 1^-$). By (3.92) we have that for $0 \leq q < 1$ we have for $0 \leq t \leq q$ that

$$\frac{\sqrt{1-t^2}}{\sqrt{1-q^2t^2}} - q < 1 - q.$$

and so

$$\int_0^q \frac{dt}{1-t}\left(\frac{\sqrt{1-t^2}}{\sqrt{1-q^2t^2}} - q\right) < \int_0^q \frac{1-q}{1-t}dt. \qquad (3.94)$$

By (3.92) the integral on the left is positive and hence both integrals in (3.94) tend to zero as $q \to 1^-$.

Using the above results in (3.93) we have,

$$\int_0^q \frac{dt}{\sqrt{1-t^2}\sqrt{1-q^2t^2}} = \frac{1}{2}\int_0^q \frac{dt}{1-t} + \mathcal{O}(1) = -\frac{1}{2}\ln(1-q) + \mathcal{O}(1) \tag{3.95}$$

It remains to show that the second integral in (3.90) is finite. Note that for $0 < q < t \leq 1$, we have

$$\sqrt{1-t^2}\sqrt{1-q^2t^2} = \sqrt{1-t}\sqrt{1+t}\sqrt{1-qt}\sqrt{1+qt} > \sqrt{1-t}\sqrt{1-q}.$$

Hence,

$$0 \leq \int_q^1 \frac{dt}{\sqrt{1-t^2}\sqrt{1-q^2t^2}} < \frac{1}{\sqrt{1-q}}\int_q^1 \frac{dt}{\sqrt{1-t}} = 2$$

and so we have proven (3.89).

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