Expansions about Free-Fermion Models

Saibal Mitra
saibalm@science.uva.nl
Instituut voor Theoretische Fysica
Universiteit van Amsterdam
1018 XE Amsterdam The Netherlands

March 28, 2022

Abstract

A simple technique for expanding the free energy of general six-vertex models about free-fermion points is introduced. This technique is used to verify a Coulomb gas prediction about the behavior of the leading singularity in the free energy of the staggered F-model at zero staggered field.

1 Definition of the staggered F-model

The staggered F-model is a special case of the six-vertex model. The six-vertex model can be defined as follows: place arrows on the edges of a square lattice so that there are two arrows pointing into each vertex. Six types of vertices can arise (hence the name of the model). These vertices are shown in fig. 1. By giving each vertex-type a (position-dependent) energy the model is defined. These models were first introduced to study (anti-)ferroelectric systems. Later it was shown that six-vertex models can be mapped to solid-on-solid models [4]. Only a few of these models can be solved exactly. These include the free-fermion models [5, 14] and models that can be solved using the Bethe Ansatz [3, 8, 9, 10, 2]. To define the staggered F-model, we divide the lattice into two sublattices A and B, such that the nearest neighbor of an A vertex is a B vertex. The vertex energies are chosen as indicated in fig. 1. When the staggered field \( s \) vanishes the model reduces to the F-model, which has been solved by Lieb [9]. At zero staggered field the model is critical. In this case the groundstate is twofold degenerate consisting of vertices of type 5 on sublattice A and vertices

\[
\begin{align*}
1 & \quad 2 & \quad 3 & \quad 4 & \quad 5 & \quad 6 \\
\epsilon & \quad \epsilon & \quad \epsilon & \quad \epsilon & \quad \pm s & \quad \mp s
\end{align*}
\]

Figure 1: The six vertices and their energies. The upper and lower signs correspond to sublattice A resp. sublattice B.
of type 6 on sublattice B, or vice versa. For $\beta \epsilon > 0$ a nonzero staggered field lifts this degeneracy, and forces the model into an ordered state \[13\].

2 Coulomb gas results

By assuming that the F-model renormalizes to the Gaussian model, it is possible to find the behavior of the staggered F-model in infinitesimal staggered fields \[11\]. It is found that the leading singularity in the free energy is:

$$F_s(\beta \epsilon, \beta s) \approx (\beta s)^{2 - \frac{2}{\pi j(\beta \epsilon)}}$$

where

$$j(\beta \epsilon) = \frac{1}{2} \arccos \left( 1 - \frac{1}{2} \exp (2\beta \epsilon) \right)$$

At the point $\beta \epsilon = \frac{1}{2} \ln (2 - \sqrt{2}) \approx -0.2674$ the exponent becomes infinite. Below this point a finite staggered field is necessary to force the model to an ordered state. In this case the transition to the ordered state happens via a Kosterlitz-Thouless (KT) transition. The existence of a line of KT transitions intersecting the point \( (\beta \epsilon = \frac{1}{2} \ln (2 - \sqrt{2}), \beta s = 0) \) has been verified by combining the results of transfer matrix studies with scaling arguments \[11\].

In this paper we will verify \[11\] by expanding around Baxter’s exact solution on the line $\beta \epsilon = \frac{1}{2} \ln 2$.

3 Baxter’s solution of the staggered F-model

Baxter has solved the staggered F-model at $\beta \epsilon = \frac{1}{2} \ln (2)$ \[1\]. Later it was found that this solution could be generalized to other models if a certain condition involving the vertex weights is met. This condition is called the free-fermion condition because for eight-vertex models satisfying this condition the problem leads to a problem of noninteracting fermions in the S-matrix formulation. Let $w_i$ be the vertex weight for a vertex of type $i$ (see fig. 1), then the free-fermion condition for six-vertex models is:

$$w_1 w_2 + w_3 w_4 - w_5 w_6 = 0$$

The weights $w_i$ may be chosen inhomogeneous. We now proceed by presenting Baxter’s solution of the staggered F-model.

Divide the lattice into two sublattices A and B. Choose the vertex energies as indicated in fig. 1. Consider the ground state in which all A-vertices are vertices of type 6, and all B-vertices are of type 5. Any state can now be represented by drawing lines on the lattice where the arrows point oppositely to the ground state configuration. In terms of these lines the six vertices are represented by vertices with either no lines, two lines at right angles, or four lines. The energies of these vertices are respectively $-s$, $\epsilon$ and $s$. The next step is to replace the original lattice by a decorated lattice by replacing each original vertex by a "city" of four internally connected points (see fig. 2).

The lines on the original lattice are regarded as dimers on the external edges of the decorated lattice. For any configuration on the original lattice, it is possible to place dimers on the internal edges of the decorated lattice, so that
the lattice becomes completely covered. Now associate to each dimer a weight as indicated in fig. 2. Demanding that the closed-packed dimer problem formulated on the decorated lattice is equivalent to our original problem yields:

\[ C = \exp \left( -\frac{1}{2} \beta s \right) \] (4)
\[ u = \frac{1}{2} \sqrt{2} \exp \left( \frac{1}{2} \beta s \right) \] (5)
\[ \beta \epsilon = \frac{1}{2} \ln (2) \] (6)

To solve the close-packed dimer problem, we use the Pfaffian method [6, 7, 12]. This method expresses the partition function \( Z \) for a closed packed dimer model on an \( N \) by \( M \) planar lattice:

\[ Z^2 = \det R \] (7)

Here \( R \) is an \( N \times M \) by \( N \times M \) anti-symmetric matrix, defined as follows. Enumerate all the \( N \times M \) vertices on the decorated lattice. If vertex \( i \) is not connected to vertex \( j \) via an edge, \( R_{i,j} = 0 \), else \( R_{i,j} = \pm \) fugacity of dimer at edge connecting \( i \) to \( j \). The way the signs have to be chosen is explained [7]. These signs define an orientation of the edges. Positive \( R_{i,j} \) is indicated by an arrow pointing from \( i \) to \( j \).

To set up a perturbation theory about \( \beta \epsilon = \frac{1}{2} \ln (2) \), we also need the inverse of \( R \). Both the determinant and the inverse of \( R \) are easily calculated by performing a similarity transformation, see [1] for details. The determinant yields the following expression for the reduced free energy per vertex (i.e. the free energy times \( -\beta \)), denoted as \( F_{\text{Baxter}} \), for an infinite by infinite lattice:

\[ F_{\text{Baxter}} = \lim_{N,M \to \infty} \frac{1}{2NM} \ln \det R \]
\[ = \frac{1}{8\pi} \int_0^{2\pi} \int_0^{2\pi} \ln \left[ 2 \cosh (2 \beta s) + 2 \cos (\theta_1) \cos (\theta_2) \right] d\theta_1 d\theta_2 \] (8)
4 Perturbation theory

We now proceed with the derivation of a perturbation theory about the free-fermion line of a six-vertex model. The Hamiltonian of a general six-vertex model can be defined as follows. One assigns an energy \( e(p, i) \) to a vertex in state \( p \) (see fig. 1) and position \( i \). The configuration of the lattice can be specified by a function \( c \) which maps a position of a vertex to a number, \( 1 \cdots 6 \), which is to be interpreted as the state of the vertex at that position. The reduced Hamiltonian \( (H) \) is defined to be the functional that assigns to each state \( c \) its energy times \(-\beta\). We can thus write

\[
H(c) = -\beta \sum_i e(c(i), i) \tag{9}
\]

For \( H \) a Hamiltonian of a general six-vertex model and \( H_0 \) a Hamiltonian of a free-fermion model, a perturbation \( V \) can be defined so that we have

\[
H = H_0 + V \tag{10}
\]

The partition function \( Z \) can be written as:

\[
Z = \sum_c \exp (H_0(c) + V(c)) = Z_0 \langle \exp (V) \rangle \tag{11}
\]

Here \( Z_0 \) is the partition function of the free-fermion model. The reduced free energy can be expressed as:

\[
F = F_0 + \ln \langle \exp (V) \rangle = F_0 + \langle V \rangle + \frac{1}{2} \langle (V - \langle V \rangle)^2 \rangle + \ldots \tag{12}
\]

Here \( F_0 \) is the reduced free energy of the free-fermion model. Now write \( V = \sum_i V_i \) with \( V_i(c(i)) \) a perturbation of the vertex energy times \(-\beta\) at position \( i \). \( \tag{12} \) can be rewritten as:

\[
F = F_0 + \sum_i \langle V_i \rangle + \frac{1}{2} \sum_{ij} [\langle V_i V_j \rangle - \langle V_i \rangle \langle V_j \rangle] + \ldots \tag{13}
\]

To compute a free-fermion average \( \langle V_{i_1} V_{i_2} \ldots V_{i_n} \rangle \), we can proceed as follows: Introduce a constraint in the free-fermion model by requiring the vertices at the positions \( i_1 \ldots i_n \) to be in the states \( x_1 \ldots x_n \). The partition function of this model is denoted by \( Z_{i_1 \ldots i_n} (x_1 \ldots x_n) \). We can then write

\[
\langle V_{i_1} V_{i_2} \ldots V_{i_n} \rangle = \frac{\sum_{x_1 \ldots x_n} Z_{i_1 \ldots i_n} (x_1 \ldots x_n) V(x_1) \ldots V(x_n)}{Z_0} \tag{14}
\]

It now remains to calculate \( Z_{i_1 \ldots i_n} (x_1 \ldots x_n) \). It is convenient to reformulate this problem as follows: Denote the state of an arrow located at the edge \( j \) by \( s_j \). Put \( s_j = 1 \) if the arrow points oppositely to the ground state configuration and \( s_j = 0 \) otherwise. Define a constrained free-fermion model by requiring the arrow at the edge \( j_r \) to be in state \( s_{j_r} \) for \( 1 \leq r \leq m \). We then want to evaluate the partition function of this model, which we denote as \( Z_{cons} (s_{j_1}, \ldots, s_{j_m}) \). The idea is to perturb the weights of the dimers on the edges \( j_r \) infinitesimally. We redefine the weight of the dimer on the edge \( j_r \) by multiplying it by \((1 + \epsilon_r)\).
The partition function of the redefined free-fermion model \( Z(\epsilon_1 \ldots \epsilon_m) \) can be written in terms of the constrained partition functions as:

\[
Z(\epsilon_1 \ldots \epsilon_m) = \sum_{\{s\}} Z^{\text{cons}}(s_{j_1} \ldots s_{j_m}) \prod_{k=1}^{m} (1 + s_j \epsilon_k)
\]

where

\[
(15)
\]

\( Z(\epsilon_1 \ldots \epsilon_m) \) can be calculated using (7), by making the necessary changes to \( R \).

We can write:

\[
R = R_0 + \sum_{k=1}^{m} \epsilon_k R_{(k)}
\]

Here \( R_0 \) is the original unperturbed matrix, \( R_{(k)} \) is defined as follows:

\[
R_{(k)}(i,j) = R_0(i,j) \quad \text{if} \quad i \text{ and } j \text{ are connected by } j_k
\]

\[
R_{(k)}(i,j) = 0 \quad \text{if} \quad i \text{ and } j \text{ are not connected by } j_k.
\]

Note that the \( R_{(k)} \) have only two nonzero matrix elements. Inserting (16) in (17) and expanding gives:

\[
Z(\epsilon_1 \ldots \epsilon_m) = \sqrt{\det R} = \sqrt{\det R_0} \exp \left( \frac{1}{2} \text{Tr} \ln \left[ 1 + \sum_{k} \epsilon_k R_0^{-1} R_{(k)} \right] \right)
\]

\[
= \sqrt{\det R_0} \left[ 1 + \frac{1}{2} \sum_{k} \epsilon_k \text{Tr} \left( R_0^{-1} R_{(k)} \right) \right]
\]

\[
+ \frac{1}{4} \sum_{k,l} \epsilon_k \epsilon_l \left[ \frac{1}{2} \text{Tr} \left( R_0^{-1} R_{(k)} \right) \text{Tr} \left( R_0^{-1} R_{(l)} \right) - \text{Tr} \left( R_0^{-1} R_{(k)} R_0^{-1} R_{(l)} \right) \right] + \ldots \]

\[
(17)
\]

Using (17) and (15) we can directly read off the constrained partition functions if all the constrained arrows point oppositely to the ground state configuration. To calculate a general constrained partition function one can apply the principle of inclusion and exclusion. E.g. consider the evaluation of \( Z(s_1, s_2, s_3, s_4, s_5) \), with \( s_1 = s_2 = 1 \) and \( s_3 = s_4 = s_5 = 0 \). Put \( t_3 = t_4 = t_5 = 1 \). According to the principle of inclusion and exclusion, we can write:

\[
Z(s_1, s_2, s_3, s_4, s_5) = Z(s_1, s_2)
\]

\[
- \left[ Z(s_1, s_2, t_3) + Z(s_1, s_2, t_4) + Z(s_1, s_2, t_5) \right]
\]

\[
+ Z(s_1, s_2, t_3, t_4) + Z(s_1, s_2, t_3, t_5) + Z(s_1, s_2, t_4, t_5)
\]

\[
- Z(s_1, s_2, t_3, t_4, t_5)
\]

\[
(18)
\]

5 First order computation for the staggered F-model

For the staggered F-model the expansion can be simplified. The vertex in the ground state at a particular point will be referred to as an a-vertex. A b-vertex
is obtained by reversing the arrows of an a-vertex. An a-vertex (b-vertex) is thus of type 5 or 6 and has an energy of $-s$ ($s$). The constrained partition function corresponding to the model with one vertex constrained to be an a-vertex (b-vertex) is denoted as $Z_a$ ($Z_b$). Note that under the transformation $s \rightarrow -s$ the role of vertices a and b are interchanged. We thus have

$$Z_a(\beta s) = Z_b(-\beta s)$$

If we put $\beta \epsilon = \frac{1}{2} \ln (2) + U$ we have, according to (13) and (14), to first order in $U$:

$$F = F_0 - \frac{Z_0 - Z_a - Z_b}{Z_0} U + O(U^2)$$

Here $F$ is the reduced free energy per vertex of the staggered F-model, and $F_0 = F_{\text{Baxter}}$ in (8). To calculate $Z_b$ we only have to constrain two opposing arrows of one vertex to point oppositely to an a-vertex. Using the formalism of the previous section, we have obtained:

$$Z_b/Z_0 = \frac{1}{64 \pi^4} \left[ \int_0^{2\pi} \int_0^{2\pi} d\theta_1 d\theta_2 \frac{\exp(-2\beta s) + \cos(\theta_1) \cos(\theta_2)}{\cosh(2\beta s) + \cos(\theta_1) \cos(\theta_2)} \right]^2$$

Using this, the first order expansion of the free energy can be written as:

$$F = F_0 + \frac{1}{2} \left[ \left( \frac{\partial F_0}{\partial \beta s} \right)^2 - 1 \right] U + \ldots$$

6 Singular behavior in the vicinity of the free-fermion line

We will now verify the Coulomb gas result (see section 2):

$$F_s \sim (\beta s)^2 \frac{1}{\sqrt{\epsilon \beta \epsilon}}$$

where

$$j(\beta \epsilon) = \frac{1}{2} \arccos \left( 1 - \frac{1}{2} \exp(2\beta \epsilon) \right)$$

If we put

$$\beta \epsilon = \frac{1}{2} \ln (2) + U$$

Expanding in powers of $U$ yields:

$$F_s = A(U)(\beta s)^2 \left[ -\frac{8}{\pi} (U + O(U^2)) \ln(\beta s) + \frac{32}{\pi^2} (U^2 + O(U^3)) \ln^2 |\beta s| + \ldots \right]$$

where the amplitude $A(U)$ is a meromorphic function. If we compare this with the non-analytical behavior at $U = 0$ (see (40) in the appendix), we find:

$$A(U) = \frac{1}{4U} + O(1)$$

It then follows that the amplitude of the term $(\beta s)^2 \ln^2 |\beta s|$ is $\frac{8}{\pi} (U + O(U^2))$. It is now a simple matter to verify this using (22) and (40). From (40) and (22)
it follows that the order $U$ contribution to the singular part of the reduced free energy, $F_1(\beta s)$, can be written as

$$F_{1,s}(\beta s) = \left[ B_1(\beta s) \ln |\beta s| + B_2(\beta s) \ln^2 |\beta s| \right] U$$

(28)

with $B_1$ and $B_2$ regular functions of $\beta s$. Inserting (40) in (22) gives

$$B_2(\beta s) = \frac{8}{\pi^2} \left[ (\beta s)^2 - \frac{2}{3} (\beta s)^4 + \frac{79}{90} (\beta s)^6 + \ldots \right]$$

(29)

We have thus verified (24) to first order in $U$.

7 Conclusions and outlook

We have presented a simple technique for expanding the free energy of six-vertex models about free-fermion points. Applying this technique to the staggered $F$-model has enabled us to verify a Coulomb gas prediction about the singular part of the free energy of this model. It would be interesting to perform such computations to higher order in the free-fermion expansion. It is possible that such an undertaking might lead to proofs of certain Coulomb gas results.

A Singular part of the free energy

In this appendix we calculate the singular part of the free energy of the staggered $F$-model at $\beta s = 0$ on the free-fermion line. Expanding the logarithm in (8) yields

$$F_{\text{Baxter}}(\beta s) = -\frac{1}{8\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} d\theta_1 d\theta_2 \sum_{n=1}^{\infty} \frac{\cos^n(\theta_1) \cos^n(\theta_2)}{n \cosh^n(2\beta s)}$$

$$= -\frac{1}{2} \sum_{n=1}^{\infty} \frac{1}{2n \cosh^n(2\beta s)} \left[ \frac{(2n)!}{4^n n!} \right]^2$$

(30)

Using the asymptotic expansion

$$n! = n^n \exp (-n) \sqrt{2\pi n} \exp \left( \sum_{k=1}^{\infty} \frac{B_{2k}}{2k (2k - 1)} \frac{1}{n^{2k-1}} \right)$$

(31)

where the $B_r$ are the Bernoulli numbers, we find

$$F_{\text{Baxter}}(\beta s) = -\frac{1}{4\pi} \sum_{n=1}^{\infty} \frac{1}{n^2 \cosh^{2n}(2\beta s)} \left[ 1 - \frac{1}{4n} + \frac{1}{32n^2} + \frac{1}{128n^3} + \ldots \right]$$

(32)

We can find the non-analytical part of the function $\sum_{n=1}^{\infty} \frac{1}{n^p \cosh^{2n}(2\beta s)}$ as follows: Put $t = \ln (\cosh^2(2\beta s))$. We then have to find the non-analytical part of the function $U_p(t)$ with

$$U_p(t) = \sum_{n=1}^{\infty} \frac{\exp (-nt)}{n^p \cosh^{2n}(2\beta s)}$$

(33)

at $t = 0$ for $p \geq 2$. From (33) it follows that

$$\frac{dU_{p+1}}{dt} = -U_p$$

(34)
We denote the non-analytical part of $U_p$ by $\tilde{U}_p$. It then follows from (34) that

$$\frac{d\tilde{U}_{p+1}}{dt} = -\tilde{U}_p$$  (35)

For $p = 1$ the sum in (33) is easily evaluated:

$$U_1(t) = -\ln (1 - \exp (-t))$$  (36)

And we see that $\tilde{U}_1(t)$ is given by

$$\tilde{U}_1(t) = -\ln (t)$$  (37)

From (37) and (35) it then follows that

$$\tilde{U}_p(t) = (-1)^p \frac{t^{p-1}}{(p-1)!} \ln (t)$$  (38)

Inserting this in (32) gives

$$F_s(\beta s) = -\frac{1}{4\pi} \left( t + \frac{t^2}{8} + \frac{t^3}{192} - \frac{t^4}{3072} + \cdots \right) \ln (t)$$  (39)

Where $F_s(\beta s)$ is the singular part of the free energy and $t = 2 \ln (\cosh (2\beta s))$. Expanding (39) in powers of $\beta s$ gives

$$F_s(\beta s) = -\frac{2}{\pi} \left[ (\beta s)^2 - \frac{1}{6} (\beta s)^4 + \frac{23}{180} (\beta s)^6 - \frac{353}{5040} (\beta s)^8 + \cdots \right] \ln |\beta s|$$  (40)

References

[1] Baxter R J 1970 Phys. Rev. B 1 2199.
[2] Baxter R J 1971 Stud. Appl. Math. (M.I.T.) 50 51
[3] Baxter R J 1972 Ann. Phys. 70 193.
[4] van Beijeren H 1977 Phys. Rev. lett. 38 993.
[5] Fan C and Wu F Y 1970 Phys. Rev. B 2 723.
[6] Hurst C A and Green H S 1960 J. Chem. Phys. 33 1059.
[7] Kasteleyn P W 1963 J. Math. Phys. 4 287.
[8] Lieb E H 1967 Phys. Rev. 162 162.
[9] Lieb E H 1967 Phys. Rev. Lett. 18 1046.
[10] Lieb E H 1967 Phys. Rev. Lett. 18 108.
[11] Luijten E, van Beijeren H, Blöte H W J 1994 Phys. Rev. Lett. 73 456.
[12] Montroll E W 1964 Combinatorial Mathematics, John Wiley & Sons, inc., New York.
[13] den Nijs M 1979 J. Phys. A 12 1857.
[14] Wu F Y and Lin K Y 1975 Phys. Rev. B 12 419.
[15] Youngblood R W and Axe J D 1980 Phys. Rev. B 21 5212.