On the thermodynamic limit of the 6-vertex model

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1 Existence of the thermodynamic limit

The 6-vertex model is an exactly soluble model of classical statistical mechanics introduced and solved in various special cases by Lieb [?, ?, ?]. A solution of the most general case was obtained by Sutherland [?]. A clear description of this model and various other soluble models can be found in Baxter's book [?]. However, as Baxter remarks, an exact solution is not the same as a rigorous solution. Already in his first article on the ice model [?], Lieb initiated the rigorous analysis of the model. A more extensive analysis was made by Lieb and Wu [?]. One major question was left open, however.

This concerns the convergence of the distribution of (quasi) wavenumbers to a continuum measure in the thermodynamic limit. A similar problem was solved in the case of the nonlinear Schroedinger model in [?]. The 6-vertex model is more complicated because we cannot in all cases use the convexity argument of Yang and Yang used there. Instead, we adjust another argument of theirs [?], and use the index theory of Leray and Schroeder [?] to prove the existence of solutions to the Bethe Ansatz equations.

We start in this section with the definition of the 6-vertex model and some general results concerning the existence of the thermodynamic limit. The transfer matrix formulation of the model and the diagonalisation of the transfer matrix by means of the Bethe Ansatz are reviewed in Section 2. The 6-vertex model is a model of classical statistical mechanics where the configurations are given by arrows on the bonds of a 2-dimensional square lattice. At each vertex only six different configurations of arrows are allowed:

Each of these vertex configurations is assigned an energy and we assume spin-flip invariance, so that the first and the second, the third and the fourth and the fifth and the sixth configuration have the same energy. We denote these energies by ϵ_1, ϵ_2 and ϵ_3. If β is the inverse temperature, the corresponding Boltzmann weights are: $w_1 = \exp[-\beta\epsilon_1]$, $w_2 = \exp[-\beta\epsilon_2]$ and $w_3 = \exp[-\beta\epsilon_3]$. The partition function of the model is a sum over all allowed configurations of a product of the Boltzmann weights of all vertices: If M is the number of rows and N is the number of columns in the lattice, and $\mathcal{C}_{M,N}$ denotes the allowed configurations and we define the total energy of a configuration $c \in \mathcal{C}_{M,N}$ by

$$E(c) = n_1(c)\,\epsilon_1 + n_2(c)\,\epsilon_2 + n_3(c)\,\epsilon_3, \tag{1.1}$$

where $n_i(c)$ is the number of vertices of type $i(a)$ or $i(b)$ then the partition function is given by

$$Z_{M,N}(w_1, w_2, w_3) = \sum_{c \in \mathcal{C}_{M,N}} e^{-\beta E(c)}. \tag{1.2}$$

Solving this model now means: finding an explicit expression for the thermodynamic limit of the free energy density, i.e.

$$f(\epsilon_1, \epsilon_2, \epsilon_3; \beta) = -\frac{1}{\beta} \lim_{N,M \to \infty} \frac{1}{NM} \ln Z_{N,M}(w_1, w_2, w_3) \tag{1.3}$$

The first question that arises is whether this limit exists. This was solved by Lieb and Wu [**?**]. For convenience we repeat their argument here. Although our proof below for the explicit formula for f includes an independent proof of the existence of this limit, we shall need the corollary that f is convex as a function of the density ρ. Here, and in the following, we shall adopt periodic boundary conditions, which means that the horizontal arrows on the left and the right boundary of a finite lattice are the same, and similarly, the vertical arrows on the top and bottom boundaries are the same. (It was proved by Brascamp et.al. [**?**] that periodic boundary conditions are equivalent to free boundary conditions in the thermodynamic limit. In the Appendix, we outline a simple alternative proof in the case of left-right symmetry, i.e. $\epsilon_2 = \epsilon_3$.) This implies that, in a given configuration, the number of up arrows in every row of vertical arrows is the same. We shall call this number divided by the maximum number N, the *density* ρ. The partition function with fixed density ρ is given by

$$Z^p_{M,N}(w_1, w_2, w_3; \rho) = \sum_{\alpha,\gamma} \sum_{c \in \mathcal{C}_{M,N}(\alpha,\alpha,\gamma,\gamma)} e^{-\beta E(c)}, \tag{1.4}$$

where $\mathcal{C}_{M,N}(\alpha, \alpha', \gamma, \gamma')$ denotes the set of configurations with given boundary arrows: α and α' for the bottom and top rows of vertical arrows, and γ and γ' for the left and right hand columns of horizontal arrows. In the following we shall write $\mathcal{C}^p_{M,N}(\alpha, \gamma)$ for $\mathcal{C}_{M,N}(\alpha, \alpha, \gamma, \gamma)$.

Theorem 1.1 *Let $Z^p_{M,N}$ denote the partition function of the six-vertex model with periodic boundary conditions and let (M_l, N_l) be a sequence tending to infinity in the sense of Van Hove, and suppose that $(\rho_l)_{l=1}^\infty$ is a sequence of* *numbers $\rho_l \in [0,1]$ tending to ρ such that $\rho_l N_l \in \mathbb{N}$. Then the corresponding free energy density $f^p(\epsilon_1, \epsilon_2, \epsilon_3; \beta, \rho)$ defined by*

$$f^p(\epsilon_1, \epsilon_2, \epsilon_3; \beta, \rho) = -\frac{1}{\beta} \lim_{l\to\infty} \frac{1}{M_l N_l} \ln Z^p_{M_l,N_l}(w_1, w_2, w_3; \rho_l) \qquad (1.5)$$

exists and is independent of the sequences (M_l, N_l) and (ρ_l). Moreover, $f^p(\epsilon_1, \epsilon_2, \epsilon_3; \beta, \rho)$ is convex as a function of ρ and concave as a function of the variables $\epsilon_1, \epsilon_2, \epsilon_3$ and β.

Proof. We start by considering special sequences. Assume first that $\rho \in [0,1] \cap \mathbb{Q}$. Take $N_0 \in \mathbb{N}$ so large that $\rho N_0 \in \mathbb{N}$, and choose $M_0 \in \mathbb{N}$ arbitrary. Consider the sequence of rectangular boxes of height $M_l = 2^l M_0$ and width $N_l = 2^l N_0$. One then proves as in Lieb and Wu [**?**] that the limit (1.5) exists, using the inequalities

$$\begin{aligned} Z_{M_l,N_l}(\beta,\rho) \geq \Gamma_{M_l,N_l}(\beta,\rho) &\geq \left(\Gamma_{M_{l-1},N_{l-1}}(\beta,\rho)\right)^4 \\ &\geq \left(Z_{M_{l-1},N_{l-1}}(\beta,\rho)\right) 2^{-4(M_0+N_0)}. \end{aligned} \qquad (1.6)$$

(We suppress the dependence on ϵ_i and on the periodic boundary conditions.) This implies that the sequence

$$f_{M_l,N_l}(\beta,\rho) = -\frac{1}{\beta M_l N_l} \ln Z_{M_l,N_l}(\beta,\rho) \qquad (1.7)$$

is essentially decreasing. As it is also bounded below, it converges.

Next we show that this definition is independent of M_0 and N_0. Let (N'_n, M'_n) be an arbitrary Van Hove sequence such that $\rho N'_n \in \mathbb{N}$ for all $n = 1, 2, \ldots$. Let $r_{n,l} = [N'_n/N_l]$ and $s_{n,l} = [M'_n/M_l]$. Given configurations $c_{i,j} \in \mathcal{C}_{M_l,N_l}(\alpha,\gamma)$ $i = 1, \ldots, r_{n,l}$, $j = 1, \ldots, s_{n,l}$ on the block (M_l, N_l), fill the remainder of the block (M'_n, N'_n) with vertices of type 2 or 3 such that the resulting configuration is periodic and has density ρ. (Notice that $\rho(N'_n - r_{n,l}N_l) \in \mathbb{N}$.) Taking the supremum over α and γ it follows that

$$\gamma_{M'_n,N'_n}(\beta,\rho) \geq (\Gamma_{M_l,N_l}(\beta,\rho))^{r_{n,l}s_{n,l}} (w_2 \wedge w_3)^{M'_n N'_n - r_{n,l}s_{n,l}N_l M_l}. \qquad (1.8)$$

As in [] this implies

$$f_{M'_n,N'_n}(\beta,\rho) \leq \alpha_{n,l} f_{M_l,N_l}(\beta,\rho) + \frac{1}{\beta}\alpha_{n,l}\left(\frac{1}{M_l} + \frac{1}{N_l}\right) \ln 2 + 2(1-\alpha_{n,l})(\epsilon_2 \vee \epsilon_3), \qquad (1.9)$$

where

$$\alpha_{n,l} = \frac{r_{n,l} s_{n,l} M_l N_l}{M'_n N'_n}. \tag{1.10}$$

Taking $n \to \infty$ and then $l \to \infty$ we obtain

$$\limsup_{n\to\infty} f_{M'_n,N'_n}(\beta,\rho) \le f(\beta,\rho). \tag{1.11}$$

Similarly, one obtains the opposite bound:

$$\liminf_{n\to\infty} f_{M'_n,N'_n}(\beta,\rho) \ge f(\beta,\rho) \tag{1.12}$$

by filling the boxes (M_l, N_l) with a maximum number of copies of (M'_n, N'_n).

We now show that $f(\beta,\rho)$ is convex as a function of ρ. (Concavity in the other variables is obvious.) Suppose $t\rho_1 + (1-t)\rho_2 = \rho$ where $t, \rho, \rho_1, \rho_2 \in \mathbb{Q}\cap[0,1]$. Given sequences $(M_l^{(1)}, N_l^{(1)})$ and $(M_l^{(2)}, N_l^{(2)})$ such that $\rho_1 N_l^{(1)} \in \mathbb{N}$ and $\rho_2 N_l^{(2)} \in \mathbb{N}$, choose p such that $tp \in \mathbb{N}$ and let $M_l = M_l^{(1)} M_l^{(2)}$ and $N_l = p N_l^{(1)} N_l^{(2)}$. Then we have

$$\Gamma_{M_l,N_l}(\beta,\rho) \ge \left(\Gamma_{M_l^{(1)},N_l^{(1)}}(\beta,\rho_1)\right)^{tpM_l^{(2)}N_l^{(2)}} \left(\Gamma_{M_l^{(2)},N_l^{(2)}}(\beta,\rho_2)\right)^{(1-t)pM_l^{(1)}N_l^{(1)}}. \tag{1.13}$$

This implies convexity of f as a function of ρ.

Finally, let $\rho_0 \in [0,1]$ be arbitrary and suppose that $\rho_n \to \rho_0$, $\rho_n \in \mathbb{Q}\cap[0,1]$ and that (M_n, N_n) is a Van Hove sequence such that $\rho_n N_n \in \mathbb{N}$. We want to prove:

$$f(\beta,\rho_0) \le \liminf_{n\to\infty} f_{M_n,N_n}(\beta,\rho_n) \le \limsup_{n\to\infty} f_{M_n,N_n}(\beta,\rho_n) \le f(\beta,\rho_0). \tag{1.14}$$

Now, since $f(\beta,\rho)$ is convex in ρ it is continuous and, given $\eta > 0$, there exists $\epsilon > 0$ such that $|f(\beta,\rho) - f(\beta,\rho')| < \eta$ if $|\rho-\rho'| < \epsilon$ and $\rho,\rho' \in \mathbb{Q}\cap[0,1]$. Choose n_0 so large that $|\rho_n - \rho_0| < \epsilon/2$ for $n \ge n_0$, and fix $\rho \in (\rho_0-\epsilon/2, \rho_0+\epsilon/2)\cap\mathbb{Q}$. Then $|\rho_n-\rho| < \epsilon$ and hence $|f(\beta,\rho_n)-f(\beta,\rho)| < \eta$. In filling up a block (M_n, N_n) with elementary blocks (M'_l, N'_l) we have to be a bit more careful. We define $s_{n,l} = [M_n/M'_l]$ and

$$r_{n,l} = \begin{cases} \left[\frac{(1-\rho_n)N_n}{(1-\rho)N'_l}\right] & \text{if } \rho_n > \rho, \\ \left[\frac{(1+\rho_n)N_n}{(1+\rho)N'_l}\right] & \text{if } \rho_0 < \rho. \end{cases} \tag{1.15}$$

This choice satisfies the requirement

$$|\rho_n N_n - \rho r_{n,l} N_l'| < N_n - r_{n,l} N_l' \tag{1.16}$$

which means that, given configurations on the blocks (M_l', N_l') with density ρ we can complement these with vertices 2 or 3 on the remainder of (M_n, N_n) to obtain a configuration with density ρ_n. We can then repeat the argument above and write an analogue of (1.8):

$$\Gamma_{M_n,N_n}(\beta,\rho_n) \geq \left(\Gamma_{M_l',N_l'}(\beta,\rho)\right)^{r_{n,l}s_{n,l}} (w_2 \wedge w_3)^{M_n N_n - r_{n,l}s_{n,l}M_l'N_l'}. \tag{1.17}$$

This implies an analogue of (1.18):

$$f_{M_n,N_n}(\beta,\rho_n) \leq \alpha_{n,l} f_{M_l',N_l'}(\beta,\rho) + \frac{1}{\beta}\alpha_{n,l}\left(\frac{1}{M_n} + \frac{1}{N_n}\right)\ln 2 + 2(1-\alpha_{n,l})(\epsilon_2 \vee \epsilon_3) \tag{1.18}$$

with

$$\alpha_{n,l} = \frac{r_{n,l}s_{n,l}M_l'N_l'}{M_n N_n}. \tag{1.19}$$

Notice that $\lim_{n\to\infty} \alpha_{n,l} = (1 \pm \rho_0)/(1 \pm \rho)$. Hence, taking $n \to \infty$ and then $l \to \infty$ in (1.18), we obtain

$$\limsup_{n\to\infty} f_{M_n,N_n}(\beta,\rho_n) \leq f(\beta,\rho) + \frac{\rho_0 \pm \rho}{1 \pm \rho}(\epsilon_2 \vee \epsilon_3). \tag{1.20}$$

The last term is bounded by a constant times ϵ so taking $\eta \to 0$, we arrive at the right-hand side of the inequality (1.14). The left hand side is proven in the same way by filling up the block (M_l', N_l') with copies of (M_n, N_n). $\square$

In the exact solution of the six-vertex model one actually takes the limits $M \to \infty$ and $N \to \infty$ consecutively, but it was also shown by Lieb and Wu [] that, for periodic boundary conditions, this yields the same limit as (1.5):

Proposition 1.1 *The double limit*

$$\tilde{f}(\epsilon_1,\epsilon_2,\epsilon_3;\beta,\rho) = -\frac{1}{\beta}\lim_{N\to\infty}\lim_{M\to\infty}\frac{1}{NM}\ln Z^p_{M,N}(w_1,w_2,w_3) \tag{1.21}$$

exists and equals $f(\epsilon_1,\epsilon_2,\epsilon_3,\beta,\rho)$.

2 The transfer matrix and its diagonalisation

The transfer matrix method for solving models of classical statistical mechanics is common knowledge. Using periodic boundary conditions one writes the partition function as a trace

$$Z_{M,N} = \text{ Trace } (V_N^M), \tag{2.1}$$

where V_N is the transfer matrix with entries between two rows of vertical arrows α and α' given by

$$(V_N)_{\alpha,\alpha'} = \sum_{\gamma} \prod_{n=1}^{N} \exp\left[-\beta \epsilon_{\alpha_n}^{\alpha'_n}(\gamma_n, \gamma_{n+1})\right]. \tag{2.2}$$

The sum runs over a row of horizontal arrows $\gamma = (\gamma_1, \ldots, \gamma_N)$, where γ_n is the horizontal arrow between the $(n-1)$-th and the$n$-th vertex. It follows that we can take the limit $M \to \infty$ to obtain

$$f(\beta, \rho) = -\frac{1}{\beta} \lim_{N\to\infty} \ln \Lambda_{\max}(N), \tag{2.3}$$

where $\Lambda_{\max}(N)$ is the maximum eigenvalue of the transfer matrix V_N which exists because V_N satisfies the conditions of the Perron-Frobenius Theorem. The transfer matrix can be diagonalised by means of the Bethe Ansatz. If we write $|x_1, \ldots, x_n\rangle$ for the row configuration with n up-arrows then a general wave function in the subspace with n up-arrows can be expressed as

$$\psi = \sum_{1\le x_1 < \cdots < x_n \le N} \psi(x_1, \ldots, x_n)\, |x_1, \ldots, x_n\rangle. \tag{2.4}$$

The Bethe Ansatz for eigenfunctions of V_N then reads:

$$\psi(x_1, \ldots, x_n) = \sum_{\sigma\in\mathcal{S}_n} A_\sigma \exp\left[i \sum_{j=1}^{n} k_{\sigma(j)} x_j\right]. \tag{2.5}$$

Here, the sum runs over the set $\mathcal{S}_n$ of all permutations of$\{1, \ldots, n\}$ and the coefficients A_σ and the wave numbers $k_1, \ldots, k_n$ are to be determined by inserting into the eigenvalue equation. This yields the following conditions:
1. The wave numbers must satisfy the simultaneous nonlinear equations:

$$e^{iNk_j} = (-1)^{n-1} \prod_{l=1;l\neq j}^{n} e^{-i\theta(k_j,k_l)}, \tag{2.6}$$

where the function θ is defined by

$$\exp\left[-i\theta(k,k')\right] = \frac{1-2\Delta e^{ik}+e^{i(k+k')}}{1-2\Delta e^{ik'}+e^{i(k+k')}} \tag{2.7}$$

with

$$\Delta = (w_2^2 + w_3^2 - w_1^2)/2w_2w_3. \tag{2.8}$$

The corresponding eigenvalue is given by

$$\Lambda(k_1,\ldots,k_n) = w_2^N \prod_{j=1}^{n} L(e^{ik_j}) + w_3^N \prod_{j=1}^{n} M(e^{ik_j}), \tag{2.9}$$

where $L(z)$ and $M(z)$ are given by

$$L(z) = \frac{w_2w_3 + (w_1^2 - w_3^2)z}{w_2^2 - w_2w_3z}, \tag{2.10a}$$

$$M(z) = \frac{w_2^2 - w_1^2 - w_2w_3z}{w_2w_3 - w_3^2z}. \tag{2.10b}$$

Of course, (2.7) only defines the function θ up to a multiple of 2π. In taking the logarithm of (2.6), we shall assume that $-\pi < \theta(k,k') \leq \pi$. We obtain

$$Nk_j = 2\pi I_j - \sum_{l=1}^{n} \theta(k_j,k_l), \tag{2.11}$$

where $I_j \in \mathbb{Z}$ if n is odd, and $I_j \in \mathbb{Z} + \frac{1}{2}$ if n is even. These equations are identical to the BA equations found by Bethe [] in his solution of the Heisenberg chain. They were analysed in detail by Yang and Yang [], who showed that the ground state of the Heisenberg chain is obtained by choosing

$$I_j = j - \frac{1}{2}(n+1). \tag{2.12}$$

They also showed that, for this choice, the equations (2.11) have a real solution for $k_1,\ldots,k_n$. Lieb [] then argued that, as the Heisenberg Hamiltonian also satisfies the conditions for the Perron-Frobenius Theorem, the corresponding eigenfunction must be positive, and hence it must also be the eigenfunction of the transfer matrix with maximum eigenvalue. We therefore have

$$\Lambda_{\max} = \Lambda(k_1,\ldots,k_n) \tag{2.13}$$

where $k_1, \ldots, k_n$ are the solutions of (2.11) in case the I_j are given by (2.12). In this paper we want to address the question of how to compute the thermodynamic limit (2.3). We want to take the limit $N \to \infty$, keeping $\rho = n/N$ fixed. One usually makes the reasonable assumption that, in this limit, the distribution of the wavenumbers $k_1, \ldots, k_n$ tends to a continuous distribution with density $\rho(k)$. In the following we shall investigate the validity of this assumption. Following Yang and Yang [], we consider separately the cases $\Delta \in [0, 1)$ and $\Delta < 0$. (The case $\Delta \geq 1$ is trivial. In the attractive case, $\Delta \in [0, 1)$, we can apply the same reasoning as in the case of the nonlinear Schroedinger model (see []) and use the convexity of a certain functional to prove the existence of a unique solution to (2.11). In the repulsive case, we extend Yang and Yang's argument to the continuum, using Leray-Schauder theory []. The solution is no longer unique, but the existence is sufficient for our purposes.

3 Thermodynamic limit in the case $\Delta \geq 0$.

In taking the thermodynamic limit we distinguish the cases $\Delta > 1$, $\Delta \in [0, 1)$, $\Delta \in (-1, 0)$ and $\Delta < -1$. The case $\Delta > 1$ is trivial (Cf. Baxter [**?**]) so we start with the case $\Delta \in [0, 1)$. We first prove an analogue of the existence and uniqueness of a solution to the Bethe Ansatz equations in the thermodynamic limit. In the present case this is analogous to the nonlinear Schrödinger problem treated in [**?**].

Theorem 3.1 *Let* $m \in \mathcal{M}_+^b\left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$ *with* $||m|| \leq 1/2$ *and* $\mathrm{supp}(m) \subset [-\pi||m||, \pi||m||]$. *In case* $||m|| = \frac{1}{2}$, *assume that there exists* $\delta_0 > 0$ *such that for* $0 < \delta \leq \delta_0$,

$$m\left(\left\{q \in [-\frac{\pi}{2}, \frac{\pi}{2}] : \frac{\pi}{2} - |q| \leq \delta\right\}\right) \leq \frac{1}{\pi}\delta. \tag{3.5}$$

(Notice that the uniform distribution satisfies this condition.) Let $\Delta = -\cos\mu$ *with* $\mu \in (\pi/2, \pi)$. *Then there exists a unique continuous function*

$k : [-\pi/2, \pi/2] \to [-\pi + \mu, \pi - \mu]$ *such that*

$$k(q) = q - \int_{-\pi/2}^{\pi/2} \theta(k(q), k(q'))\, m(dq'). \tag{3.6}$$

Proof. Define the new function $\rho(q)$ by

$$e^{ik(q)} = \frac{e^{i\mu} - e^{\rho(q)}}{e^{i\mu+\rho(q)} - 1}. \tag{3.7}$$

Then $k(q) = R(\rho(q))$ where $R : \mathbb{R} \to (-\pi/2, \pi/2)$ is an increasing function given by

$$R(\alpha) = \int_0^\alpha \frac{\sin\mu}{\cosh\beta - \cos\mu} d\beta = 2\tan^{-1}\frac{\tanh(\alpha/2)}{\tan(\mu/2)}. \tag{3.8}$$

It follows that $\rho(q)$ must satisfy:

$$R(\rho(q)) = q - \int_{-\pi/2}^{\pi/2} \omega(\rho(q) - \rho(q'))\, m(dq') \tag{3.9}$$

where

$$\omega(\alpha) = -2\tan^{-1}\left(\frac{\tanh(\alpha/2)}{\tan(\mu)}\right). \tag{3.10}$$

Notice that

$$\omega'(\alpha) = -\frac{\sin(2\mu)}{\cosh\alpha - \cos(2\mu)} > 0. \tag{3.11}$$

As in [**?**], we now define a functional $B[\rho]$ on the space $L^2(\mathbb{R}, m)$ by

$$B[\rho] = \int S(\rho(q))\, m(dq) - \int q\rho(q) m(dq) \tag{3.12}$$

$$+\frac{1}{2}\int\int \Omega(\rho(q) - \rho(q'))\, m(dq)m(dq'), \tag{3.13}$$

where $S(\alpha) = \int_0^\alpha R(\beta)d\beta$ and $\Omega(\alpha) = \int_0^\alpha \omega(\beta)d\beta$.

This is well-defined because $0 \le S(\alpha) \le \frac{1}{2}R'(0)\alpha^2$, where $R'(0) = \frac{\sin\mu}{1-\cos\mu}$, and similarly, $0 \le \Omega(\alpha) \le \frac{1}{2}\omega'(0)\alpha^2$, where $\omega'(0) = -\frac{\sin(2\mu)}{1-\cos(2\mu)}$. It is also easily seen to be continuous. The Gateaux derivative in the direction of a function f is given by

$$DB[\rho]f = \int \left\{ R(\rho(q)) - q + \int \omega(\rho(q) - \rho(q'))m(dq') \right\} f(q)m(dq). \quad (3.14)$$

It follows that the solution to (3.4) is a stationary point of B. Moreover, B is convex as

$$\begin{aligned} \frac{d^2}{dt^2} B[\rho + tf] &= \int R'(\alpha(q)) f(q)^2 m(dq) \\ &+ \frac{1}{2} \int \int \omega'(\rho(q) - \rho(q'))(f(q) - f(q'))^2 m(dq)\, m(dq') \geq 0 \end{aligned} \quad (3.15)$$

by (3.6). This proves the uniqueness of the solution. To prove the existence, we need to find a compact set which contains the minimiser.

Consider first the case that $||m|| < \frac{1}{2}$. Now, as $\alpha \to \pm\infty$, $R(\alpha) \to \pm(\pi - \mu)$ and $\omega(\alpha) \to \pm(2\mu - \pi)$. Let M be so large that $\pi - \mu - |R(\alpha)| < \epsilon$ and $(2\mu - \pi) - \omega(\alpha) < \epsilon$ for $|\alpha| > M$, where ϵ is to be determined later. Consider the set

$$\Gamma_M = \{q \in [-\pi||m||, \pi||m||] : \rho(q) > M\}. \quad (3.16)$$

For M large enough, we can assume that $m(\Gamma_M) < \epsilon$. We now replace ρ on the set Γ_{2M} by $\pm 2M$, i.e. we set

$$\tilde{\rho}(q) = \mathrm{sgn}\,(\rho(q))(|\rho(q)| \wedge (2M)). \quad (3.17)$$

By convexity of the functions Ω and S we then have

$$\begin{aligned} & B[\rho] - B[\tilde{\rho}] = \\ &= \int (S(\rho(q)) - S(\tilde{\rho}(q)))\, m(dq) - \int q\, (\rho(q) - \tilde{\rho}(q))\, m(dq) \\ &\quad + \frac{1}{2} \int \int (\Omega(\rho(q) - \rho(q')) - \Omega(\tilde{\rho}(q) - \tilde{\rho}(q')))\; m(dq)m(dq') \\ &\geq \int_{\Gamma_{2M}} (|\rho(q)| - 2M)(R(2M) - |q|)\, m(dq) \\ &\quad + \int_{\Gamma_{2M}} m(dq) \int_{\Gamma_{2M}^c} m(dq')\, (\Omega(\rho(q) - \rho(q')) - \Omega(\tilde{\rho}(q) - \rho(q'))) \end{aligned} \quad (3.18)$$

where we used the convexity of the function S and the fact that if $q, q' \in \Gamma_{2M}$ then the second term is zero whereas the first term is positive since $\Omega \geq 0$.

Next using the convexity of Ω and the above bounds on the derivatives we get

$$
\begin{aligned}
&B[\rho]-B[\tilde\rho] = \\
&\quad\geq \int_{\Gamma_{2M}} (|\rho(q)|-2M)(R(2M)-|q|)\,m(dq) \\
&\qquad + \int_{\Gamma_{2M}} m(dq) \int_{\Gamma^c_{2M}} m(dq')\omega(2M-|\rho(q')|)(|\rho(q)|-2M) \\
&\quad\geq \int_{\Gamma_{2M}} (|\rho(q)|-2M)(\pi-\mu-|q|-\epsilon)m(dq) \\
&\qquad + \int_{\Gamma_{2M}} m(dq) \int_{\Gamma^c_{M}} m(dq')\,((2\mu-\pi)-\epsilon)\,(|\rho(q)|-2M) \\
&\quad\geq \int_{\Gamma_{2M}} m(dq)(|\rho(q)|-2M)\,(\pi-\mu-|q|-\epsilon \\
&\qquad + ((2\mu-\pi)-\epsilon)\,m(\Gamma^c_M)) \\
&\quad\geq \int_{\Gamma_{2M}} m(dq)(|\rho(q)|-2M)\,(\pi-\mu-|q|-\epsilon \\
&\qquad + ((2\mu-\pi)-\epsilon)\,(||m||-\epsilon)) \\
&\quad\geq \int_{\Gamma_{2M}} m(dq)(|\rho(q)|-2M)\,((\pi-\mu)(1-2||m||)-\epsilon(1+2\mu-\pi+||m||))>0
\end{aligned}
\tag{3.19}
$$

provided

$$\epsilon < \frac{(\pi-\mu)(1-2||m||)}{1+2\mu-\pi+||m||}.$$

We conclude that the minimiser must satisfy $||\rho||_\infty \leq 2M$ and is a fortiori contained in the ball $\{\rho \in L^2(m) : ||\rho||_2 \leq 2M\}$. This ball is bounded and therefore weakly compact. But the functional $B[\rho]$ is norm continuous and convex and therefore lower semicontinuous for the weak topology, see e.g. [?], Prop. 1.5 of Chap. 2. It follows that it attains its minimum on a compact set.

Next consider the case $||m|| = \frac{1}{2}$. In that case we cannot prove that the minimiser is bounded, so we need a more sophisticated bound. We use the function

$$f(q) = -2\ln\left(\frac{\pi}{2}-|q|\right).$$

Given $M > 0$ and $\delta > 0$, we define the sets

$$\Gamma_0^M = \{q \in [-\frac{1}{2}\pi, \frac{1}{2}\pi] : |\rho(q)| > M, |q| < \frac{\pi}{2} - \delta\} \tag{3.20}$$

and

$$\Gamma_k = \left\{q \in [\frac{1}{2}\pi, \frac{1}{2}\pi] : |\rho(q)| > f(q), \frac{\pi}{2} - \gamma^{-k+1}\delta \le |q| < \frac{\pi}{2} - \gamma^{-k}\delta \right\}, \tag{3.21}$$

where $\gamma > 1$ is a parameter to be determined later.

We now write

$$\Gamma^M = \Gamma_0^M \cup \bigcup_{k \ge 1} \Gamma_k$$

and consider the decomposition

$$\begin{aligned} &\{(q, q') : q \in \Gamma^M \text{ or } q' \in \Gamma^M\} = \\ &= \bigcup_{k \ge 0} \left(\Gamma_k \times \left(\bigcup_{l \ge k} \Gamma_l \right)^c \cup \left(\bigcup_{l \ge k} \Gamma_l \right)^c \times \Gamma_k \cup (\Gamma_k \times \Gamma_k) \right). \end{aligned} \tag{3.22}$$

Note that this is a disjoint union. Replacing now $\rho(q)$ by

$$\tilde{\rho}(q) = \operatorname{sgn}(\rho(q)) \left(|\rho(q)| \wedge \left(f(q)\chi_{\Gamma^M \setminus \Gamma_0^M} + 2M\chi_{\Gamma_0^M} \right) \right)$$

we have first of all

$$\begin{aligned} &\int (S(\rho(q)) - S(\tilde{\rho}(q)))\, m(dq) - \int q\,(\rho(q) - \tilde{\rho}(q))\, m(dq) \ge \\ &\ge \int_{\Gamma_0^{2M}} m(dq)(|\rho(q)| - 2M)(R(2M) - |q|) \\ &\quad + \sum_{k=1}^{\infty} \int_{\Gamma_k} m(dq)\,(|\rho(q)| - f(q))\,(R(f(q)) - |q|) \\ &\ge \int_{\Gamma_0^{2M}} m(dq)(|\rho(q)| - 2M)(\pi - \mu - |q| - \eta) \\ &\quad + \sum_{k=1}^{\infty} \int_{\Gamma_k} m(dq)\,(|\rho(q)| - f(q)) \\ &\qquad \times \left(\pi - \mu - \frac{\pi}{\tan(\mu/2)} \left(\frac{\pi}{2} - |q| \right)^2 - |q| \right), \end{aligned} \tag{3.23}$$

where we used the bound

$$R(f(q)) > \pi - \mu - \frac{4}{\tan(\mu/2)} \left(\frac{\pi}{2} - |q| \right)^2 \tag{3.24}$$

which follows from the inequalities

$$\tan^{-1}(x - \delta) > \tan^{-1}(x) - \delta$$

and

$$\tanh(x) > 1 - 2e^{-|x|}.$$

For the term

$$\frac{1}{2} \int \int (\Omega(\rho(q) - \rho(q')) - \Omega(\tilde{\rho}(q) - \tilde{\rho}(q')))\ m(dq) m(dq')$$

we consider the contributions from the decomposition (3.22) separately:

$$\begin{aligned} &\int_{\Gamma_0^M} \int_{(\Gamma^M)^c} (\Omega(\rho(q) - \rho(q')) - \Omega(\tilde{\rho}(q) - \tilde{\rho}(q')))\ m(dq) m(dq') \\ &\qquad \geq \int_{\Gamma_0^{2M}} m(dq) (2\mu - \pi - \eta) m((\Gamma^M)^c) \end{aligned} \tag{3.25}$$

as before. Combining this with the first term of (3.23) gives a positive contribution provided M is so large that $m(\Gamma^M) < \epsilon$ and $R(2M) > \pi - \mu - \eta$ and $\omega(M) > 2\mu - \pi - \eta$ where $\frac{3}{2}\eta + \pi\epsilon < \delta$.

Next consider a term of the form

$$\int_{\Gamma_k} \int_{(\cup_{l \geq k} \Gamma_k)^c} (\Omega(\rho(q) - \rho(q')) - \Omega(\tilde{\rho}(q) - \tilde{\rho}(q')))\ m(dq) m(dq').$$

Assuming $\delta < \delta_0$, this is bounded by

$$\begin{aligned} &\int_{\Gamma_k} \int_{(\cup_{l \geq k} \Gamma_k)^c} (\Omega(\rho(q) - \rho(q')) - \Omega(\tilde{\rho}(q) - \tilde{\rho}(q')))\ m(dq) m(dq') \geq \\ &\geq \int_{\Gamma_k} m(dq) \left(|\rho(q)| - f(q) \right) \\ &\qquad \times \left[2\mu - \pi - \frac{4}{\tan(\pi - \mu)} \left(\frac{\pi}{2} - |q| \right)^2 \right] m \left[\left(\bigcup_{l \geq k} \Gamma_l \right)^c \right]. \end{aligned} \tag{3.26}$$

Since

$$\bigcup_{l\geq k}\Gamma_l \subset \left\{q\in\left[-\frac{\pi}{2},\frac{\pi}{2}\right]:\ \frac{\pi}{2}-\gamma^{-k+1}\delta\leq |q|\right\}$$

we have by the assumption about m,

$$m\left(\bigcup_{l\geq k}\Gamma_l\right)\leq \frac{1}{\pi}\gamma^{-k+1}\delta. \tag{3.27}$$

Therefore

$$\begin{aligned}&\int_{\Gamma_k}\int_{(\cup_{l\geq k}\Gamma_k)^c}\left(\Omega(\rho(q)-\rho(q'))-\Omega(\tilde\rho(q)-\tilde\rho(q'))\right)\,m(dq)m(dq')\geq\\ &\quad\geq \int_{\Gamma_k} m(dq)\,(|\rho(q)|-f(q))\\ &\qquad\times\left[2\mu-\pi-\frac{4}{\tan(\pi-\mu)}\left(\frac{\pi}{2}-|q|\right)^2\right]\left(\frac{1}{2}-\frac{1}{\pi}\gamma^{-k+1}\delta\right).\end{aligned} \tag{3.28}$$

Combining this with the corresponding term of (3.23) we have

$$\begin{aligned}&\int (S(\rho(q))-S(\tilde\rho(q)))\,m(dq)-\int q\,(\rho(q)-\tilde\rho(q))\,m(dq)\\ &+\int_{\Gamma_k}\int_{(\cup_{l\geq k}\Gamma_k)^c}\left(\Omega(\rho(q)-\rho(q'))-\Omega(\tilde\rho(q)-\tilde\rho(q'))\right)\,m(dq)m(dq')\\ &\quad\geq\int_{\Gamma_k} m(dq)\,(|\rho(q)|-f(q))\\ &\qquad\times\left[\pi-\mu-\frac{\pi}{\tan(\mu/2)}\left(\frac{\pi}{2}-|q|\right)^2-|q|\right.\\ &\qquad\left.+\left(2\mu-\pi-\frac{4}{\tan(\pi-\mu)}\left(\frac{\pi}{2}-|q|\right)^2\right)\left(\frac{1}{2}-\frac{1}{\pi}\gamma^{-k+1}\delta\right)\right].\end{aligned} \tag{3.29}$$

Since $\frac{\pi}{2}-\gamma^{-k+1}\delta\leq|q|<\frac{\pi}{2}-\gamma^{-k}\delta$ for $q\in\Gamma_k$, we have

$$\begin{aligned}&\pi-\mu-c_1\left(\frac{\pi}{2}-|q|\right)^2-|q|\\ &+\left(2\mu-\pi-c_2\left(\frac{\pi}{2}-|q|\right)^2\right)\left(\frac{1}{2}-\frac{1}{\pi}\gamma^{-k+1}\delta\right)\\ &\quad\geq\frac{\pi}{2}-\mu-c_1\left(\gamma^{-k+1}\delta\right)^2+\gamma^{-k}\delta\\ &\qquad+\mu-\frac{\pi}{2}-\frac{1}{2}c_2\left(\gamma^{-k+1}\delta\right)^2-\frac{2\mu-\pi}{\pi}\gamma^{-k+1}\delta\\ &=\left(1-\frac{2\mu-\pi}{\pi}\gamma\right)\gamma^{-k}\delta-c\gamma^{-2k+2}\delta^2,\end{aligned} \tag{3.30}$$

where

$$c_1 = \frac{4}{\tan(\mu/2)}, \quad c_2 = \frac{4}{\tan(\pi-\mu)}, \text{ and } c = c_1 + \frac{1}{2}c_2.$$

Hence

$$\begin{aligned}
&\int (S(\rho(q)) - S(\tilde\rho(q)))\, m(dq) - \int q\,(\rho(q) - \tilde\rho(q))\, m(dq) \\
&+ \int_{\Gamma_k} \int_{(\cup_{l\geq k}\Gamma_k)^c} (\Omega(\rho(q)-\rho(q')) - \Omega(\tilde\rho(q)-\tilde\rho(q')))\ m(dq)m(dq') \\
&\quad \geq \int_{\Gamma_k} m(dq)\, (|\rho(q)| - f(q)) \\
&\qquad \times \left[\left(1 - \frac{2\mu-\pi}{\pi}\gamma\right) \gamma^{-k}\delta - c\gamma^{-2k+2}\delta^2 \right]. \qquad (3.31)
\end{aligned}$$

Finally consider the terms

$$\frac{1}{2}\int_{\Gamma_k} m(dq) \int_{\Gamma_k} m(dq')\, (\Omega(\rho(q)-\rho(q')) - \Omega(f(q)-f(q')))\,.$$

Since $0 \leq \Omega(\alpha) \leq (2\mu-\pi)|\alpha|$, these can be bounded by

$$\begin{aligned}
&\frac{1}{2}\int_{\Gamma_k} m(dq) \int_{\Gamma_k} m(dq')\, (\Omega(\rho(q)-\rho(q')) - \Omega(f(q)-f(q'))) \\
&\quad \geq -(\mu - \frac{\pi}{2}) \int_{\Gamma_k} m(dq) \int_{\Gamma_k} m(dq')\, |f(q) - f(q')| \\
&\quad \geq \pi \ln(\gamma^{-k}\delta) m(\Gamma_k)^2 \geq \pi(\gamma^{-k}\delta)^2 \ln(\gamma^{-k}\delta). \qquad (3.32)
\end{aligned}$$

In all, we get

$$\begin{aligned}
&\int (S(\rho(q)) - S(\tilde\rho(q)))\, m(dq) - \int q\,(\rho(q) - \tilde\rho(q))\, m(dq) \\
&+ \int_{\Gamma_k} \int_{(\cup_{l\geq k}\Gamma_k)^c} (\Omega(\rho(q)-\rho(q')) - \Omega(\tilde\rho(q)-\tilde\rho(q')))\ m(dq)m(dq') \\
&+ \frac{1}{2}\int_{\Gamma_k} m(dq) \int_{\Gamma_k} m(dq')\, (\Omega(\rho(q)-\rho(q')) - \Omega(f(q)-f(q'))) \\
&\quad \geq \int_{\Gamma_k} m(dq)\, (|\rho(q)| - f(q)) \\
&\qquad \times \left[\left(1 - \frac{2\mu-\pi}{\pi}\gamma\right) \gamma^{-k}\delta - c\gamma^{-2k+2}\delta^2 + \pi(\gamma^{-k}\delta)^2 \ln(\gamma^{-k}\delta) \right] \qquad (3.33)
\end{aligned}$$

Choosing $\gamma < \frac{2\mu-\pi}{\pi}$ (which is possible as $\mu < \pi$) and δ small enough, this is positive.

□

Theorem 3. *The mapping $m \mapsto k_m$ defined by Theorem 2 is continuous, that is, if $m_n \to m$* weakly *then $k_{m_n} \to k_m$ in norm.*

Proof. Let $m_n^{(1)}$ be a subsequence. Notice that $||k_{m_n}|| \leq \pi - \mu$ and k_{m_n} is also equicontinuous because

$$\frac{\partial}{\partial k}\theta(k,k') = \Delta \frac{\cos k' + \cos\mu}{\Delta^2 \sin^2(k-k')/2 + [\cos(k+k')/2 - \Delta\cos(k-k')/2]^2} \geq 0 \tag{3.11}$$

for $-\pi + \mu \leq k' \leq \pi - \mu$. Hence

$$k'_{m_n}(q) = \left\{1 + \int \frac{\partial\theta}{\partial k}(k_{m_n}(q) - k_{m_n}(q'))m_n(dq')\right\}^{-1} \in (0,1) \tag{3.12}$$

Therefore, $|k_{m_n}(q) - k_{m_n}(q')| \leq |q - q'|$ uniformly in n. It follows that there exists a subsequence $m_n^{(2)}$ of $m_n^{(1)}$ such that $k_{m_n^{(2)}}$ converges to a continuous function k uniformly on $[-\pi/2, \pi/2]$. We must show that $k = k_m$. But θ is uniformly continuous on $[-\pi+\mu, \pi-\mu]^2$ so $\theta(k_{m_n^{(2)}}(q) - k_{m_n^{(2)}}(\cdot)) \to \theta(k(q) - k(\cdot))$ in norm, and hence

$$\int \theta(k_{m_n^{(2)}}(q) - k_{m_n^{(2)}}(q'))m_n^{(2)}(dq') \to \int \theta(k(q) - k(q'))m(dq').$$

It follows that $k(q) = k_m(q)$. □

Corollary. *If $m_n \to m$ weakly, and $\tilde{m}_n$ is the image measure of m_n under the mapping k_{m_n} then $\tilde{m}_n \to \tilde{m} = k_m(m)$.*

Proof. Let $F \in \mathcal{C}([-\pi+\mu, \pi-\mu])$. Then $\int F(k)\tilde{m}_n(dk) = \int F(k_{m_n}(q))m_n(dq)$ and

$$\begin{aligned}\left|\int F(k)\tilde{m}_n(dk) - \int F(k)\tilde{m}(dk)\right| &\leq \int |F(k(q)) - F(k_m(q))|m_n(dq) \\ &+ \left|\int F(k_m(q))m_n(dq) - \int F(k_m(q))m(dq)\right|.\end{aligned} \tag{3.13}$$

The right-hand side tends to zero as $n \to \infty$ because $k_{m_n} \to k_m$ uniformly and k_m is continuous. □

Theorem 4. *Let*

$$m_N = \frac{1}{N} \sum_{j=1}^{n_N} \delta_{q_j}, \tag{3.14}$$

where $q_j = \frac{2\pi}{N}(j - \frac{1}{2}(n_N + 1))$ *and* $n_N \leq N/2$*. Assume that* $n_N/N \to \rho$ *as* $N \to \infty$*. Then* $m_N \to \frac{1}{2\pi} dq$ *on* $[-\pi\rho, \pi\rho]$ *and* $\tilde{m}_n \to \tilde{m}$*, where* $\tilde{m}$ *is absolutely continuous with respect to the Lebesgue measure and symmetric, and there exists* $Q \in [0, \pi - \mu]$ *such that* $\operatorname{supp}(m) = [-Q, Q]$*.*

Proof. Let $F \in \mathcal{C}([-\pi/2, \pi/2])$. Then

$$\begin{aligned} \int F(q)\, m_N(dq) &= \frac{1}{N} \sum_{j=1}^{n_N} F\left(\frac{2\pi}{N}(i - \frac{1}{2}(n_N + 1))\right) \\ &\to \int_{-\pi\rho}^{\pi\rho} F(q) \frac{dq}{2\pi}. \end{aligned} \tag{3.15}$$

Hence $\tilde{m}_N \to \tilde{m}$ and we must show that $\tilde{m}$ is absolutely continuous and even. To that end, let $\epsilon > 0$. We must show that there exists $\delta > 0$ such that $\tilde{m}(k_0 - \delta, k_0 + \delta) < \epsilon$ for all k_0. Now, $\tilde{m}(k_0 + \delta, k_0 + \delta) = \int_{k_m^{-1}(k_0 - \delta, k_0 + \delta)} \frac{dq}{2\pi}$ and we have seen that k_m is continuous and increasing: $[-\pi/2, \pi/2] \to [-\pi + \mu, \pi - \mu]$. Therefore k_m^{-1} is continuous and $\forall \epsilon > 0\, \exists \delta > 0 : k_m^{-1}(k_0 - \delta, k_0 + \delta) \subset (q_0 - \pi\epsilon, q_0 + \pi\epsilon)$ where $k_m(k_0) = q_0$. Hence $\int_{k_m^{-1}(k_0 - \delta, k_0 + \delta)} \frac{dq}{2\pi} < \epsilon$. □