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Finding Equilibrium Macrostates of the Face-Cubic Model

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Abstract

In this report we study equilibrium macrostates of the Face-Cubic model on the complete graph. Specifically, we analyse the high temperature case for $d = 3$ with non-zero field. We derive a function $\tilde{G}_{\beta,h}$ which can be minimised in order to identify equilibrium macrostates. By bounding the function below by a convex quadratic, we prove existence of a global minimum point. Through analysis of the partial derivatives of $\tilde{G}_{\beta,h}$ we show that the global minimum is unique and specify bounds for the point.

Acknowledgements

I would primarily like to thank my supervisor A/Prof Tim Garoni for his guidance and mentorship throughout this project. I am truly grateful for the time he dedicated to providing insightful feedback and sharing his expertise. Furthermore, I would like to thank Aram Perez for his constructive suggestions and willingness to provide assistance throughout the project. Finally, I would like to thank AMSI for the opportunity to undertake a project over the summer.

Contents

1 Introduction

The Ising model is a fundamental model in statistical mechanics. The model consists of spins arranged on the nodes of a graph, with edges representing an interaction between adjacent spins. An external field h also interacts with the spins. The spins are discrete random variables taking values in $\{-1, +1\}$ and the overall energy of the system can be described by its Hamiltonian function.

The Ising model can be simplified by using a mean-field approximation, whereby each spin is assumed to interact with every other spin. Doing so can make it possible to analyse the macroscopic behaviour of a system through explicit computations [1]. This approximation is known as the Curie-Weiss model, and can be thought of as the Ising model on the complete graph.

In this study we generalise the Curie-Weiss model to higher dimensional spaces by allowing the spins to take values in $\mathbb{R}^d$. Specifically, we restrict the spin-state space to vectors with precisely one non-zero entry: either $+1$ or -1. Formally, this is the set

$$\Omega_d = \{c_1\mathbf{e}_1 + ... + c_n\mathbf{e}_d : c_i \in \{-1, 0, 1\} \text{ for all } i = 1, ..., d \text{ and precisely one } c_i \text{ is non-zero}\}. \tag{1.1}$$

We call this the Face-Cubic model as the possible spin states are unit vectors pointing to the faces of a d-dimensional cube.

To generalise the Curie-Weiss Hamiltonian function to higher dimensions, we replace the product of spins with a dot product. For a collection of spins $\sigma = (\sigma_1, ..., \sigma_n)$, $\sigma_i \in \Omega_d$ for all $i = 1, ..., n$, inverse temperature β and external magnetic field $h \in \mathbb{R}^d$, the Curie-Weiss Hamiltonian is defined as

$$H_{n;\beta;h}(\sigma) := -\frac{d\beta}{n}\sum_{i,j=1}^{n}\sigma_i \cdot \sigma_j - h \cdot \sum_{i=1}^{n}\sigma_i \ . \tag{1.2}$$

We can then introduce the Gibbs measure, which gives the probability of a system having spin configuration σ,

$$P^{\beta}(\sigma) = \frac{\exp(-\beta H_{n;\beta;h}(\sigma))}{Z_n(\beta, h)} \ . \tag{1.3}$$

The partition function in the denominator serves as a normalising term and is given by

$$Z_n(\beta, h) = \sum_{\sigma \in \Omega_d^n} \exp(-\beta H_{n;\beta;h}(\sigma)) \ . \tag{1.4}$$

To analyse the global behaviour of a system we introduce a quantity called the magnetisation which can be thought of as an 'average' of the spins in a system,

$$m_n(\sigma) := \frac{1}{n}\sum_{i=1}^{n}\sigma_i \ . \tag{1.5}$$

We are interested in where the magnetisation asymptotically converges to as n becomes large. This is well understood in the $d = 1$ case with zero external field (see e.g. [1]). At high temperature ($\beta \le \beta_c$), the spin-to-spin interactions are small and the magnetisation converges to zero. Conversely, at low temperature ($\beta > \beta_c$) the spin interactions are stronger and the magnetisation converges with equal probability to either of the two ground states with all spins equal. Here β_c is the inverse critical temperature and $\beta_c = d$ for $d \leq 3$. It has been shown that $m_n(\sigma)$ satisfies a large deviation principle with respect to P^β, with non-negative rate function I^β [4]. This leads to the following result

$$P^\beta(m_n = x) \simeq \exp(-nI^\beta(x)) \ . \tag{1.6}$$

As n goes to infinity, (1.6) tells us that the probability of a particular magnetisation will become small unless the rate function is zero. The values of x at which the rate function vanishes are called equilibrium macrostates. The $d = 1$ case described above is illustrated in Figure 1.

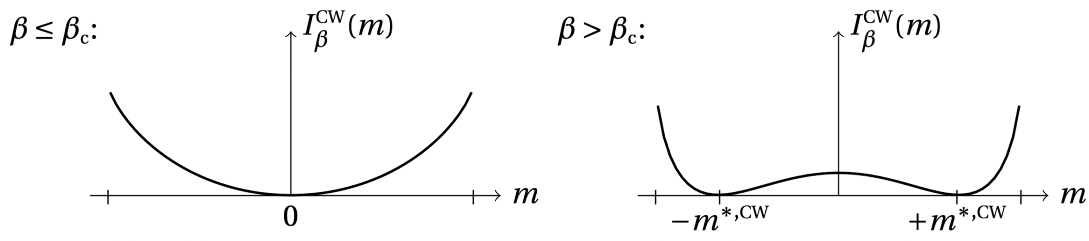

Figure 1: The rate function of the Curie-Weiss model when $d = 1$ and $h = 0$. Extracted from Friedli, S & Velenik, Y 2017 [1].

When considering the general d case in the absence of an external field, finding the equilibrium macrostates is equivalent to minimising the function G_β [3], which is given by

$$G_\beta(x) = \frac{\beta}{2}\langle x, x\rangle - \ln\sum_{j=1}^{d}\cosh(\beta x_j) + \ln(d) \ , x \in \mathbb{R}^d \ . \tag{1.7}$$

In this report we derive a similar function for non-zero field and identify the equilibrium macrostates for the high temperature case when $d = 3$.

1.1 Statement of Authorship

The background and motivation of this report follows closely to work done by Tim Garoni, Aram Perez and Zongzheng Zhou in [2]. In particular Lemma 2.1 is adapted from Lemma 4.1 in [2], with the difference being the inclusion of an additional term for external field. The content of Lemmas 2.2 - 2.5 is original work for which I was responsible. I acknowledge however the direction Tim and Aram gave me in pursuing these ideas and the suggestions they offered in refining my arguments.

2 Identifying Equilibrium Macrostates with an External Field for $d = 3$

Lemma 2.1. *Let $\beta \in (0,\infty)$, $h \in \mathbb{R}^d$ and $r \in \mathbb{R}^d$. Define $S_n(\sigma) := \sum_{i=1}^n \sigma_i$ and $G_{\beta,h}(x) := \frac{\beta}{2}\langle x,x\rangle - \ln\left(\sum_{j=1}^d \cosh(\beta(h_j + x_j))\right)$. The moment generating function of S_n/n^δ for the d-dimensional Face-Cubic model is given by*

$$M_n(r) = \exp\left(-\frac{n^{1-2\delta}}{2\beta}\langle r,r\rangle\right)\frac{\int_{\mathbb{R}^d}\exp[\langle r,x\rangle - nG_{\beta,h}(\frac{x}{n^{1-\delta}})]\,dx}{\int_{\mathbb{R}^d}\exp[-nG_{\beta,h}(\frac{x}{n^{1-\delta}})]\,dx}\,. \tag{2.1}$$

Proof. Let $a_n = \sqrt{\beta/n}$. We have from the definition of the moment generating function

$$\begin{aligned}
M_n(r) &= \sum_{\sigma\in\Omega^n}\exp\left(\frac{1}{n^\delta}\langle r,S_n\rangle\right)\left(\frac{\exp(\frac{\beta}{2n}\langle S_n,S_n\rangle + \beta\langle h,S_n\rangle)p(\sigma)}{\sum_{\sigma\in\Omega^n}\exp(\frac{\beta}{2n}\langle S_n,S_n\rangle + \beta\langle h,S_n\rangle)p(\sigma)}\right)\,,\\
&= \frac{\sum_{\sigma\in\Omega^n}\exp(\frac{1}{a_n n^\delta}\langle r,a_nS_n\rangle)\exp(\frac{1}{2}\langle a_nS_n,a_nS_n\rangle)\exp(na_n\langle h,a_nS_n\rangle)p(\sigma)}{\sum_{\sigma\in\Omega^n}\exp(\frac{1}{2}\langle a_nS_n,a_nS_n\rangle)\exp(na_n\langle h,a_nS_n\rangle)p(\sigma)}\,,\\
&= \frac{T_n(r)}{T_n(0)}\,,
\end{aligned}$$

where $T_n(r) := \sum_{\sigma\in\Omega^n}\exp(\frac{1}{a_n n^\delta}\langle r,a_nS_n\rangle)\exp(\frac{1}{2}\langle a_nS_n,a_nS_n\rangle)\exp(na_n\langle h,a_nS_n\rangle)p(\sigma)$. We then apply the identity $\exp(\frac{1}{2}\langle y,y\rangle) = \frac{1}{(2\pi)^{d/2}}\int_{\mathbb{R}^d}\exp(\langle y,x\rangle - \frac{1}{2}\langle x,x\rangle)\,dx$ to $T_n(r)$,

$$\begin{aligned}
T_n(r) &= \sum_{\sigma\in\Omega^n}\exp\left(\frac{1}{a_n n^\delta}\langle r,a_nS_n\rangle + na_n\langle h,a_nS_n\rangle\right)p(\sigma)\frac{1}{(2\pi)^{d/2}}\int_{\mathbb{R}^d}\exp\left(\langle x,a_nS_n\rangle - \frac{1}{2}\langle x,x\rangle\right)dx\,,\\
&= \left(\frac{1}{\sqrt{2\pi}}\right)^d\sum_{\sigma\in\Omega^n}\int_{\mathbb{R}^d}\exp\left(\frac{1}{n^\delta a_n}\langle r,a_nS_n\rangle + na_n\langle h,a_nS_n\rangle + \langle x,a_nS_n\rangle - \frac{1}{2}\langle x,x\rangle\right)p(\sigma)\,dx\,,\\
&= \left(\frac{1}{\sqrt{2\pi}}\right)^d\sum_{\sigma\in\Omega^n}\int_{\mathbb{R}^d}\exp\left(\langle\frac{r}{n^\delta} + na_n^2h + a_nx, S_n\rangle - \frac{1}{2}\langle x,x\rangle\right)p(\sigma)\,dx\,,\\
&= \left(\frac{1}{\sqrt{2\pi}}\right)^d\int_{\mathbb{R}^d}\exp\left(-\frac{1}{2}\langle x,x\rangle\right)\sum_{\sigma\in\Omega^n}\prod_{i=1}^n\exp\left(\langle\frac{r}{n^\delta} + na_n^2h + a_nx,\sigma_i\rangle\right)\frac{1}{2d}\,dx\,.
\end{aligned}$$

Swapping the product and the sum gives

$$\begin{aligned}
T_n(r) &= \left(\frac{1}{\sqrt{2\pi}}\right)^d\int_{\mathbb{R}^d}\exp\left(-\frac{1}{2}\langle x,x\rangle\right)\prod_{i=1}^n\sum_{j=1}^d\frac{1}{d}\cosh\left(\frac{r_j}{n^\delta} + na_n^2h_j + a_nx_j\right)dx\,,\\
&= \left(\frac{1}{\sqrt{2\pi}}\right)^d\int_{\mathbb{R}^d}\exp\left[-\frac{1}{2}\langle x,x\rangle + n\ln\left(\sum_{j=1}^d\cosh\left(\frac{r_j}{n^\delta} + na_n^2h_j + a_nx_j\right)\right) - n\ln d\right]dx\,.
\end{aligned}$$

We make the substitution $x \to \frac{1}{a_n}(\frac{\beta x}{n^{1-\delta}} - \frac{r}{n^\delta})$ and define $c_n(\beta) = (\frac{1}{\sqrt{2\pi}})^d(\frac{\beta}{a_n n^{1-\delta}})^d$ such that

$$\begin{aligned}
T_n(r) &= c_n(\beta)\int_{\mathbb{R}^d}\exp\left[-\frac{1}{2a_n^2}\langle\frac{\beta x}{n^{1-\delta}} - \frac{r}{n^\delta},\frac{\beta x}{n^{1-\delta}} - \frac{r}{n^\delta}\rangle + n\ln\left(\sum_{j=1}^d\cosh\left(na_n^2h_j + \frac{\beta x_j}{n^{1-\delta}}\right)\right) - n\ln d\right]dx\,,\\
&= c_n(\beta)\int_{\mathbb{R}^d}\exp\left[\langle r,x\rangle - \frac{n^{1-2\delta}}{2\beta}\langle r,r\rangle - \frac{n}{2\beta}\langle\frac{\beta x}{n^{1-\delta}},\frac{\beta x}{n^{1-\delta}}\rangle + n\ln\left(\sum_{j=1}^d\cosh\left(na_n^2h_j + \frac{\beta x_j}{n^{1-\delta}}\right)\right) - n\ln d\right]dx\,.
\end{aligned}$$

Recalling the definition of $G_{\beta,h}$ we have

$$\begin{aligned} M_n(r) &= \frac{T_n(r)}{T_n(0)} \,, \\ &= \exp\left(-\frac{n^{1-2\delta}}{2\beta}\langle r,r\rangle\right)\frac{\int_{\mathbb{R}^d}\exp[\langle r,x\rangle - nG_{\beta,h}(\frac{x}{n^{1-\delta}})]\,dx}{\int_{\mathbb{R}^d}\exp[-nG_{\beta,h}(\frac{x}{n^{1-\delta}})]\,dx} \quad . \end{aligned}$$

□

Lemma 2.2. *Let $f:\mathbb{R}^d\to\mathbb{R}, f\in C^0$ and $a>0$ such that $f(x)\geq a|x|^2$ for all $x\in\mathbb{R}^d$. Then f has at least one global minimum point on $\mathbb{R}^d$.*

Proof. Set $M=f(0)\geq 0$ and $x^*=\sqrt{\frac{M+1}{a}}$. Since f is continuous, by the Extreme Value Theorem it has a minimum on the compact ball $B=\{x\in\mathbb{R}^d:|x|\leq x^*\}$. So there exists $x_0\in B$ such that

$$f(x_0)\leq f(x) \text{ for all } x\in B \,. \tag{2.2}$$

In particular,

$$f(x_0)\leq f(0)=M \,, \tag{2.3}$$

since $0\in B$. Suppose $x\in\mathbb{R}\backslash B=\{x\in\mathbb{R}^d:|x|>x^*\}$. Then using the fact that $a>0$,

$$\begin{aligned} f(x) &\geq a|x|^2 \,, \\ &> ax^{*2} \,, \\ &= a\left(\sqrt{\frac{M+1}{a}}\right)^2 \,, \\ &= M+1 \,, \\ &> M \,, \\ &\geq f(x_0) \,. \end{aligned} \tag{2.4}$$

Hence, from (2.2) and (2.4), $f(x_0)\leq f(x)$ for all $x\in\mathbb{R}^d$. So f has a global minimum point at x_0. □

Lemma 2.3. *Let $\beta\in(0,\infty)$ and $h\in\mathbb{R}^d$. Then $\tilde{G}_{\beta,h}(u):=G_{\beta,h}(u-h)$ has at least one global minimum point on $\mathbb{R}^d$.*

Proof. Applying the change of variables $x=u-h$ to the function $G_{\beta,h}(x)$ gives

$$\begin{aligned} \tilde{G}_{\beta,h}(u):=G_{\beta,h}(u-h) &= \frac{\beta}{2}\langle u,u\rangle - \ln\left(\sum_{j=1}^{d}\cosh(\beta u_j)\right) - \beta\langle u,h\rangle + \frac{\beta}{2}\langle h,h\rangle \,, \\ &= G_\beta(u) - \beta\langle u,h\rangle + \frac{\beta}{2}\langle h,h\rangle \,, \\ &\geq G_\beta(u) - \beta\langle u,h\rangle \,. \end{aligned} \tag{2.5}$$

Lemma 6.4.1. from [3] implies $G_\beta(u) \geq \frac{\beta}{4}\langle u,u\rangle + \frac{\beta}{4}\sum_{j=1}^d (u_j-2)^2 - d\beta - \ln(d)$ for all $u \in \mathbb{R}^d$. Therefore,

$$\begin{aligned} \tilde{G}_{\beta,h}(u) &\geq \frac{\beta}{4}\langle u,u\rangle + \frac{\beta}{4}\sum_{j=1}^d (u_j-2)^2 - d\beta - \ln(d) - \beta\langle u,h\rangle \ , \\ &= \frac{\beta}{2}\langle u,u\rangle - \beta\sum_{j=1}^d u_j - \ln(d) - \beta\langle u,h\rangle \ . \end{aligned} \tag{2.6}$$

Let $\mathbf{1} = \sum_{j=1}^d \mathbf{e}_j$ and $c(h) = \frac{\beta}{2}\langle h+\mathbf{1}, h+\mathbf{1}\rangle + \ln(d)$. Then

$$\begin{aligned} \tilde{G}_{\beta,h}(u) &\geq \frac{\beta}{2}\langle u,u\rangle - \beta\langle u, h+\mathbf{1}\rangle - \ln(d) \ , \\ &= \frac{\beta}{2}\langle u-(h+\mathbf{1}), u-(h+\mathbf{1})\rangle - \frac{\beta}{2}\langle h+\mathbf{1}, h+\mathbf{1}\rangle - \ln(d) \ , \\ &= \frac{\beta}{2}|u-(h+\mathbf{1})|^2 - c(h) \ , \\ \Rightarrow \tilde{G}_{\beta,h}[u+(h+\mathbf{1})] + c(h) &\geq \frac{\beta}{2}|u|^2 \ . \end{aligned} \tag{2.7}$$

Since $\frac{\beta}{2} > 0$, $\tilde{G}_{\beta,h}[u+(h+\mathbf{1})]+c(h)$ has at least one global minimum point on $\mathbb{R}^d$ by Lemma 2.2. By translation, this implies the same for $\tilde{G}_{\beta,h}$. □

Lemma 2.4. *Let $\beta \in (0,\beta_c)$ and $d=3$. For all $u_1,u_2,u_3 \in \mathbb{R}$ and any $i \in [d]$,*

$$\frac{\beta\cosh(\beta u_i)}{\sum_{j=1}^3 \cosh(\beta u_j)} - \frac{\beta\sinh^2(\beta u_i)}{(\sum_{j=1}^3 \cosh(\beta u_j))^2} < 1 \ . \tag{2.8}$$

When $\beta = \beta_c$,

$$\frac{\beta\cosh(\beta u_i)}{\sum_{j=1}^3 \cosh(\beta u_j)} - \frac{\beta\sinh^2(\beta u_i)}{(\sum_{j=1}^3 \cosh(\beta u_j))^2} \leq 1 \ , \tag{2.9}$$

with equality if and only if $u_1=u_2=u_3=0$.

Proof. Let $u_1,u_2,u_3 \in \mathbb{R}$ and $d=3$. Without loss of generality we set $i=1$ and observe the following

$$\begin{aligned} \frac{\beta\cosh(\beta u_i)}{\sum_{j=1}^3 \cosh(\beta u_j)} - \frac{\beta\sinh^2(\beta u_i)}{(\sum_{j=1}^3 \cosh(\beta u_j))^2} &= \frac{\beta\cosh(\beta u_1)(\sum_{j=1}^3 \cosh(\beta u_j)) - \beta\sinh^2(\beta u_1)}{(\sum_{j=1}^3 \cosh(\beta u_j))^2} \ , \\ &= \frac{\beta[\cosh^2(\beta u_1) - \sinh^2(\beta u_1) + \cosh(\beta u_1)\cosh(\beta u_2) + \cosh(\beta u_1)\cosh(\beta u_3)]}{(\sum_{j=1}^3 \cosh(\beta u_j))^2} \ , \\ &= \frac{\beta[1+\cosh(\beta u_1)(\cosh(\beta u_2)+\cosh(\beta u_3))]}{(\sum_{j=1}^3 \cosh(\beta u_j))^2} \ . \end{aligned} \tag{2.10}$$

Let $x = \cosh(\beta u_1)$ and $y = \cosh(\beta u_2) + \cosh(\beta u_3)$ so that $x \geq 1$ and $y \geq 2$. Then

$$\frac{\beta\cosh(\beta u_i)}{\sum_{j=1}^3 \cosh(\beta u_j)} - \frac{\beta\sinh^2(\beta u_i)}{(\sum_{j=1}^3 \cosh(\beta u_j))^2} = \frac{\beta(1+xy)}{(x+y)^2} \ . \tag{2.11}$$

Recall that $\beta_c = d$ for $d \leq 3$. Hence when $\beta \in (0,\beta_c)$, we have

$$\frac{\beta\cosh(\beta u_i)}{\sum_{j=1}^3 \cosh(\beta u_j)} - \frac{\beta\sinh^2(\beta u_i)}{(\sum_{j=1}^3 \cosh(\beta u_j))^2} < \frac{3(1+xy)}{(x+y)^2} \ . \tag{2.12}$$

In the case $\beta = \beta_c$, we have

$$\frac{\beta \cosh(\beta u_i)}{\sum_{j=1}^{3} \cosh(\beta u_j)} - \frac{\beta \sinh^2(\beta u_i)}{(\sum_{j=1}^{3} \cosh(\beta u_j))^2} = \frac{3(1+xy)}{(x+y)^2} \ . \tag{2.13}$$

Define $q(x,y) = \frac{1}{4}(2x-y)^2 + \frac{3}{4}(y^2-4)$. For all $(x,y) \in [1,\infty) \times [2,\infty)$, we have $y^2 - 4 \geq 0$. So $q(x,y) \geq \frac{1}{4}(0) + \frac{3}{4}(0) = 0$. Therefore

$$\begin{aligned} 0 &\leq \frac{1}{4}(2x-y)^2 + \frac{3}{4}(y^2-4) \ , \qquad (\star) \\ &= \frac{1}{4}(4x^2 - 4xy + y^2) + \frac{3}{4}(y^2-4) \ , \\ &= x^2 - xy + y^2 - 3 \ . \end{aligned}$$

Rearranging gives

$$3xy + 3 \leq x^2 + 2xy + y^2 \ ,$$

and so

$$\frac{3(1+xy)}{(x+y)^2} \leq 1 \ , \tag{2.14}$$

for all $(x,y) \in [1,\infty) \times [2,\infty)$. Hence (2.8) follows from (2.12) and (2.9) follows from (2.13). We will now show that there is equality in (2.9) if and only if $u_1 = u_2 = u_3 = 0$. Let $\beta = \beta_c$ and suppose $u_i = 0$ for all $i \in [d]$. Then

$$\begin{aligned} \frac{\beta \cosh(\beta u_i)}{\sum_{j=1}^{3} \cosh(\beta u_j)} - \frac{\beta \sinh^2(\beta u_i)}{(\sum_{j=1}^{3} \cosh(\beta u_j))^2} &= \frac{3 \cosh(3(0))}{\sum_{j=1}^{3} \cosh(3(0))} - \frac{3 \sinh^2(3(0))}{(\sum_{j=1}^{3} \cosh(3(0)))^2} \ , \\ &= \frac{3}{3} \ , \\ &= 1 \ . \end{aligned} \tag{2.15}$$

Now let $\beta = \beta_c$ and suppose $\frac{\beta \cosh(\beta u_i)}{\sum_{j=1}^{3} \cosh(\beta u_j)} - \frac{\beta \sinh^2(\beta u_i)}{(\sum_{j=1}^{3} \cosh(\beta u_j))^2} = 1$. From (2.13), this implies

$$\frac{3(1+xy)}{(x+y)^2} = 1 \ , \tag{2.16}$$

where $x = \cosh(\beta u_1)$ and $y = \cosh(\beta u_2) + \cosh(\beta u_3)$, so that $x \geq 1$ and $y \geq 2$. From $(\star)$ it follows that

$$\frac{1}{4}(2x-y)^2 + \frac{3}{4}(y^2-4) = 0 \ . \tag{2.17}$$

This forces $y = 2$ and $x = 1$. Therefore $u_1 = u_2 = u_3 = 0$. □

Lemma 2.5. *Let $\beta \in (0, \beta_c]$, $d = 3$ and $h = (\eta_1, \eta_2, \eta_3) \in \mathbb{R}^d$. There exists a unique global minimum point $\bar{v} = (\bar{v}_1, \bar{v}_2, \bar{v}_3)$ of $\tilde{G}_{\beta,h}(x)$. For each $i \in [d]$, $\bar{v}_i \in (0, 1+\eta_i)$ if $\eta_i > 0$, $\bar{v}_i = 0$ if $\eta_i = 0$ and $\bar{v}_i \in (\eta_i - 1, 0)$ if $\eta_i < 0$.*

Proof. Let $\beta \in (0, \beta_c]$ and $d = 3$. Recall the definition of $\tilde{G}_{\beta,h}$ from Lemma 2.3. From Lemma 2.3, $\tilde{G}_{\beta,h}$ has at least one global minimum point. Note that $\tilde{G}_{\beta,h} \in C^\infty$. Then if $\bar{v}$ is a global minimum point of $\tilde{G}_{\beta,h}$ it must satisfy

$$\begin{aligned} \frac{\partial \tilde{G}_{\beta,h}(u)}{\partial u_i}|_{u=\bar{v}} = \beta\left(\bar{v}_i - \frac{\sinh(\beta\bar{v}_i)}{\sum_{j=1}^3 \cosh(\beta\bar{v}_j)} - \eta_i\right) = 0\ , \\ \Rightarrow \bar{v}_i - \frac{\sinh(\beta\bar{v}_i)}{\sum_{j=1}^3 \cosh(\beta\bar{v}_j)} - \eta_i = 0\ , \end{aligned} \tag{2.18}$$

for all $i \in [d]$.

Fix u_2 and $u_3 \in \mathbb{R}$ and define the following function

$$f(u_1) := u_1 - \frac{\sinh(\beta u_1)}{\sum_{j=1}^3 \cosh(\beta u_j)} - \eta_1\ , \tag{2.19}$$

such that $\bar{v}_1$ satisfies $f(\bar{v}_1) = 0$. Let $\eta_1 > 0$. Then we observe for fixed choices of u_2 and u_3

$$f(0) = -\eta_1 < 0\ , \tag{2.20}$$

and

$$\begin{aligned} f(1+\eta_1) &= 1 - \frac{\sinh(\beta(1+\eta_1))}{\cosh(\beta(1+\eta_1)) + \cosh(\beta u_2) + \cosh(\beta u_3)}\ , \\ &> 1 - \tanh(\beta(1+\eta_1))\ , \\ &> 1 - 1\ , \\ &= 0\ . \end{aligned} \tag{2.21}$$

Now suppose $\eta_1 = 0$. Trivially, for any fixed u_2 and u_3,

$$f(0) = 0\ . \tag{2.22}$$

Finally, suppose $\eta_1 < 0$. For fixed choices of u_2 and u_3, using the fact that sinh is odd we have

$$\begin{aligned} f(\eta_1 - 1) &= -1 + \frac{\sinh(\beta|\eta_1 - 1|)}{\cosh(\beta|\eta_1 - 1|) + \cosh(\beta u_2) + \cosh(\beta u_3)}\ , \\ &< -1 + \tanh(\beta|\eta_1 - 1|)\ , \\ &< -1 + 1\ , \\ &= 0\ , \end{aligned} \tag{2.23}$$

and

$$f(0) = -\eta_1 > 0\ . \tag{2.24}$$

Since f is a smooth function, we have shown that f has at least one root for any $\eta_1 \in \mathbb{R}$. To prove the uniqueness of this solution, we will show that for any choices of u_2 and u_3 and any $\eta_1 \in \mathbb{R}$, f is strictly monotone.

Consider the derivative

$$f'(u_1) = -\frac{\beta\cosh(\beta u_1)}{\sum_{j=1}^3 \cosh(\beta u_j)} + \frac{\beta\sinh^2(\beta u_1)}{(\sum_{j=1}^3 \cosh(\beta u_j))^2} + 1\ . \tag{2.25}$$

When $\beta \in (0, \beta_c)$, Lemma 2.4 tells us that for any fixed choices of u_2 and u_3 and for all $u_1 \in \mathbb{R}$,

$$\frac{\beta\cosh(\beta u_1)}{\sum_{j=1}^3 \cosh(\beta u_j)} - \frac{\beta\sinh^2(\beta u_1)}{(\sum_{j=1}^3 \cosh(\beta u_j))^2} < 1\ .$$

It follows that

$$
\begin{aligned}
-\frac{\beta\cosh(\beta u_1)}{\sum_{j=1}^{3}\cosh(\beta u_j)} + \frac{\beta\sinh^2(\beta u_1)}{(\sum_{j=1}^{3}\cosh(\beta u_j))^2} &> -1\ , \\
f'(u_1) = -\frac{\beta\cosh(\beta u_1)}{\sum_{j=1}^{3}\cosh(\beta u_j)} + \frac{\beta\sinh^2(\beta u_1)}{(\sum_{j=1}^{3}\cosh(\beta u_j))^2} + 1 &> 0\ .
\end{aligned}
\tag{2.26}
$$

So f is an increasing function of u_1 for any fixed choices of u_2 and u_3 when $\beta \in (0, \beta_c)$.

Now consider $\beta = \beta_c$. From Lemma 2.4, (2.26) holds unless $u_1 = u_2 = u_3 = 0$, in which case $f'(u_1) = 0$. So for any fixed choices of u_2 and u_3 where at least one of u_2 and u_3 is non-zero, f is an increasing function of u_1 with a positive derivative. If $u_2 = u_3 = 0$, then f is increasing on u_1 and instantaneously stationary at $u_1 = 0$. In any case f is strictly monotone so its root v_1 must be unique. From the calculations above, $\bar{v}_1 \in (0, 1 + \eta_1)$ when $\eta_1 > 0$, $\bar{v}_1 \in (\eta_1 - 1, 0)$ when $\eta_1 < 0$. When $\eta_1 = 0$, $\bar{v}_1 = 0$. By symmetry, the same arguments hold for $\bar{v}_2$ and $\bar{v}_3$.

Since $\tilde{G}_{\beta,h}$ has at least one global minimum point by Lemma 2.3 and $\bar{v}$ is the only point satisfying (2.18), $\bar{v}$ is the unique global minimum point of $\tilde{G}_{\beta,h}$.

□

3 Further Study

In this report we were able to specify the equilibrium macrostate for the case $d = 3$ and $\beta \in (0, \beta_c]$ with non-zero field. A natural next step would be to further understand the $d = 3$ case by identifying the equilibrium macrostates when $\beta \in (\beta_c, \infty)$ with non-zero field. In the $d = 1$ case, $G_{\beta,h}$ may have up to three stationary points depending on the magnitude of h when $\beta \in (\beta_c, \infty)$ as shown in Figure 2. The function has a unique global minimum point when the field is non-zero.

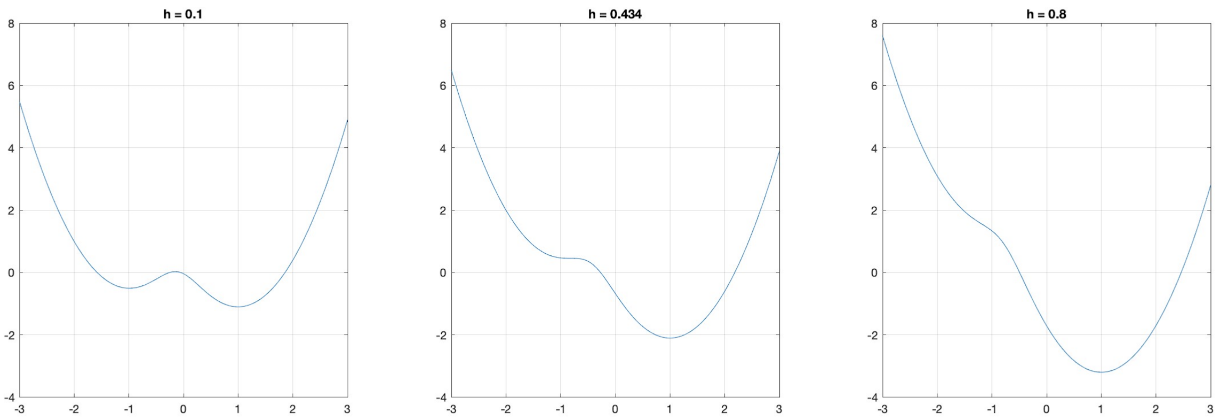

Figure 2: $G_{\beta,h}$ plotted for $\beta = 3$ and various values of h.

As such, extending the $\beta \in (0, \beta_c]$ case to $d = 3$ will likely be less straightforward than the case studied in this report. Lemmas 2.1 - 2.3 hold in this scenario, meaning that the existence of at least one global minimum point of $\tilde{G}_{\beta,h}$ is known. We expect the multivariate function to have more than one local minimum which will need to be accounted for when determining uniqueness of a global minimum and dependence of its position on h.

Furthermore, using the results from this report we may be able to identify the critical exponent δ when $d = 3$. To understand this exponent we first introduce the specific Gibbs free energy, which is given by

$$\psi(\beta, h) := \lim_{n\to\infty} \frac{1}{n} \log Z_n(\beta, h) \,, \tag{3.1}$$

where $Z_n(\beta, h)$ is the partition function. The Hubbard-Stratonovich transformation and Laplace's method may be used to show the following equivalence [2],

$$\psi(\beta, h) = \inf_{u\in\mathbb{R}^d} \tilde{G}_{\beta,h}(u). \tag{3.2}$$

We then introduce another quantity called the specific magnetisation, which is defined as

$$M(\beta, h) := \frac{\partial}{\partial h}\psi(\beta, h). \tag{3.3}$$

As $||h|| \to 0$, we say that $M(\beta_c, h) \asymp ||h||^{\frac{1}{\delta}}$. Since the existence and uniqueness of $\inf_{u\in\mathbb{R}^d} \tilde{G}_{\beta,h}(u)$ has been proven in this report when $\beta = \beta_c$, we may use (2.18) and (3.2) to specify the Gibbs free energy and therefore deduce the critical exponent δ. In the $d = 3$ case, we expect that $\delta = 5$ [2].

4 Conclusion

By deriving and minimising a function $\tilde{G}_{\beta,h}$, we were able to prove the existence and uniqueness of an equilibrium macrostate of the Face-Cubic model when $d = 3$ and $\beta \in (0, \beta_c]$ with non-zero field. By bounding $\tilde{G}_{\beta,h}$ below by a convex quadratic, we were able to show existence of a global minimum point. In order to demonstrate uniqueness, we analysed the partial derivatives of $\tilde{G}_{\beta,h}$. By considering them as functions of one variable, fixing the other variables to any values in $\mathbb{R}$ and demonstrating the strict monotonicity of these functions, we proved the uniqueness of each component of a global minimum vector for given h. For an external field $h = (\eta_1, \eta_2, \eta_3) \in \mathbb{R}^3$, we were able to place bounds on the equilibrium macrostate $\bar{v} = (\bar{v}_1, \bar{v}_2, \bar{v}_3)$. We showed that for each $i \in \{1, 2, 3\}$, $\bar{v}_i \in (0, 1 + \eta_i)$ if $\eta_i > 0$, $\bar{v}_i = 0$ if $\eta_i = 0$ and $\bar{v}_i \in (\eta_i - 1, 0)$ if $\eta_i < 0$.

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