CURVATURE AND STATISTICS

BY YU WANG

A dissertation submitted to the
Graduate School—New Brunswick
Rutgers, The State University of New Jersey
in partial fulfillment of the requirements
for the degree of
Doctor of Philosophy
Graduate Program in Mathematics

Written under the direction of
Michael Kiessling
and approved by

New Brunswick, New Jersey
October, 2013

ABSTRACT OF THE DISSERTATION

Curvature and Statistics

by Yu Wang

Dissertation Director: Michael Kiessling

This thesis consists of two parts: In part I we apply the statistical mechanics techniques to a generalization of the prescribed Q-curvature problem, especially on the D-dim sphere $\mathbb{S}^{\mathrm{D}}$. We introduce a coupling constant c on top of the configurational canonical ensemble and study the weak convergence of this new canonical ensemble. In this part, the Q-curvature does not change sign. In part II the statistical mechanics technique is generalized to the prescribed Q-curvature problem with sign-change, while the mechanical interpretation will be lost. We decompose a single differential equation into a system of two differential equations, and the statistical mechanics technique can be applied to each equation.

Acknowledgements

I would like to express my sincere gratitude to my advisor Prof. Michael Kiessling for his continuous support, meticulous guidance and numerous patience during my Ph.D study. Without his help, the thesis would not be possible.

Besides, I would like to thank the other members of my thesis committee, Prof. Sagun Chanillo, Marcello Lucia, A. Shadi Tahvildar-Zadeh, for their advice in the preparation and review of my thesis.

I would also like to thank Prof. Anders Buch, Richard Falk, Zhengchao Han, Xiaojun Huang, Joel Lebowitz, Young-Ju Lee, Yanyan Li, Jian Song, Richard Wheeden, Doron Zeilberger, and other faculty members in the math department for their help and encouragement during my years in Rutgers. Moreover, I want to thank Prof. Terence Butler, Amy Cohen-Corwin, Michael Weingart, for their valuable suggestions in my teaching performance.

I here also thank my fellow graduate students and friends, Ke Wang, Tianling Jin, Hui Wang, Ming Xiao, Tian Yang, Jinwei Yang, Yunpeng Wang, Yuan Yuan, Yuan Zhang, Ming Shi, Jin Wang, Nan Li, Biao Yin, Xukai Yan, Bin Guo, Zhuohui Zhang, Lihua Huang, Zahra Aminzare, Edward Chien, Simao Herdade, Hui Li, and many others for accompanying me through my years at Rutgers.

Last but not least, I would like to express my appreciation towards my family for their love and support in my life.

Dedication

This thesis is dedicated to my dear parents, Guoqin Wang and Shichen Yu.

Table of Contents

Chapter 1

Introduction

Let a 2-dim surface $S \subset \mathbb{R}^3$ be parametrized by $\vec{r} = \vec{r}(s,t)$ with (s,t) in some domain $\Lambda \subset \mathbb{R}^2$. Let $\mathcal{W}$ denote the Weingarten transform from the tangent space of S at P_0 to itself, defined by (cf. [PeCh02]):

$$\mathcal{W}(a\vec{r}_s + b\vec{r}_t) = -(a\vec{n}_s + b\vec{n}_t), \tag{1.1}$$

here $\vec{n}$ is the unit vector in the direction of $\vec{r}_s \times \vec{r}_t$ at P_0. The Weingarten transform does not rely on the choice of parametrization for the surface S, and it has the coefficient matrix with respect to the basis $\{\vec{r}_s, \vec{r}_t\}$ as

$$\frac{1}{EG - F^2} \begin{pmatrix} LG - MF & ME - LF \\ MG - NF & NE - MF \end{pmatrix}, \tag{1.2}$$

where E, F and G are the coefficients in the first fundamental form of S, and L, M and N are the coefficients in the second fundamental form of S. The product of the two eigenvalues of $\mathcal{W}$ is called the *Gaussian curvature* K, which can be calculated as

$$K = \frac{LN - M^2}{EG - F^2}. \tag{1.3}$$

According to Gauss' "Theorema Egregium" or notable theorem, the Gaussian curvature is independent of the embedding of the surface in higher dimension spaces, i.e. the Gaussian curvature is an intrinsic property of the surface. Hence, by making smart choices of parametrization of the surface, K can have simpler expressions. In particular, the so called "isothermal[1] parametrization" $(s,t) \to (x_1, x_2)$ yields $E = G$ and $F = 0$,

[1]The coordinates leading to (1.5) are called "isothermal coordinates", or sometimes "isothermic parameters". This terminology goes back to Gabriel Lamé who used the phrase "thermometric parameters".

such that K is neatly expressed by

$$K = -\frac{1}{2E}(\partial_{x_1}^2 \ln E + \partial_{x_2}^2 \ln E); \tag{1.4}$$

the pair of isothermal coordinates (x_1, x_2) plays the role of two Cartesian coordinates. Furthermore, set $2u = \ln E$, then

$$K = -e^{-2u}\Delta_{\mathbb{R}^2} u \tag{1.5}$$

The specific local coordinates chosen above correspond to the surface metric $g = e^{2u}g_0$, conformal to the 2-dim standard Euclidean metric $g_0 = \mathrm{d}x_1^2 + \mathrm{d}x_2^2$. Such surfaces are called conformally flat. Similarly, a conformal deformation of the 2-dim standard sphere $\mathbb{S}^2 \subset \mathbb{R}^3$ also corresponds to a metric $g = e^{2u}g_0$, and here (with some abuse of notations) $g_0 = \mathrm{d}x_1^2 + \mathrm{d}x_2^2 + \mathrm{d}x_3^2$ is the 3-dim standard metric restricted to $\mathbb{S}^2$. The Gaussian curvature K_g of $(\mathbb{S}^2, g)$ is calculated by the following formula, with the function u given:

$$K_g = \frac{1 - \Delta_{\mathbb{S}^2} u}{e^{2u}} \tag{1.6}$$

here $1 (= K_{g_0})$ is the Gaussian curvature of the standard metric. For a more general 2-dim Riemannian manifold (M, g_0), an analogous formula can be derived:

$$K_g = \frac{K_{g_0} - \Delta_M u}{e^{2u}} \tag{1.7}$$

here K_g is the Gaussian curvature for the metric g which is conformal to the metric g_0, and K_{g_0} is the Gaussian curvature for the metric g_0.

Incidentally, we here mention already that in recent years also higher order curvatures, the so called Q-curvatures, which are related to conformally covariant higher order (pseudo)partial differential operators, the so-called GJMS operators [GJMS92], have been considered. rf.[Cha08] , etc. Specifically, in 4-dim, the prescribed Q-curvature [Cha96, Bra87] reads as

$$Q = [-\frac{1}{6}\Delta R + \frac{1}{6}R^2 - \frac{1}{2}R^{ab}R_{ab}] \tag{1.8}$$

where R is the scalar curvature of the metric g, and the GJMS operator is known as the Paneitz operator, given by

$$P = \Delta^2 + div(\frac{2}{3}RI - 2Ric)\mathrm{d}, \tag{1.9}$$

see [Pan08, Cha96]. There will be more on this in a moment.

Continuing with the 2-dim setting, we note that the above formulas (1.5), (1.6) allow us to compute the Gaussian curvature K_g if the conformal deformation $g_0 \to g = e^{2u} g_0$ is known. The inverse problem is to find a conformal deformation, i.e. to find u, which results in a surface with a desired Gaussian curvature K_g. This is known as the "prescribed Gaussian curvature problem": Given a function K, does there exist a function u such that the metric $g = e^{2u} g_0$ has Gaussian curvature $K_g = K$? To answer this question, one has to solve equations (1.5) and (1.6), or in general (1.7), which are now nonlinear partial differential equations for the unknown u. This is equivalent to look for the existence of solutions to the equation:
in the conformally flat case,

$$\Delta_{\mathbb{R}^2} u + K e^{2u} = 0; \tag{1.10}$$

in the conformally round case,

$$\Delta_{\mathbb{S}^2} u + K e^{2u} = 1; \tag{1.11}$$

and more generally,

$$\Delta_{g_0} u + K e^{2u} = K_{g_0}; \tag{1.12}$$

all these equations have to be supplemented by suitable boundary conditions for u. Alternatively, suppose $\bar{u}$ is a harmonic function satisfying the required boundary condition, then the difference $u - \bar{u}$ should satisfy the same type of equation (1.10), (1.11) or (1.12) as that of u but with a zero boundary condition, and with K changed into $\bar{K} = K e^{2\bar{u}}$.

The 2-dim prescribed Gaussian curvature problem has an analogue in D-dim, the prescribed Q-curvature problem. The prescribed Q-curvature problem, on $\mathbb{S}^4$ in particular reads

$$Pu = Q e^{4u} - 6. \tag{1.13}$$

In general, on the D-dim sphere $\mathbb{S}^{\mathrm{D}}$, the prescribed Q-curvature equation is

$$Pu = Q e^{\mathrm{D}u} - (\mathrm{D} - 1)! \tag{1.14}$$

while the conformal covariant operator is defined by

$$P_{\mathrm{D}} = \begin{cases} \prod_{k=0}^{\frac{\mathrm{D}-2}{2}} (-\Delta + k(\mathrm{D} - k - 1)) & \text{when D is even} \\ (-\Delta + (\frac{\mathrm{D}-1}{2})^2)^{\frac{1}{2}} \prod_{k=0}^{\frac{\mathrm{D}-3}{2}} (-\Delta + k(\mathrm{D} - k - 1)) & \text{when D is odd} \end{cases} \tag{1.15}$$

It has been studied, rf. [Kie00, Pan08, Cha96, Bra87, Cha08, Li95B, Li96], etc. We will come back to this at the end of this introduction.

Of course, there is an even vaster literature on the prescribed Gaussian curvature problems. Thus the conformally flat case was studied in [Sat72, Aub79, Ni82, McO85, Avi86, ChNi91A, ChNi91B, ChKi94, ChLi97, ChLi98A, ChLi98B, ChKi00]. The conformally round case is the well-known Nirenberg problem; see [Mos71, Oba71, Mos73, KaWa74, Ono82, Bra87, ChYa87, ChYa88, Han90, CaLo92, Bec93, Li95B, Ma98, Kie00, KiWa12]. More generally, the prescribed Gaussian curvature problems are studied on Riemannian manifolds, [Li95A, DJLW97, Tar97].

Although the prescribed Gaussian curvature problems, in particular the Nirenberg problem, are PDE problems coming from the area of differential geometry, the name "isothermal coordinates" indicates a connection with the science of thermodynamics. Indeed, consider the self-gravitating ideal gas in thermal and mechanical equilibrium. The gravitational potential satisfies the following Poisson's equation

$$\Delta\Phi = 4\pi G\rho \tag{1.16}$$

where ρ is the mass density, assuming that Φ is continuously differentiable without specific boundary condition and decreases like $-G\frac{M}{r}$ outside of the domain, with $M = \int_\Lambda \rho$. Besides, the gravitational force density is equal to $\rho(-\nabla\Phi)$. When the gas reaches mechanical equilibrium, the pressure gradient and the gravitational force density should add up to zero, i.e.,

$$-\nabla P - \rho\nabla\Phi = 0 \tag{1.17}$$

The above two equations (1.16) and (1.17) with three unknowns Φ, ρ and P don't make a closed system. We postulate the ideal gas law

$$P = \rho kT \tag{1.18}$$

where T is the thermodynamic temperature in Kelvins. Here, T is a constant because the gas is in thermal equilibrium. This makes a complete system for Φ, ρ and P.

We now eliminate the variable P by substituting (1.18) into (1.17), and get

$$-kT\nabla\rho - \rho\nabla\Phi = 0 \tag{1.19}$$

then after rearrangement,

$$\frac{\nabla\rho}{\rho} = -\frac{1}{kT}\nabla\Phi \tag{1.20}$$

the left side above is equal to $\nabla \ln \frac{\rho}{\rho_0}$, where ρ_0 is a constant with the dimension of mass density so that $\frac{\rho}{\rho_0}$ is dimensionless. Thus $\ln \frac{\rho}{\rho_0} + \frac{\Phi}{kT}$ is a constant, denoted by θ, i.e.,

$$\rho = \rho_0 e^{\theta - \frac{\Phi}{kT}}. \tag{1.21}$$

Plug (1.21) into (1.16) and obtain the so-called isothermal Lane-Emden equation:

$$\Delta\Phi = 4\pi G\rho_0 e^{\theta - \frac{\Phi}{kT}}. \tag{1.22}$$

If we rename the exponent $-\frac{\Phi}{kT}$ on the right side as $2u$, then an equation of u is derived

$$-\Delta u = \frac{2\pi G\rho_0}{kT} e^{\theta + 2u}. \tag{1.23}$$

Denote the constant $\frac{2\pi G\rho_0}{kT} e^{\theta}$ on the right hand side of the equation by K, and then the equation looks like

$$-\Delta u = K e^{2u}, \tag{1.24}$$

the same form as (1.10), except for the difference in dimensions. Notice that the physics here is done in a 3-dim domain, but nothing prevents us from considering (1.10) as the 2-dim caricature of the 3-dim real world.

Thus, two different fields of science, geometry and thermodynamics, contain problems that lead to the same equations. This leads to the following interesting perspective: In the 19th century, mathematicians and physicists began to implement atomistic ideas to derive the known laws of continuum physics, in particular, thermodynamics, from deeper physical principles. According to these ideas, the formulas of continuum physics, using partial differential equations, are approximate descriptions of an underlying atomistic reality, governed by finitely many ordinary differential equations, namely Newton's equations of motion of N atoms. Formally at least, the continuum laws should emerge in the limit as $N \to \infty$ of a system containing N atoms. This means if these derivations can be proved rigorously, they not only substantiate the physical understanding of the world, but also provide an alternative way of looking at partial differential equations.

To see this more clearly, we revisit the ideal gas model with N being the total number of particles in the domain (or a "container"), and let $k = \frac{k_{\mathrm{B}}}{m}$, where k_{B} is the Boltzmann's constant, m a suitable mass unit, and $\nu = \frac{\rho}{m}$ the number of particles per volume. Then the equation (1.21) of ρ turns into an equation of ν,

$$\nu = \nu_0 e^{\theta - \frac{m\Phi}{k_{\mathrm{B}}T}}. \tag{1.25}$$

Since now the integral $\int \nu dV$ taken over the domain is equal to N, we have

$$N = \nu_0 e^{\theta} \int e^{-\frac{m\Phi}{k_{\mathrm{B}}T}}, \tag{1.26}$$

and (1.25) transforms into

$$\nu = N \frac{e^{-\frac{m\Phi}{k_{\mathrm{B}}T}}}{\int e^{-\frac{m\Phi}{k_{\mathrm{B}}T}}}. \tag{1.27}$$

Plug (1.27) into (1.16) and obtain

$$\Delta\Phi = 4\pi G m N \frac{e^{-\frac{m\Phi}{k_{\mathrm{B}}T}}}{\int e^{-\frac{m\Phi}{k_{\mathrm{B}}T}}} \tag{1.28}$$

Note that this equation is different from its counterpart with an extra normalization denominator. Yet if we regard κ as a rescaling of K with the relation $\kappa = K \int e^{2u} \mathrm{d}^2 x$ in (1.10), then an equation of the form (1.28) shows up. Of course, (1.28) is still a continuum equation in appearance, but now it has a different interpretation, namely as the continuum *approximation* to a discrete distribution with N atoms. In concert with (1.23), it reveals the N-scaling in which the underlying discrete distribution should converge to the proper continuum equations[2], namely

$$\Phi = N\phi \tag{1.29}$$

[2]Later it will prove convenient to rescale $\Phi = (N-1)\phi$ and $T = (N-1)\Theta$.

and

$$T = N\Theta, \tag{1.30}$$

both in the leading order N, where ϕ and Θ are "$O(1)$" quantities.

Among the first rigorous results in this direction was the work [MeSp82] by Messer and Spohn. They treated the case of bounded Lipschitz continuous pairwise interactions, and derived an integral equation which is equivalent to a regularized isothermal Lane-Emden equation.

Later, this technique was generalized to the point vortex interactions with logarithmic singularities, independently by [CLMP92] and [Kie93], and further developed in [CLMP95] and [KiLe97]. It can be applied to study Nirenberg's problem in 2-dim, see [Kie00, Kie11, KiWa12], etc.

To illustrate how the idea works in 2-dim, we follow [Kie11]. In 2-dim Newtonian physics, points on the 2-dim sphere can be interpreted as particles that move according to the Newtonian equation of motion with pairwise logarithmic interactions, i.e.,

$$\ddot{\mathbf{s}}_k(t) + |\dot{\mathbf{s}}_k(t)|^2 \mathbf{s}_k(t) = -\gamma \sum_{1\le j\le N, j\neq k} \Pi^{\perp}_{\mathbf{s}_k(t)} \frac{\mathbf{s}_k(t) - \mathbf{s}_j(t)}{|\mathbf{s}_k(t) - \mathbf{s}_j(t)|^2} \tag{1.31}$$

here $\Pi^{\perp}_{\mathbf{s}_k(t)} = 1 - \mathbf{s}_k(t) \otimes \mathbf{s}_k(t)$ is the projection from[3] $\mathbb{R}^3$ onto the tangent space to $\mathbb{S}^2$ at $\mathbf{s}_k(t) \in \mathbb{S}^2 \subset \mathbb{R}^3$. Here, $\gamma = +1$ is for the gravitational interactions, and $\gamma = -1$ for the electrical interactions. The mechanical energy of the system,

$$H^{(N)}(\mathbf{s}_1, \mathbf{p}_1; \dots; \mathbf{s}_N, \mathbf{p}_N) = \sum_{1\le j\le N} \frac{1}{2}|\mathbf{p}_j|^2 + \frac{1}{2}\sum\sum_{j\neq k} \gamma U(|\mathbf{s}_j - \mathbf{s}_k|), \tag{1.32}$$

is preserved, with the particles located at $(\mathbf{s}_1, \dots, \mathbf{s}_N)$ in the configurational space $\Lambda^N = (\mathbb{S}^2)^N$ and their momenta as $(\mathbf{p}_1, \dots, \mathbf{p}_N) \in \prod_k (T^*_{\mathbf{s}_k}\mathbb{S}^2) \subset \mathbb{R}^{3N}$. As the number of particles increases, there is no way for us to know the exact state of each specific particle, but by looking at an ensemble of systems all with fixed energy E, the so-called *microcanonical ensemble*, we can determine the "typical" macrostate of the system as

[3] We emphasize that $\mathbb{R}^3$ here is *not* the physical space. The embedding $\mathbb{S}^2 \subset \mathbb{R}^3$ is for mathematical convenience only.

a whole. More precisely, if the law of large numbers holds, then the empirical measures

$$\begin{aligned}\underline{\Delta}^{(1)}_{X_t^{(N)}}(\mathbf{s},\mathbf{p}) &= \tfrac{1}{N}\sum_{1\le j\le N}\delta_{s_j(t)}(\mathbf{s})\delta_{p_j(t)}(\mathbf{p})\\ \underline{\Delta}^{(2)}_{X_t^{(N)}}(\mathbf{s},\mathbf{p};\mathbf{s}',\mathbf{p}') &= \tfrac{2}{N(N-1)}\sum\sum_{1\le j\ne k\le N}\delta_{s_j(t)}(\mathbf{s})\delta_{s_k(t)}(\mathbf{s}')\delta_{p_j(t)}(\mathbf{p})\delta_{p_k(t)}(\mathbf{p}');\end{aligned} \tag{1.33}$$

and higher order U-statistics $\underline{\Delta}^{(n)}_{X_t^{(N)}}(\mathbf{s}_1,\mathbf{p}_1;\ldots;\mathbf{s}_n,\mathbf{p}_n)$ will each converge in probability to some "typical" distribution $\varrho^{(n)}_{typ}$ i.e.

$$Prob\Big(Dist(\underline{\Delta}^{(n)}_{X_t^{(N)}},\varrho^{(n)}_{typ})>\delta\Big)\to 0,\ \text{as}\, N\to\infty, \forall\delta>0 \tag{1.34}$$

More generally, the typical state does not have to be unique. It can even be an orbit $\mathcal{O}[\varrho^{(n)}_{typ}]$, so that the above equation becomes

$$Prob(Dist(\underline{\Delta}^{(n)}_{X_t^{(N)}},\mathcal{O}[\varrho^{(n)}_{typ}])>\delta)\to 0,\ \text{as}\, N\to\infty, \forall\delta>0 \tag{1.35}$$

The question is now how to prove the law of large numbers and what specifically it says for the microcanonical ensemble.

The *microcanonical ensemble* is a family $\{(\mathbf{S}^{(N)}_k,\mathbf{P}^{(N)}_k)|k\in\mathbb{N}\}$ of i.i.d. (independent and identically distributed) copies of a random vector $(\mathbf{S}^{(N)},\mathbf{P}^{(N)})$ taking values $(S^{(N)},P^{(N)})\in(T^*\mathbb{S}^2)^N\subset\mathbb{R}^{6N}$, with stationary[4] single-system probability measure

$$\mathrm{d}\mu^{(N)}_{\mathcal{E}} = {\Omega'_N}^{-1}(\mathcal{E})\delta\big(\mathcal{E}-H^{(N)}\big)\mathrm{d}^2p^N\mathrm{d}^2\underline{\alpha}^N, \tag{1.36}$$

which also defines the *microcanonical ensemble partition function*, as

$$\Omega'_N(\mathcal{E}) = \int\int\delta\Big[\mathcal{E}-H^{(N)}\big(S^{(N)},P^{(N)}\big)\Big]\,\mathrm{d}^2p^N\mathrm{d}^2\underline{\alpha}^N; \tag{1.37}$$

with $\mathrm{d}^2\underline{\alpha}=\frac{1}{4\pi}\mathrm{d}^2\alpha$, and $\mathrm{d}^2\alpha$ the standard uniform measure on $\mathbb{S}^2$. Besides, Ω'_N means the derivative of

$$\Omega_N(\mathcal{E}) = \int\int\chi_{\{H^{(N)}(S^{(N)},P^{(N)})<\mathcal{E}\}}\mathrm{d}^2p^N\mathrm{d}^2\underline{\alpha}^N \tag{1.38}$$

with respect to $\mathcal{E}$, where χ_B is the characteristic function of the Borel set $B\subset(\mathbb{S}^2)^N$.

Indeed, when the Hamiltonian $H^{(N)}$ is fixed to some value $\mathcal{E}$, several main results for the typical distribution have been proved in [Kie11]:

[4] Stationary w.r.t. the flow generated by the Hamilton function $H^{(N)}(S^{(N)})$.

Theorem 1. *For N large enough, the ensemble entropy defined by $\ln \Omega'_N(\mathcal{E})$ has the asymptotic behavior*[5]

$$\ln \Omega'_N(N^2\varepsilon) = N\mathscr{S}(\varepsilon) + o(N), \tag{1.39}$$

with ε independent of N.

The term $\mathscr{S}$ is the so-called "entropy per particle", which will be studied in the next chapter in detail, and is characterized by the maximizers of the following entropy variational principle, see [Kie11]:

Theorem 2. *The entropy per particle $\mathscr{S}$ is equal to the maximum of an entropy variational principle $-\mathscr{H}_{\mathrm{B}}(\rho)$, i.e.,*

$$\mathscr{S}(\varepsilon) = -\mathscr{H}_{\mathrm{B}}(\rho_\varepsilon) \tag{1.40}$$

where ρ_ε is a minimizer of the (negative)[6] *entropy functional $\mathscr{H}_{\mathrm{B}}$, defined by*

$$\mathscr{H}_{\mathrm{B}}(\rho) = \int\int \rho(s,p)\ln\rho(s,p)\mathrm{d}^2p\mathrm{d}^2\underline{\alpha}(s), \tag{1.41}$$

over the set $\mathfrak{A}_\varepsilon = \{\rho \in (\mathfrak{P}\cap\mathfrak{L}^1\ln\mathfrak{L}^1)(T^*\mathbb{S}^2, \mathrm{d}^2p\mathrm{d}^2\underline{\alpha}) : \mathcal{E}(\rho) = \varepsilon\}$. Here,

$$\mathcal{E}(\rho) = \iint \frac{1}{2}|p|^2\rho(s,p)\mathrm{d}^2p\mathrm{d}^2\alpha + \iiiint \frac{1}{2}\gamma U(|s,s'|)\rho(s,p)\rho(s',p')\mathrm{d}^2p\mathrm{d}^2\alpha\mathrm{d}^2p'\mathrm{d}^2\alpha' \tag{1.42}$$

Furthermore, the minimizers of $\mathscr{H}_{\mathrm{B}}$ satisfy the Euler-Lagrange equation

$$\rho(s) = \frac{e^{-\beta\gamma\int U(s,s')\rho(s')\mathrm{d}^2\alpha(s')}}{\int e^{-\beta\gamma\int U(s,s')\rho(s')\mathrm{d}^2\alpha(s')}\mathrm{d}^2\alpha(s)} \tag{1.43}$$

with U being the Green's function of the Laplace-Beltrami operator on $\mathbb{S}^2$, and β the Lagrange multiplier for the constraint

$$\mathcal{E}(\rho) = \varepsilon. \tag{1.44}$$

---

[5] *In statistical physics, the microcanonical ensemble measure often has a factor $\frac{1}{N!}$ in the front to eliminate the overcounting from labeling, and correspondingly, the asymptotic behavior of $\ln\Omega'_N(\mathcal{E})$ will have an extra term $-N(\ln N - 1)$.*

[6] *The term "entropy" has different signs in physics and probablity: while physicists define "entropy" as $\ln\Omega$ in units of Boltzmann's constant k_{B}, mathematicians and statisticians prefer $-\int f\ln f$ which is the negative of the physical definition.*

The next result relates the minimizers of $\mathscr{H}_{\mathrm{B}}$ (or equivalently, the maximizers of $-\mathscr{H}_{\mathrm{B}}$) to the typical distribution of the microcanonical ensemble measure, see [Kie11]:

Theorem 3. *Suppose the (negative) entropy functional $\mathscr{H}_{\mathrm{B}}(\rho)$ has a unique minimizer ρ_ε. For any fixed positive integer n, the sequence of the n-th marginal measure of $\mu^{(N)}_{N(N-1)\varepsilon}$, denoted by ${}^{(n)}\mu^{(N)}_{N(N-1)\varepsilon}$, converges, up to the extraction of a subsequence, in probability to the tensor product of ρ_ε, i.e.,*

$$\lim_{N\to\infty} {}^{(n)}\mu^{(N)}_{N(N-1)\varepsilon} = \rho_\varepsilon^{\otimes n} \tag{1.45}$$

In general, $\mathscr{H}_{\mathrm{B}}(\rho)$ can have a family of minimizers, then the sequence ${}^{(n)}\mu^{(N)}_{N(N-1)\varepsilon}$ converges, modulo the extraction of a subsequence, to a superposition of these maximizers, namely,

$$\lim_{N\to\infty} {}^{(n)}\mu^{(N)}_{N(N-1)\varepsilon} = {}^{(n)}\mu_\varepsilon = \int_{\mathfrak{P}(\mathbb{S}^2)} \zeta^{\otimes n}\nu(d\zeta|\mu_\varepsilon) \tag{1.46}$$

where the measure $\nu(d\zeta|\mu_\varepsilon)$ for the convex decomposition of ${}^{(n)}\mu_\varepsilon$ is concentrated on the set of minimizers of $\mathscr{H}_{\mathrm{B}}$ on $\mathfrak{A}_\varepsilon$.

In the case that $\nu(d\zeta|\mu_\varepsilon)$ is not a singleton but a convex linear combination of maximizers of the entropy functional $-\mathscr{H}_{\mathrm{B}}$, the "implicitly defined" typical distribution can be only one of these maximizers.

Remark 1. *For a detailed explanation of "convex decomposition" into product measures, the readers is refered to the references [deF37, Dyn53, HeSa55].*

Among these results, we take a look specifically at the equation (1.43) of ρ. Apply the substitution $2u = -\beta\gamma\int U(s,s')\rho(s')\mathrm{d}^2\alpha'$ so that the equation turns into an equation for u:

$$-\Delta u = \tfrac{1}{2}\beta\gamma\frac{e^{2u}}{\int e^{2u}\mathrm{d}^2\alpha} - \frac{1}{4\pi} \tag{1.47}$$

with the same form as the equation of the prescribed Gaussian curvature problem. Here, of course, the Gaussian curvature $K = \dfrac{\beta\gamma}{2\int e^{2u}\mathrm{d}^2\alpha}$ is constant, and $K > 0$ for $\gamma = 1$ and $K < 0$ for $\gamma = -1$.

The microcanonical ensemble is tricky and difficult to deal with, and it may look like "magic" how (1.47) emerged from (1.36). However, the derivation becomes more transparent if we shift the problem to the *canonical* level — possibly with some loss of information — by applying the bilateral Laplace transform to the microcanonical ensemble partition function (1.37). Taking $\frac{1}{N-1}\beta$ as the conjugate variable of $\mathcal{E}$, we obtain the canonical ensemble partition function

$$\begin{aligned}
&\int_{\mathbb{R}} e^{-\frac{1}{N-1}\beta\mathcal{E}}\Omega'_N(\mathcal{E})\mathrm{d}\mathcal{E} \\
=\ &\int_{\mathbb{R}} e^{-\frac{1}{N-1}\beta\mathcal{E}} \int_{(\mathbb{S}^2)^N}\int_{\prod\limits_k (T^*_{s_k}\mathbb{S}^2)} \delta\Big[\mathcal{E} - H^{(N)}\big(S^{(N)}, P^{(N)}\big)\Big]\,\mathrm{d}^2p^N\mathrm{d}^2\underline{\alpha}^N\mathrm{d}\mathcal{E} \\
=\ &\int_{(\mathbb{S}^2)^N}\int_{\prod\limits_k (T^*_{s_k}\mathbb{S}^2)} e^{-\frac{1}{N-1}\beta\left(\sum\limits_j \frac{1}{2}|p_j|^2 + \frac{1}{2}\sum\sum\limits_{j\neq k}\gamma U(|\mathbf{s}_j - \mathbf{s}_k|)\right)}\mathrm{d}^2p^N\mathrm{d}^2\underline{\alpha}^N
\end{aligned} \tag{1.48}$$

The last double integral can be factored into two integrals–one in terms of the momentum p, the other in term of the position s. The former part can be calculated explicitly,

$$\int_{\prod\limits_k (T^*_{s_k}\mathbb{S}^2)} e^{-\frac{1}{N-1}\beta\sum\limits_j \frac{1}{2}|p_j|^2}\mathrm{d}^2p^N = \left(\int_{T^*_{\mathbf{n}}\mathbb{S}^2} e^{-\frac{1}{N-1}\beta\frac{1}{2}|p|^2}\mathrm{d}^2p\right)^N = \left(\frac{2(N-1)}{\beta}\pi\right)^N, \tag{1.49}$$

where $\mathbf{n}$ is the north pole of the sphere, leaving the latter part

$$\int_{(\mathbb{S}^2)^N} e^{-\frac{1}{N-1}\beta\frac{1}{2}\sum\sum\limits_{j\neq k}\gamma U(|\mathbf{s}_j - \mathbf{s}_k|)}\mathrm{d}^2\underline{\alpha}^N,$$

namely the configurational integral, to be considered. Moreover, the measure

$$\mathrm{d}\mu^{(N)} = \frac{e^{-\frac{1}{N-1}\beta\frac{1}{2}\sum\sum\limits_{j\neq k}\gamma U(|\mathbf{s}_j - \mathbf{s}_k|)}}{\int e^{-\frac{1}{N-1}\beta\frac{1}{2}\sum\sum\limits_{j\neq k}\gamma U(|\mathbf{s}'_j - \mathbf{s}'_k|)}\mathrm{d}^2\underline{\alpha}'^N}\mathrm{d}^2\underline{\alpha}^N \tag{1.50}$$

is the configurational canonical ensemble measure. Then the "typicality" problem of the microcanonical ensembles shifts to the limiting behavior of the canonical ensemble measures, and it leads to the results above except that the $\mathcal{E}$-constraint is gone. To see this, notice that a law of large numbers for (1.50) suggests that if the configurational empirical measure

$$\underline{\Delta}^{(1)}_{Q^{(N)}_t}(\mathbf{s}) = \int \underline{\triangle}^{(1)}_{X^{(N)}_t}(\mathbf{s},\mathbf{p})\mathrm{d}^2p \rightharpoonup \rho(s) \tag{1.51}$$

as $N \to \infty$, then

$$\frac{1}{N-1}\sum_{k\neq j}\gamma U(|s_k - s_j|) \approx \gamma \int U(|s_j - s|)\rho(s)\mathrm{d}\underline{\alpha} \tag{1.52}$$

so that

$$d\mu^{(N)} \approx \prod_{j=1}^{N} \frac{e^{-\beta\gamma\int U(|s_j-s'|)\rho\mathrm{d}\underline{\alpha}'}}{\int e^{-\beta\gamma\int U(|s_j-s'|)\rho\mathrm{d}\underline{\alpha}'}\mathrm{d}\underline{\alpha}}\mathrm{d}\underline{\alpha}^N. \tag{1.53}$$

This plausibility reasoning can indeed be made rigorous, as first done by Messer and Spohn [MeSp82] (for Lipschitz continuous and bounded interactions).

In the above sketched examples, the Gaussian curvature obtained from statistical techniques is a constant, either positive or negative, depending on whether $\gamma = +1$ or $\gamma = -1$. However, by adding a so-called external potential term $\sum_k \psi(s_k)$ to the Hamiltonian (1.32), one can produce a non-constant Gaussian curvature $K \propto \pm e^{\beta\psi}$.

One of the shortcomings of this method, apparently, is that the prescribed Gaussian curvatures, or Q-curvatures in higher dimensions, never change sign. This fact let Prof. Alice Chang raise the question: Can one generalize this technique to the type of curvatures that change sign? This thesis is in part concerned with answering Prof. Chang's question.

Another part of this thesis is concerned with the direct application of the statistical mechanical approach to other types of differential-geometric partial differential equations, like the equation of the immersed tori [Abr87]

$$-\Delta u = \sinh u \tag{1.54}$$

in 2-dim and its higher dimensional analogues.

The rest of the thesis, therefore, consists of two parts:

In Part I, we will apply established statistical mechanics techniques to study a generalization of the prescribed Q-curvature problem on the D-dimensional sphere. While the Gaussian curvature corresponds to the Laplace operator $-\Delta$, Q-curvature is related to the GJMS [GJMS92, Cha08] operators P_{2k}^{D}. The GJMS operators have order $2k$, and the leading term is $(-\Delta)^k$. In particular, when $\mathrm{D} = 2k$, the kernel of P_{2k}^{D} has $\ln\frac{1}{|x|}$ as its leading order, similar to that of the Laplacian in 2-dim. So we can treat the prescribed

Q-curvature problem of all dimensions in one setup, see [Kie00]. We will show that this statistical mechanics strategy can also handle a generalized prescribed Q-curvature problem which in particular contains the equation $Pu = \sinh u$ as a special case.

Before dealing with the problem itself, however, we will first review the results without external fields of Messer and Spohn, in Section 2.1. Then in Section 2.2 we discuss the proof technique of Messer-Spohn. More to the point, we recall the properties of entropy in Subsection 2.2.1, then discuss the continuum limit proved by Messer-Spohn in Subsection 2.2.2. The incorporation of external fields is an immediate generalization, studied in Section 2.3; and another generalization involving a coupling constant, the distribution of which is presumed, is in Section 2.4. Then in Chapter 3, we apply the Messer-Spohn technique to a generalization of the prescribed Q-curvature problem which contains the latter as a special case; however, the Q-curvature is without sign-change.

In Part II, we will generalize the technique of Messer-Spohn to the prescribed Q-curvature problem with sign-change. In order to fulfill the task, we decompose the equation into a pair of equations without changing sign. In the view of statistics, neither the system nor the ensemble of systems contains just one species of particles, but two species of particles. Besides, the interactions are no longer symmetric, voiding the Hamiltonian mechanical interpretation. Instead, we will give an interpretation in terms of biological populations. In contrast to Part I, Part II is not concerned with the application of established rigorous techniques, but with the development of a conceptually new method.

Part I

Application of Statistical Mechanics Techniques to a Generalization of the Prescribed Q-Curvature Problem on $\mathbb{S}^{\mathrm{D}}$

Chapter 2

Introduction to statistical mechanics technique

In this chapter, we introduce the readers to the technique of Messer and Spohn [MeSp82]. For the sake of simplicity and to emphasize the essence, we focus on the pairwise interactions with Lipschitz continuity and boundedness and work in a bounded region of the flat space $\mathbb{R}^{\mathrm{D}}$. Subsequently when we treat the interactions with logarithmic singularities, we will have to change the topology of the function spaces in order to discuss the convergence of measures.

2.1 The Main Results of Messer-Spohn

Assume that the function $U \in C_b^0(\Lambda^2)$ satisfies $U(x,y) = U(y,x)$ for $x, y \in \Lambda \subset \mathbb{R}^{\mathrm{D}}$, where Λ is a bounded domain, and D is a positive integer. The fixed point problem

$$\rho(x) = \frac{e^{-\int_\Lambda U(x,y)\rho(y)\mathrm{d}y}}{\int_\Lambda e^{-\int_\Lambda U(x,y)\rho(y)\mathrm{d}y}\mathrm{d}x}. \tag{2.1}$$

is the Euler-Lagrange equation associated with the problem for finding $\min\limits_{\rho} \mathcal{F}(\rho)$, where $\mathcal{F}$ is the *free energy functional* defined by

$$\mathcal{F}(\rho) = \frac{1}{2}\int_\Lambda\int_\Lambda U(x,y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y + \int_\Lambda \rho(x)\ln(|\Lambda|\rho(x))\mathrm{d}x \tag{2.2}$$

for all $\rho \in (\mathfrak{P} \cap \mathfrak{L}^1 \cap \mathfrak{L}^1 \ln \mathfrak{L}^1)(\Lambda)$.

The functional $\mathcal{F}$ is known in the physics literature as the thermodynamic configurational free energy of ρ, and ρ is a particle density function. The first integral in $\mathcal{F}$ is the potential (configurational) energy of ρ, the second is the negative of the entropy of ρ relative to uniform Lebesgue measure. Messer and Spohn studied $\mathcal{F}$ using statistical mechanics tools and showed that there exists a solution of the Euler-Lagrange equation (2.1). However, in general this procedure won't give all solutions.

More precisely, Messer and Spohn studied the canonical ensemble measures

$$\mu^{(N)}(\mathrm{d}x_1, \cdots, \mathrm{d}x_N) = Z(N)^{-1} \exp\Big[- \frac{1}{2(N-1)} \sum\sum_{1 \le j \ne k \le N} U(x_j, x_k) \Big] \mathrm{d}^N x, \qquad (2.3)$$

where

$$Z(N) = \int \exp\Big[- \frac{1}{2(N-1)} \sum\sum_{1 \le j \ne k \le N} U(x_j, x_k) \Big] \mathrm{d}^N x \qquad (2.4)$$

is the canonical partition function. They showed that as $N \to \infty$ the limit of the canonical measures (2.3) can be characterized as follows:

Definition 1. (Marginal Measure) *For any positive integer $n \le N$, define the n-th marginal measure of a measure μ_N on Λ^N by*

$$^{(n)}\mu_N(\mathrm{d}^n x) := \int_{\Lambda^{N-n}} \mu_N(\mathrm{d}^n x \mathrm{d}^{N-n} x). \qquad (2.5)$$

Result 1. *Suppose the free energy functional $\mathfrak{F}$ has a unique minimizer ρ, then the sequence of the n-th marginal measures $\{^{(n)}\mu^{(N)}\}_{N=1}^{\infty}$ converges weakly to an n-th tensor product of ρ, i.e.,for any positive integer n,*

$$^{(n)}\mu^{(N)} \rightharpoonup \rho^{\otimes n} \in \mathfrak{P}(\Lambda^n), \ \text{as } N \to \infty. \qquad (2.6)$$

We can consider the measures $\mu^{(N)}$ as probability measures on the infinite product of the space Λ, namely $\Lambda^{\mathbb{N}}$, in the following sense [HeSa55]:

Let $B(\Lambda)$ be the σ-algebra of Borel subsets of Λ, and $\mathfrak{P}(\Lambda)$ the set of probability measures on Λ. Now let $\Lambda^{\mathbb{N}}$ be the countably infinite Cartesian product of Λ equipped with product topology, and denote τ_N the projection mapping from $\Lambda^{\mathbb{N}}$ to Λ^N. Then a measure μ_N on the σ-algebra of subsets of Λ^N can be considered equivalent to a measure $\tilde{\mu}_N$ on $\Lambda^{\mathbb{N}}$ in the sense that for any product set $E_1 \times \cdots \times E_N \subset \Lambda^N$,

$$\mu_N(E_1 \times \cdots \times E_N) = \tilde{\mu}_N \circ \tau_N^{-1}(E_1 \times \cdots \times E_N) \qquad (2.7)$$

In this sense, the weak limit point μ of (2.3) is an infinite tensor product of ρ, i.e.,

$$\mu = \rho \otimes \rho \otimes \rho \otimes \cdots \in \mathfrak{P}(\Lambda^{\mathbb{N}}). \qquad (2.8)$$

For each canonical ensemble measure $\mu^{(N)}$, define its free energy by[1]

$$\mathcal{G}^{(N)}(\mu^{(N)}) = \frac{1}{2N}\int_{\Lambda^N}\sum_{1\le k\ne l\le N}\sum U(x_k,x_l)\mathrm{d}\mu^{(N)} + \int_{\Lambda^N}\ln\left(|\Lambda|^N\frac{\mathrm{d}\mu^{(N)}}{\mathrm{d}^N x}\right)\mathrm{d}\mu^{(N)}. \quad (2.9)$$

The so-called "free energy per particle" stands for the limit

$$\lim_{N\to\infty}\frac{1}{N}\mathcal{G}(\mu^{(N)}). \quad (2.10)$$

Result 2. *For the sequence of canonical ensemble measures $\{\mu^{(N)}\}_{N=1}^{\infty}$, the set of its weak limit points consists of minimizers for the functional $\mathcal{F}$, i.e., suppose μ is a weak limit point of $\{\mu^{(N)}\}_{N=1}^{\infty}$, then*

$$\lim_{N\to\infty}\frac{1}{N}\mathcal{G}(\mu^{(N)}) = \lim_{n\to\infty}\frac{1}{n}\mathcal{G}({}^{(n)}\mu) = \inf_{\rho}\mathcal{F}(\rho). \quad (2.11)$$

Result 3. *In general, $\mathcal{F}$ may have a family of minimizers, then each weak limit point μ is a superposition of these minimizers, in the sense that*

$$\mu = \int_{\mathfrak{P}(\Lambda)}\zeta^{\otimes\mathbb{N}}\nu(\mathrm{d}\zeta|\mu), \quad (2.12)$$

or equivalently, for any positive integer n,

$$^{(n)}\mu = \int_{\mathfrak{P}(\Lambda)}\zeta^{\otimes n}\nu(\mathrm{d}\zeta|\mu), \quad (2.13)$$

where the decomposition measure $\nu(\mathrm{d}\zeta|\mu)$ has its support within the set of minimizers of $\mathcal{F}$.

2.2 The Proof Technique of Messer-Spohn

In this section we recall the technique of Messer and Spohn, and in later sections, two generalizations will be discussed.

2.2.1 Properties of Entropy

First, we need some general facts about "the entropy" of some classes of probability measures:

---

[1] In fact, a factor $\frac{1}{N-1}$ instead of the $\frac{1}{2N}$ in front of the first integral will make the following calculation technically easier, and does not change the asymptotic behavior of $\mathcal{G}$ when N is large.

Definition 2. (Entropy) *Let $\mu_N(d^N x) \in \mathfrak{P}(\Lambda^N)$ be a probability measure which is permutation invariant (or permutational symmetric), with $\Lambda^N \subset \mathbb{R}^{N\mathrm{D}}$ bounded. We define its entropy as*

$$\mathcal{S}(\mu_N) = \begin{cases} -\displaystyle\int_{\Lambda^N} \ln(|\Lambda|^N \frac{\mathrm{d}\mu_N}{\mathrm{d}^N x})\mu_N(\mathrm{d}^N x) & \textit{if } \mu_N(\mathrm{d}x^N) \ll \mathrm{d}^N x \textit{ and } \frac{\mathrm{d}\mu_N^{(N)}}{\mathrm{d}^N x} \in \mathfrak{L}^1 \ln \mathfrak{L}^1(\Lambda^N) \\ -\infty & \textit{otherwise} \end{cases} \tag{2.14}$$

For a marginal measure, the entropy $\mathcal{S}({}^{(n)}\mu_N)$ is defined analogously. Entropy of the marginal measure has the following properties:

Property 1. (Decrease of Entropy) *For any positive integers n and m, satisfying $n < m \leq N$, the entropy of the m-th marginal measure cannot be greater than the entropy of the n-th marginal measure, i.e.,*

$$\mathcal{S}({}^{(m)}\mu_N) \leq \mathcal{S}({}^{(n)}\mu_N), \ \forall n < m \leq N. \tag{2.15}$$

Indeed, by setting

$$\begin{aligned} {}^{(m)}\mu_N(\mathrm{d}^m x) \quad &= \quad \rho_m(x_1, \ldots, x_m)\mathrm{d}^m x \\ \text{we have} \quad & \quad -\textstyle\int \rho_m \ln(|\Lambda|^m \rho_m)\mathrm{d}^m x + \int \rho_n \ln(|\Lambda|^n \rho_n)\mathrm{d}^n x \\ &= \quad -\textstyle\int \rho_m \ln \rho_m \mathrm{d}^m x + \int \rho_n \ln \rho_n \mathrm{d}^n x - \ln|\Lambda|^m + \ln|\Lambda|^n \\ &= \quad -\textstyle\int \rho_m \ln \rho_m \mathrm{d}^m x + \int \rho_n \ln \rho_n \mathrm{d}^n x - \ln|\Lambda|^{m-n} \\ &= \quad -\textstyle\int \rho_m \ln \frac{\rho_m}{\rho_n} \mathrm{d}^m x - \ln|\Lambda|^{m-n} \\ &= \quad \langle \ln \tfrac{\rho_n}{\rho_m} \rangle - \ln|\Lambda|^{m-n} \\ &\leq \quad \ln\langle \tfrac{\rho_n}{\rho_m} \rangle - \ln|\Lambda|^{m-n} \\ &= \quad \ln \textstyle\int \rho_m \frac{\rho_n}{\rho_m} \mathrm{d}^m x - \ln|\Lambda|^{m-n} \\ &= \quad \ln \textstyle\int \rho_n \mathrm{d}^m x - \ln|\Lambda|^{m-n} \\ &= \quad \ln|\Lambda|^{m-n} - \ln|\Lambda|^{m-n} = 0 \end{aligned}$$

The "$\leq$" comes from Jensen's inequality, since the function $\ln x$ is concave, then $\langle \ln \cdot \rangle \leq \ln\langle \cdot \rangle$, here the notation $\langle \cdot \rangle$ represents the average with respect to ρ_m.

Property 2. (Subadditivity of Entropy) *For positive integers m and n, the entropy of the $(m+n)$-th marginal measure cannot exceed the sum of the two entropies for the two marginal measures, i.e.,*

$$\mathcal{S}({}^{(m+n)}\mu_N) \leq \mathcal{S}({}^{(m)}\mu_N) + \mathcal{S}({}^{(n)}\mu_N). \tag{2.16}$$

Indeed,

$$\begin{aligned}
& -\int \rho_{m+n} \ln(|\Lambda|^{m+n}\rho_{m+n})\mathrm{d}^{m+n}x + \int \rho_m \ln(|\Lambda|^m \rho_m)\mathrm{d}^m x + \int \rho_n \ln(|\Lambda|^n \rho_n)\mathrm{d}^n x \\
= \; & \int \rho_{m+n} \ln \tfrac{\rho_m \rho_n}{\rho_{m+n}} \mathrm{d}^{m+n}x \\
\leq \; & \ln \int \rho_{m+n} \tfrac{\rho_m \rho_n}{\rho_{m+n}} \mathrm{d}^{m+n}x \\
= \; & \ln \int \rho_m \rho_n \mathrm{d}^{m+n}x \\
= \; & \ln(\int \rho_m \mathrm{d}^m x \int \rho_n \mathrm{d}^n x) = \ln 1 = 0
\end{aligned}$$

Again, the "$\leq$" comes from Jensen's inequality.

Property 3. (Negativity of Entropy)*: For any $N \in \mathbb{N}$, the entropy of μ_N is always non-positive, i.e.*

$$\mathcal{S}(\mu_N) \leq 0. \tag{2.17}$$

The equality occurs if and only if the measure μ_N is the normalized uniform Lebesgue measure on Λ^N, i.e. $\mu_N(\mathrm{d}^N x) = \frac{1}{|\Lambda|^N}\mathrm{d}^N x$.

Indeed, a) if $\mu_N(\mathrm{d}^N x) = \frac{1}{|\Lambda|^N}\mathrm{d}^N x$, then

$$\ln(|\Lambda|^N \frac{\mathrm{d}\mu_N}{\mathrm{d}^N x}) = \ln 1 = 0;$$

b) using the fact that the function $x \mapsto x \ln x$ is convex, we have

$$\begin{aligned}
& -\int \ln(|\Lambda|^N \tfrac{\mathrm{d}\mu_N}{\mathrm{d}x^N})\mu_N(\mathrm{d}^N x) \\
= \; & -\int \ln(|\Lambda|^N \rho_N)\rho_N \mathrm{d}^N x \\
= \; & -\int \ln(|\Lambda|^N \rho_N)|\Lambda|^N \rho_N \tfrac{\mathrm{d}^N x}{|\Lambda|^N} \\
\leq \; & -\int (|\Lambda|^N \rho_N)\tfrac{1}{|\Lambda|^N}\mathrm{d}^N x \cdot \ln \int (|\Lambda|^N \rho_N)\tfrac{1}{|\Lambda|^N}\mathrm{d}^N x \\
= \; & -\ln 1 = 0
\end{aligned}$$

Once again, the "$\leq$" comes from Jensen's Inequality, with $x \ln x$ convex.

Remark 2. *The combination of subadditivity and negativity properties of entropy actually implies the decrease property of entropy.*

Now we extend the concept of entropy to compatible sequences of probability measures $\{^{(1)}\mu, {}^{(2)}\mu, {}^{(3)}\mu, \cdots\}$. By "compatibility", we mean the marginal measures of lower indices can be obtained from integrating the marginal measures of higher indices, i.e.,

$$^{(n)}\mu = \int_{\Lambda^{m-n}} {}^{(m)}\mu(\mathrm{d}^n x \mathrm{d}^{m-n} x), \ \forall m > n. \tag{2.18}$$

Definition 3. (Mean Entropy) *For a sequence of "compatible" probability measures* $\mu = \{^{(1)}\mu, {}^{(2)}\mu, {}^{(3)}\mu, \cdots\}$ *we define the mean entropy of* μ *by*

$$\mathscr{S}(\mu) := \lim_{n\to\infty} \frac{1}{n} \mathcal{S}(^{(n)}\mu), \tag{2.19}$$

where $\mathcal{S}(^{(n)}\mu) := -\int_{\Lambda^n} {}^{(n)}\mu \ln(|\Lambda|^n \, {}^{(n)}\mu) d^n x$ *as before.*

Theorem 4. $\mathscr{S}$ *is well-defined, in the sense that* $\mathscr{S}$ *might be* $-\infty$*, but if* $\inf \frac{1}{n}\mathcal{S}(^{(n)}\mu) > -\infty$*, then a unique finite limit* $\lim_{n\to\infty} \frac{1}{n}\mathcal{S}(^{(n)}\mu)$ *exists and equals* $\inf \frac{1}{n}\mathcal{S}(^{(n)}\mu)$*.*

Proof of Theorem 4. Assume $\inf \frac{1}{n}\mathcal{S}(^{(n)}\mu) = c > -\infty$, then for any $\varepsilon > 0$, there always exists $n_0 \in \mathbb{N}$, such that

$$c \leq \frac{1}{n_0}\mathcal{S}(^{(n_0)}\mu) < c + \varepsilon. \tag{2.20}$$

Now for any $n \in \mathbb{N}$, with the chosen n_0, there exist positive integers A and B, satisfying $0 \leq B < n_0$, such that

$$n = An_0 + B. \tag{2.21}$$

Using the subadditivity and decrease of entropy, we have

$$\begin{aligned} \tfrac{1}{n}\mathcal{S}(^{(n)}\mu) &\leq \tfrac{A}{n}\mathcal{S}(^{(n_0)}\mu) + \tfrac{1}{n}\mathcal{S}(^{(B)}\mu) \\ &\leq \tfrac{A}{n} n_0 (c+\varepsilon) + \tfrac{B}{n}\mathcal{S}(^{(1)}\mu) \end{aligned} \tag{2.22}$$

Let $n \to \infty$, $\frac{A}{n} \to n_0$, so

$$\limsup_{n\to\infty} \frac{1}{n}\mathcal{S}(^{(n)}\mu) \leq c + \varepsilon. \tag{2.23}$$

Then by the arbitrariness of ε, we get our desired limit

$$\lim_{n\to\infty} \frac{1}{n}\mathcal{S}(^{(n)}\mu) = c = \inf \frac{1}{n}\mathcal{S}(^{(n)}\mu). \tag{2.24}$$

Property 4. *The mean entropy functional is affine linear, i.e. for all $\alpha \in [0,1]$,*

$$\mathscr{S}\big(\alpha\mu + (1-\alpha)\nu\big) = \alpha\mathscr{S}(\mu) + (1-\alpha)\mathscr{S}(\nu). \tag{2.25}$$

Remark 3. *The convex linear combination of permutational symmetric probability measures is still a permutational symmetric probability measure, i.e., $\alpha\mu+(1-\alpha)\nu \in \mathfrak{P}(\Lambda^{\mathbb{N}})$ for $\mu, \nu \in \mathfrak{P}(\Lambda^{\mathbb{N}})$.*

Proof of Property 4. a) Let $\rho(x)$ and $\varrho(x)$ be the density functions of μ and ν, respectively. Since the function $f(x) = x\ln x$ is convex, by the definition of convexity, i.e. $f[\alpha\rho + (1-\alpha)\varrho] \le \alpha f(\rho) + (1-\alpha)f(\varrho)$, we have

$$[\alpha\rho + (1-\alpha)\varrho]\ln[\alpha\rho + (1-\alpha)\varrho] \le \alpha\rho\ln\rho + (1-\alpha)\varrho\ln\varrho \tag{2.26}$$

Using the definition of mean entropy,

$$\mathscr{S}(\alpha\mu + (1-\alpha)\mu) \ge \alpha\mathscr{S}(\mu) + (1-\alpha)\mathscr{S}(\mu) \tag{2.27}$$

b) Let ρ_n and ϱ_n be the density functions of μ_n and ν_n respectively. Simply notice that ρ_n and ϱ_n are non-negative, so that for $0 \le \alpha \le 1$,

$$\frac{\alpha\rho_n + (1-\alpha)\varrho_n}{\rho_n} \ge \frac{\alpha\rho_n}{\rho_n} = \alpha \tag{2.28}$$

and similarly,

$$\frac{\alpha\rho_n + (1-\alpha)\varrho_n}{\rho_n} \ge \frac{(1-\alpha)\rho_n}{\varrho_n} = 1-\alpha \tag{2.29}$$

Then

$$\begin{aligned}
& \textstyle\int[\alpha\rho_n + (1-\alpha)\varrho_n]\ln[\alpha\rho_n + (1-\alpha)\varrho_n]\mathrm{d}^n x \\
& -\alpha\textstyle\int\rho_n\ln\rho_n\mathrm{d}^n x - (1-\alpha)\int\varrho_n\ln\varrho_n\mathrm{d}^n x \\
= \ & \alpha\textstyle\int\rho_n\ln\dfrac{\alpha\rho_n + (1-\alpha)\varrho_n}{\rho_n}\mathrm{d}^n x + (1-\alpha)\int\varrho_n\ln\dfrac{\alpha\rho_n + (1-\alpha)\varrho_n}{\varrho_n}\mathrm{d}^n x \\
\ge \ & \alpha\textstyle\int\rho_n\ln\alpha\mathrm{d}^n x + (1-\alpha)\int\varrho_n\ln(1-\alpha)\mathrm{d}^n x \\
= \ & \alpha\ln\alpha + (1-\alpha)\ln(1-\alpha).
\end{aligned}$$

Now divide the inequality above by n and take the limit $n \to \infty$, then the right hand side implies $\lim\limits_{n\to\infty}\frac{1}{n}[\alpha\ln\alpha + (1-\alpha)\ln(1-\alpha)] = 0$, and thus

$$\alpha\mathscr{S}(\mu) + (1-\alpha)\mathscr{S}(\mu) \ge \mathscr{S}(\alpha\mu + (1-\alpha)\mu). \tag{2.30}$$

Put parts a) and b) together, we get the desired equality

$$\alpha\mathscr{S}(\mu) + (1-\alpha)\mathscr{S}(\mu) = \mathscr{S}(\alpha\mu + (1-\alpha)\mu). \tag{2.31}$$

2.2.2 The Continuum Limit

Messer-Spohn's convergence result implies that there is a solution to the Euler-Lagrange equation,

$$\rho(x) = \frac{e^{-\int_\Lambda U(x,y)\rho(y)\mathrm{d}y}}{\int e^{-\int_\Lambda U(x,y)\rho(y)\mathrm{d}y}\mathrm{d}x},$$

associated with the problem for finding $\min_\rho \mathcal{F}(\rho)$, with

$$\mathcal{F}(\rho) = \frac{1}{2}\int_\Lambda\int_\Lambda U(x,y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y + \int_\Lambda \rho(x)\ln(|\Lambda|\rho(x))\mathrm{d}x$$

where $\rho \in (\mathfrak{P}\cap\mathfrak{L}^1\cap\mathfrak{L}^1\ln\mathfrak{L}^1)(\Lambda)$. Here, for simplicity, the interaction U is continuous and bounded, the domain Λ is simply connected and bounded. Moreover, whenever a unique minimizer exists, there exists an approximating sequence. The whole procedure runs as follows:

Step 1. *We define a functional $\mathcal{G}^{(N)}$ on $(\mathfrak{P}\cap\mathfrak{L}^1\cap\mathfrak{L}^1\ln\mathfrak{L}^1)(\Lambda^N)$ by*

$$\mathcal{G}^{(N)}(\mu_N) = \frac{1}{2N}\int_{\Lambda^N}\sum\sum_{1\le k\ne l\le N} U(x_k,x_l)\mathrm{d}\mu_N + \int_{\Lambda^N}\ln\left(|\Lambda|^N\frac{\mathrm{d}\mu_N}{\mathrm{d}^N x}\right)\mathrm{d}\mu_N \tag{2.32}$$

for any permutational symmetric distribution measure $\mu_N \in (\mathfrak{P}\cap\mathfrak{L}^1\cap\mathfrak{L}^1\ln\mathfrak{L}^1)(\Lambda^N)$. It is known that $\mathcal{G}^{(N)}(\mu_N)$ has a unique minimizer in $(\mathfrak{P}\cap\mathfrak{L}^1\cap\mathfrak{L}^1\ln\mathfrak{L}^1)(\Lambda^N)$ given by

$$\mathrm{d}\mu^{(N)}(x_1,\cdots,x_N) = \frac{\exp\{-\frac{1}{2N}\sum\sum_{1\le k\ne l\le N} U(x_k,x_l)\}}{\int\exp\{-\frac{1}{2N}\sum\sum_{1\le k\ne l\le N} U(x_k,x_l)\}\mathrm{d}^N x}\mathrm{d}^N x. \tag{2.33}$$

Indeed, let $\mu'_N(x_1,\cdots,x_N)$ be the Radon-Nikodym derivative (probability density function) of μ_N with respect to $\mathrm{d}x^N$, and naturally require[2] that $\mathcal{G}(\mu'_N) = \mathcal{G}(\mu_N)$. Then we vary the probability density μ'_N by $\varepsilon\delta_{\mu'_N}$ for a "compatible" density function $\delta_{\mu'_N}$

[2]Here there is a little abuse of notation, as $\mathcal{G}$ is originally defined on the space of distribution measures, but it does not hurt to let $\mathcal{G}$ act "alternatively" on corresponding distribution density functions with the same image values.

such that $\mu'_N + \varepsilon\delta_{\mu'_N}$ is still a probability density function. Thus, with a Lagrange multiplier η for the constraint $\int(\mu'_N + \varepsilon\delta_{\mu'_N})\mathrm{d}x^N = 1$,

$$\begin{aligned} & \mathcal{G}^{(N)}(\mu'_N + \varepsilon\delta_{\mu'_N}) + \eta(\textstyle\int_{\Lambda^N}(\mu'_N + \varepsilon\delta_{\mu'_N})\mathrm{d}x^N - 1) \\ = \; & \tfrac{1}{2N}\textstyle\int_{\Lambda^N}\sum\sum_{1\le k\ne l\le N} U(x_k,x_l)(\mu'_N + \varepsilon\delta_{\mu'_N})\mathrm{d}x^N \\ & + \textstyle\int_{\Lambda^N}(\mu'_N + \varepsilon\delta_{\mu'_N})\ln\left(|\Lambda|^N(\mu'_N + \varepsilon\delta_{\mu'_N})\right)\mathrm{d}x^N + \eta\Big[\int_{\Lambda^N}(\mu'_N + \varepsilon\delta_{\mu'_N})\mathrm{d}x^N - 1\Big] \end{aligned}$$

Differentiate the equation above with respect to ε and evaluate at $\varepsilon = 0$, we get

$$\begin{aligned} & \frac{\partial}{\partial\varepsilon}\Big|_{\varepsilon=0}\Big\{\mathcal{G}^{(N)}(\mu'_N + \varepsilon\delta_{\mu'_N}) + \eta(\int_{\Lambda^N}(\mu'_N + \varepsilon\delta_{\mu'_N})\mathrm{d}x^N - 1)\Big\} \\ = \; & \tfrac{1}{2N}\textstyle\int_{\Lambda^N}\sum\sum_{1\le k\ne l\le N} U(x_k,x_l)\delta_{\mu'_N}\mathrm{d}x^N + \int_{\Lambda^N}\delta_{\mu'_N}\Big[\ln\left(|\Lambda|^N\mu'_N\right) + 1\Big]\mathrm{d}x^N + \eta\int_{\Lambda^N}\delta_{\mu'_N}\mathrm{d}x^N, \end{aligned}$$

which equals 0 for all "compatible" density function $\delta_{\mu'_N}$, if μ'_N is a minimizer of $\mathcal{F}$. So that

$$\frac{1}{2N}\sum\sum_{1\le k\ne l\le N} U(x_k,x_l) + \Big[\ln\left(|\Lambda|^N\mu'_N\right) + 1\Big] + \eta = 0$$

and thus

$$\mu'_N = \frac{1}{|\Lambda|^N}\exp\{-1 - \eta - \frac{1}{2N}\sum\sum_{1\le k\ne l\le N} U(x_k,x_l)\}$$

Finally, by the constraint that $\int\mu'_N\mathrm{d}x^N = 1$, we arrive at the representation of the density functions of minimizers

$$\mu'_N(x_1,\cdots,x_N) = \frac{\exp\Big[-\tfrac{1}{2N}\sum\sum_{1\le k\ne l\le N} U(x_k,x_l)\Big]}{\int_{\Lambda^N}\exp\Big[-\tfrac{1}{2N}\sum\sum_{1\le k\ne l\le N} U(x_k,x_l)\Big]\mathrm{d}x^N}$$

This shows (2.33).

Step 2. *We show that* $\inf_\rho \mathcal{F}(\rho) \ge \limsup_{N\to\infty}\frac{1}{N}\mathcal{G}^{(N)}(\mu^{(N)})$.

Proof of Step 2. For any product measure with its density denoted by $\rho^{\otimes N}$, we compute $\mathcal{G}^{(N)}(\rho^{\otimes N})$ as follows:

$$\begin{aligned}
\mathcal{G}^{(N)}(\rho^{\otimes N}) &= \tfrac{1}{2N}\int_{\Lambda^N}\sum_{1\le k\ne l\le N}\sum U(x_k,x_l)\rho^{\otimes N}(x_1,\cdots,x_N)\mathrm{d}x_1\cdots\mathrm{d}x_N \\
&\quad + \int_{\Lambda^N}\rho^{\otimes N}(x_1,\cdots,x_N)\ln\big(|\Lambda|^N\rho^{\otimes N}(x_1,\cdots,x_N)\big)\mathrm{d}x_1\cdots\mathrm{d}x_N \\
&= \tfrac{1}{2N}\sum_{1\le k\ne l\le N}\sum\int_{\Lambda^N}U(x_k,x_l)\rho(x_1)\cdots\rho(x_N)\mathrm{d}x_1\cdots\mathrm{d}x_N \\
&\quad + \int_{\Lambda^N}\rho(x_1)\cdots\rho(x_N)\ln\big(|\Lambda|^N\rho(x_1)\cdots\rho(x_N)\big)\mathrm{d}x_1\cdots\mathrm{d}x_N \\
&= \tfrac{1}{2N}\sum_{1\le k\ne l\le N}\sum\int_{\Lambda^2}U(x_k,x_l)\rho(x_k)\rho(x_l)\mathrm{d}x_k\mathrm{d}x_l \\
&\quad + \int_{\Lambda^N}\rho(x_1)\cdots\rho(x_N)\sum_{i=1}^{N}\ln\big(|\Lambda|\rho(x_i)\big)\mathrm{d}x_1\cdots\mathrm{d}x_N \\
&= \tfrac{N(N-1)}{2N}\int_{\Lambda^2}U(x,y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y + \sum_{i=1}^{N}\int_{\Lambda}\rho(x_i)\ln\big(|\Lambda|\rho(x_i)\big)\mathrm{d}x_i \\
&= \tfrac{N-1}{2}\int_{\Lambda^2}U(x,y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y + N\int_{\Lambda}\rho(x)\ln\big(|\Lambda|\rho(x)\big)\mathrm{d}x
\end{aligned}$$

Divide by N to get

$$\begin{aligned}
\tfrac{1}{N}\mathcal{G}^{(N)}(\rho^{\otimes N}) &= \tfrac{N-1}{2N}\int_{\Lambda^2}U(x,y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y + \int_{\Lambda}\rho(x)\ln\big(|\Lambda|\rho(x)\big)\mathrm{d}x \\
&= \mathcal{F}(\rho) - \tfrac{1}{2N}\int_{\Lambda^2}U(x,y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y.
\end{aligned}$$

Since U is continuous and bounded, $\frac{1}{2N}\int_{\Lambda^2}U(x,y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y \to 0$ as $N\to\infty$, thus

$$\frac{1}{N}\mathcal{G}^{(N)}({\mu'_N}^{(N)}) \le \frac{1}{N}\mathcal{G}^{(N)}(\rho^{\otimes N}) \le \mathcal{F}(\rho) + O(\frac{1}{N}) \tag{2.34}$$

and hence, as $N\to\infty$,

$$\limsup_{N\to\infty}\frac{1}{N}\mathcal{G}^{(N)}({\mu'_N}^{(N)}) \le \mathcal{F}(\rho),\ \forall\rho. \tag{2.35}$$

Finally, taking infimum with respect to ρ, we get

$$\limsup_{N\to\infty}\frac{1}{N}\mathcal{G}^{(N)}({\mu'_N}^{(N)}) \le \inf_{\rho}\mathcal{F}(\rho). \tag{2.36}$$

Step 3. *In the following, we want to show that*

$$\liminf_{N\to\infty}\frac{1}{N}\mathcal{G}^{(N)}({\mu'_N}^{(N)}) \ge \inf_{\rho}\mathcal{F}(\rho), \tag{2.37}$$

so that together with the previous step, the limit $\lim_{N\to\infty}\frac{1}{N}\mathcal{G}^{(N)}({\mu'_N}^{(N)})$ *exists and equals to* $\inf_{\rho}\mathcal{F}(\rho)$.

Step 3a) Consider the marginal measure ${}^{(n)}\mu^{(N)}(d^n x) := \int_{\Lambda^{N-n}}\mu^{(N)}(d^n x d^{N-n}x)$. Since Λ is bounded, $\bar{\Lambda}$ is compact, then $\mathfrak{P}(\bar{\Lambda}^n)$ is a compact and convex set. (Remark:

$\mathfrak{P}(\bar{\Lambda}^{\mathbb{N}})$ is also compact by Tychonoff's Theorem.) So by extracting a subsequence (if necessary), there exists a permutational symmetric probability measure ${}^{(n)}\mu$, such that

$$ {}^{(n)}\mu^{(N)} \rightharpoonup {}^{(n)}\mu \text{ as } N \to \infty \tag{2.38}$$

the notation "$\rightharpoonup$" represents weak convergence, i.e.

$$\int_{\Lambda^n} \psi(x_1, \cdots, x_n)^{(n)}\mu^{(N)} d^n x \to \int_{\Lambda^n} \psi(x_1, \cdots, x_n)^{(n)}\mu d^n x, \ \forall \psi \in C_b^0(\Lambda^N) \tag{2.39}$$

In particular,

$$\int_\Lambda \int_\Lambda U(x,y)^{(2)}\mu^{(N)} \mathrm{d}x\mathrm{d}y \to \int_\Lambda \int_\Lambda U(x,y)^{(2)}\mu \mathrm{d}x\mathrm{d}y, \text{ as } N \to \infty. \tag{2.40}$$

Step 3b) Fix n, similar to (2.21), $N = Mn+L$, where $0 \le L < n$. Then by subadditivity and negativity of entropy,

$$\begin{aligned} \tfrac{1}{N}\mathcal{S}(\mu^{(N)}) &= \tfrac{1}{N}\mathcal{S}({}^{(Mn+L)}\mu^{(N)}) \le \tfrac{1}{N}\mathcal{S}({}^{(Mn)}\mu^{(N)}) + \tfrac{1}{N}\mathcal{S}({}^{(L)}\mu^{(N)}) \\ &\le \tfrac{M}{N}\mathcal{S}({}^{(n)}\mu^{(N)}) + \tfrac{1}{N}\mathcal{S}({}^{(L)}\mu^{(N)}) \le \tfrac{M}{N}\mathcal{S}({}^{(n)}\mu^{(N)}) \end{aligned} \tag{2.41}$$

Notice that:

1) $\frac{M}{N} \to \frac{1}{n}$ as $N \to \infty$;

2) $\limsup_{N\to\infty} \mathcal{S}({}^{(n)}\mu^{(N)}) \le \mathcal{S}({}^{(n)}\mu)$ by the upper semi-continuity of entropy (cf. Theorem 4.2.9 in [Kel98]; Propositions 3 and 4 in [RoRu67])[3].

Combining 1) and 2), we deduce

$$\limsup_{N\to\infty} \frac{1}{N}\mathcal{S}(\mu^{(N)}) \le \frac{1}{n}\mathcal{S}({}^{(n)}\mu) \tag{2.42}$$

where the right hand side depends on n, but the left hand side is independent of n.

Step 3c) Let $n \to \infty$, since $\lim_{N\to\infty} \frac{1}{n}\mathcal{S}({}^{(n)}\mu) = \mathscr{S}(\mu)$ by the definition of *entropy per particle* ("mean entropy of the state μ" in [RoRu67]),

$$\limsup_{N\to\infty} \frac{1}{N}\mathcal{S}(\mu^{(N)}) \le \mathscr{S}(\mu). \tag{2.43}$$

Step 3d) Together with the fact that the energy functional $\mathcal{E}$ defined by

$$\mathcal{E}(\mu_N) = \frac{1}{2N}\int_{\Lambda^N} \sum\sum_{1\le k\ne l\le N} U(x_k, x_l)\mathrm{d}\mu_N \tag{2.44}$$

---

[3]The main idea of the proof, which is omitted here, is to express the entropy functional as the limit of a decreasing sequence of continuous functionals. Moreover, it can be shown that each continuous functional is concave.

is linear, so far we have

$$\liminf_{N\to\infty}\frac{1}{N}\mathcal{G}^{(N)}(\mu^{(N)})=\liminf_{N\to\infty}\frac{1}{N}\Big[\mathcal{E}(\mu^{(N)})-\mathcal{S}(\mu^{(N)})\Big]\geq\inf_{\mu}\mathscr{F}(\mu) \tag{2.45}$$

where μ is any weak limit point of the sequence $\mu^{(N)}$, and functional $\mathscr{F}$ is the "free energy per particle" defined as $\mathscr{F}(\mu)=\lim\limits_{N\to\infty}\frac{1}{n}\Big[\mathcal{E}(^{(n)}\mu)-\mathcal{S}(^{(n)}\mu)\Big]$. The job left is to transfer $\mathscr{F}(\mu)$ to $\mathcal{F}(\rho)$. Indeed, any weak limit point of $\{\mu^{(N)}\}$ is a permutation invariant measure on $\Lambda^{\mathbb{N}}$. Moreover, Hewitt and Savage [HeSa55] proved that $\forall\mu\in\mathfrak{P}(\Lambda^{\mathbb{N}}),\exists\pi\in\mathfrak{P}(\mathfrak{P}(\Lambda))$, s.t.

$$\mu=\int_{\mathfrak{P}(\Lambda)}\rho^{\otimes\mathbb{N}}\mathrm{d}\pi(\rho|\mu),\ {}^{(n)}\mu=\int_{\mathfrak{P}(\Lambda)}\rho^{\otimes n}\mathrm{d}\pi(\rho|\mu) \tag{2.46}$$

Note that ρ here is the integration variable.[4] Hence, utilizing the affine linearity of entropy, we have the following:

$$\begin{aligned}\mathscr{F}(\mu) &= \int_{\mathfrak{P}(\Lambda)}\Big\{\tfrac{1}{2}\int_\Lambda\int_\Lambda U(x,y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y+\int_\Lambda\rho(x)\ln(|\Lambda|\rho(x))\mathrm{d}x\Big\}\mathrm{d}\pi(\rho|\mu)\\ &\geq \inf_\rho\mathcal{F}(\rho)\end{aligned} \tag{2.47}$$

Combining the steps 2 and 3 above, we proved that $\lim\limits_{N\to\infty}\frac{1}{N}\mathcal{G}^{(N)}(\mu^{(N)})$ exists and equals to $\inf\limits_\mu\mathscr{F}(\mu)=\inf\limits_\rho\mathcal{F}(\rho)$. Moreover, since $\inf\limits_\mu\mathscr{F}(\mu)$ is attained by any limit point, it is actually $\min\limits_\mu\mathscr{F}(\mu)$. Finally, notice that if μ is a weak limit point of the sequence $\{\mu^{(N)}\}$, then the decomposition measure $\pi(\mathrm{d}\rho|\mu)$ has to concentrate on the set of minimizers of $\mathcal{F}$, because otherwise the equality $\mathscr{F}(\mu)=\inf\limits_\rho\mathcal{F}(\rho)$ would be violated. As a result,

$$\mathscr{F}(\mu)=\frac{1}{2}\int_\Lambda\int_\Lambda U(x,y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y+\int_\Lambda\rho(x)\ln(|\Lambda|\rho(x))\mathrm{d}x, \tag{2.48}$$

for any ρ a minimizer of the free energy functional $\mathcal{F}$.

As a summary, when the uniqueness of solution ρ to the equation (2.1) holds, then an approximating sequence $\{^{(1)}\mu^{(N)}\}_{N=1}^\infty$ exists, each term of which is the first marginal measure of an explicitly represented minimizer $\mu^{(N)}$ of the free energy functional $\mathcal{G}^{(N)}$.

---

[4] One can think this integral on the functional space $\mathfrak{P}(\Lambda)$ as a "weighted average" of all product measures $\rho^{\otimes\mathbb{N}}$ and $\rho^{\otimes n}$ respectively, for $\rho\in\mathfrak{P}(\Lambda)$. The decomposition measure $\mathrm{d}\pi$ tells the weight on each $\rho\in\mathfrak{P}(\Lambda)$, which is determined by the "resulted average" μ.

More generally, when the uniqueness does not hold, the technique of Messer-Spohn still proves the existence of solutions, but does not provide an approximating sequence for any of them.

2.3 An Immediate Generalization: Incorporating External Fields

In this section, we generalize the canonical ensembles (2.3) to the following canonical ensembles with the external field ψ:

$$\mu^{(N)}(\mathrm{d}x_1, \cdots, \mathrm{d}x_N) = Z(N)^{-1} \exp\Big[\sum_{k=1}^{N} \psi(x_k) - \frac{1}{2(N-1)} \sum\sum_{1\le j\ne k\le N} U(x_j, x_k)\Big] \mathrm{d}^N x, \tag{2.49}$$

where the corresponding canonical partition function is modified into

$$Z(N) = \int \exp\Big[\sum_{k=1}^{N} \psi(x_k) - \frac{1}{2(N-1)} \sum\sum_{1\le j\ne k\le N} U(x_j, x_k)\Big] \mathrm{d}^N x. \tag{2.50}$$

The weak limit points μ of the sequence $\{\mu^{(N)}\}_{N=1}^{\infty}$ are superpositions of the solutions ρ to the following Euler-Lagrange equation:

$$\rho(x) = \frac{e^{\psi(x) - \int U(x,y)\rho(y)\mathrm{d}y}}{\int e^{\psi(x) - \int U(x,y)\rho(y)\mathrm{d}y} \mathrm{d}x}. \tag{2.51}$$

If we set $J(x) = e^{\psi(x)}$, then the equation above can be rewritten as

$$\rho(x) = \frac{J(x) e^{-\int_\Lambda U(x,y)\rho(y)\mathrm{d}y}}{\int J(x) e^{-\int_\Lambda U(x,y)\rho(y)\mathrm{d}y} \mathrm{d}x}, \tag{2.52}$$

the same type of equation as (2.1), but with an extra factor $J(x)$. When the function J does not change its sign — naturally satisfied by the construction $J(x) = e^{\psi}$ — the equation (2.52) can be translated into the original fixed point equation (2.1) easily. There are two ways to do so, one is to absorb J into U, while the other is to absorb J into $\mathrm{d}x$.

Method 1. *Absorb $J(x)$ into $U(x, y)$.*

This method works pretty smoothly when J is bounded away from zero in Λ, even when J takes on only negative values.

<u>*Case 1.*</u> $J \in C_b^0(\Lambda)$, $J \geq C_0 > 0$, for some $C_0 \in \mathbb{R}^+$. $\rho \in (\mathfrak{P} \cap \mathfrak{L}^1 \cap \mathfrak{L}^1 \ln \mathfrak{L}^1)(\Lambda)$.

Let $\tilde{U}(x,y) = U(x,y) - \ln J(x) - \ln J(y)$, then

$$\begin{aligned} \int_\Lambda \tilde{U}(x,y)\rho(y)\mathrm{d}y &= \int_\Lambda U(x,y)\rho(y)\mathrm{d}y - \int_\Lambda \ln J(x)\rho(y)\mathrm{d}y - \int_\Lambda \ln J(y)\rho(y)\mathrm{d}y \\ &= -C - \ln J(x) + \int_\Lambda U(x,y)\rho(y)\mathrm{d}y \end{aligned} \tag{2.53}$$

where we denote $\int_\Lambda \rho(y)\ln J(y)\mathrm{d}y$ by C. Now

$$e^{-\int_\Lambda \tilde{U}(x,y)\rho(y)\mathrm{d}y} = e^C J(x) e^{-\int_\Lambda U(x,y)\rho(y)\mathrm{d}y} \tag{2.54}$$

and thus

$$\frac{e^{-\int_\Lambda \tilde{U}(x,y)\rho(y)\mathrm{d}y}}{\int e^{-\int_\Lambda \tilde{U}(x,y)\rho(y)\mathrm{d}y}\mathrm{d}x} = \frac{e^C J(x) e^{-\int_\Lambda U(x,y)\rho(y)\mathrm{d}y}}{e^C \int J(x) e^{-\int_\Lambda U(x,y)\rho(y)\mathrm{d}y}} = \rho(x) \tag{2.55}$$

i.e. equation (2.52) becomes

$$\rho(x) = \frac{e^{-\int_\Lambda \tilde{U}(x,y)\rho(y)\mathrm{d}y}}{\int e^{-\int_\Lambda \tilde{U}(x,y)\rho(y)\mathrm{d}y}\mathrm{d}x} \tag{2.56}$$

which has the same form as our original problem (2.1). Note that the $\tilde{U}$ here also belongs to $C_b^0(\Lambda^2)$, same as U does. Hence all the tricks we did for (2.1) work here.

<u>*Case 2.*</u> $J \in C_b^0(\Lambda)$, $J \leq C_0 < 0$, for some $C_0 \in \mathbb{R}^+$. $\rho \in (\mathfrak{P} \cap \mathfrak{L}^1 \cap \mathfrak{L}^1 \ln \mathfrak{L}^1)(\Lambda)$.

Let $\tilde{J}(x) = -J(x)$, then equation (2.52) is equivalent to

$$\rho(x) = \frac{\tilde{J}(x) e^{-\int_\Lambda U(x,y)\rho(y)\mathrm{d}y}}{\int \tilde{J}(x) e^{-\int_\Lambda U(x,y)\rho(y)\mathrm{d}y}\mathrm{d}x} \tag{2.57}$$

where $\tilde{J} \in C_b^0(\Lambda)$, $\tilde{J} \geq C_0 > 0$. In this way, we transform case 2) to case 1).

<u>**Method 2.**</u> *Absorb* $J(x)$ *into* $\mathrm{d}x$.

This method may seem "unnatural" at the first glance. As we'll see, however, it gives us more advantage to generalize problem (2.52) to its counterpart with a wider class of ρ's.

<u>*Case 1.*</u> To warm up with this method, let's put aside the generalization first, and return to our original problem (2.1), with a normalized uniform measure defined as $\mathrm{d}\lambda = \frac{1}{|\Lambda|}\mathrm{d}x$. The motivation is to make $\mathrm{d}\lambda$ a probability measure, and at the same time to eliminate the $|\Lambda|$ inside "ln" in the definition of entropy.

For any probability measure μ, let $\rho(x)$ be its density function with respect to $\mathrm{d}x$, and $\tilde{\rho}(x) = \frac{\mathrm{d}\mu}{\mathrm{d}\lambda}$ be the relative density with respect to $\mathrm{d}\lambda$. We show that the variational problem for finding $\min_{\tilde{\rho}} \mathcal{F}(\tilde{\rho})$, where $\mathcal{F}(\tilde{\rho}) := \mathcal{F}(\rho)$, gives the same equation as (2.1). Indeed, by using Lagrange multiplier, define

$$\begin{aligned} F(\tilde{\rho},\sigma) &= \tfrac{1}{2}\int_\Lambda\int_\Lambda U(x,y)\tilde{\rho}(x)\tilde{\rho}(y)\mathrm{d}\lambda(x)\mathrm{d}\lambda(y) + \int_\Lambda \tilde{\rho}(x)\ln(\tilde{\rho}(x))\mathrm{d}\lambda(x) \\ &\quad +\sigma[\textstyle\int_\Lambda \tilde{\rho}(x)\mathrm{d}\lambda(x) - 1] \end{aligned} \tag{2.58}$$

With a similar procedure as in Subsection 2.2.2 Step 1, we get the Euler-Lagrange equation for $\min \mathcal{F}(\tilde{\rho})$,

$$\tilde{\rho}(x) = \frac{e^{-\int_\Lambda U(x,y)\tilde{\rho}(y)d\lambda(y)}}{\int_\Lambda e^{-\int_\Lambda U(x,y)\tilde{\rho}(y)d\lambda(y)}d\lambda(x)} \tag{2.59}$$

which coincides with the original equation (2.1).

<u>Case 2.</u> Now, coming back to problem (2.1), we define $d\lambda = \frac{J(x)}{\int_\Lambda J(y)\mathrm{d}y}\mathrm{d}x$, we again check that the variational problem also gives the same problem as (2.1). In fact, the new λ here satisfies $\int_\Lambda d\lambda = 1$. For $\mu(\mathrm{d}x) = \rho(x)d\lambda$ and the functional

$$\mathcal{F}(\rho) = \frac{1}{2}\int_\Lambda\int_\Lambda U(x,y)\rho(x)\rho(y)d\lambda(x)d\lambda(y) + \int_\Lambda \rho(x)\ln[|\Lambda|^n\rho(x)]\mathrm{d}x, \tag{2.60}$$

we define, analogously to (34),

$$\begin{aligned} F(\rho,\sigma) &= \tfrac{1}{2}\int_\Lambda\int_\Lambda U(x,y)\rho(x)\rho(y)d\lambda(x)d\lambda(y) + \int_\Lambda \rho(x)\ln[|\Lambda|^n\rho(x)]\mathrm{d}x \\ &\quad +\sigma[\textstyle\int_\Lambda \rho(x)d\lambda(x) - 1] \end{aligned} \tag{2.61}$$

Imitating the process for Case 1, the following procedure goes through again:

$$\begin{aligned} F(\rho+\varepsilon\delta_{\tilde{\rho}},\sigma) &= \tfrac{1}{2}\int_\Lambda\int_\Lambda U(x,y)(\rho+\varepsilon\delta_{\tilde{\rho}})(x)(\rho+\varepsilon\delta_{\tilde{\rho}})(y)d\lambda(x)d\lambda(y) \\ &\quad + \textstyle\int_\Lambda(\rho+\varepsilon\delta_{\tilde{\rho}})(x)\ln[|\Lambda|^n(\rho+\varepsilon\delta_{\tilde{\rho}})(x)]\mathrm{d}x \\ &\quad +\sigma[\textstyle\int_\Lambda(\rho+\varepsilon\delta_{\tilde{\rho}})(x)d\lambda(x) - 1] \\ \frac{\partial F(\rho+\varepsilon\delta_{\tilde{\rho}},\sigma)}{\partial\varepsilon}\Big|_{\varepsilon=0} &= \textstyle\int_\Lambda\int_\Lambda U(x,y)\rho(y)\delta_{\tilde{\rho}}(x)d\lambda(x)d\lambda(y) \\ &\quad + \textstyle\int_\Lambda \big(\delta_{\tilde{\rho}}(x)\ln[|\Lambda|^n\rho(x)] + \frac{\delta_{\tilde{\rho}}(x)}{|\Lambda|^n}\big)d\lambda(x) + \sigma\int_\Lambda \delta_{\tilde{\rho}}(x)d\lambda(x) \\ &= \textstyle\int_\Lambda \big\{ \int_\Lambda U(x,y)\rho(y)d\lambda(y) + \ln|\Lambda|^n\rho(x) + \frac{1}{|\Lambda|^n} + \sigma\big\}\delta_{\tilde{\rho}}(x)d\lambda(x) \\ &= 0 \end{aligned}$$

Thus,

$$\int_\Lambda U(x,y)\rho(y)d\lambda(y) + \ln|\Lambda|^n\rho(x) + \frac{1}{|\Lambda|^n} + \sigma = 0 \tag{2.62}$$

and then

$$\rho(x) = \frac{1}{|\Lambda|^n} e^{-\frac{1}{|\Lambda|^n} - \sigma} e^{-\int_\Lambda U(x,y)\rho(y)d\lambda(y)} \tag{2.63}$$

Integrate both side with respect to $d\lambda$, we get

$$1 = \int_\Lambda \rho(x)d\lambda(x) = \frac{1}{|\Lambda|^n} e^{-\frac{1}{|\Lambda|^n} - \sigma} \int_\Lambda e^{-\int_\Lambda U(x,y)\rho(y)d\lambda(y)} d\lambda(x) \tag{2.64}$$

and

$$\frac{1}{|\Lambda|^n} e^{-\frac{1}{|\Lambda|^n} - \sigma} = \Big[\int_\Lambda e^{-\int_\Lambda U(x,y)\rho(y)d\lambda(y)} d\lambda(x) \Big]^{-1}$$

Finally, the following equation is deduced

$$\rho(x) = \frac{e^{-\int_\Lambda U(x,y)\rho(y)d\lambda(y)}}{\int_\Lambda e^{-\int_\Lambda U(x,y)\rho(y)d\lambda(y)} d\lambda(x)} \tag{2.65}$$

At this point, the extra function J is gone, and the technique of Messer-Spohn introduced can work smoothly again.

2.4 Another Generalization: A Random Coupling Constant c

In this section we introduce the generalization of Messer and Spohn's technique to a model with coupling constants, i.e., the canonical ensemble measure is now defined by

$$\mu^{(N)}(\mathrm{d}x_1, \cdots, \mathrm{d}x_N) = Z(N)^{-1} \exp\Big[-\frac{1}{2} \sum_{1\le j\ne k\le N}\sum c_j c_k U(|\mathbf{s}_j - \mathbf{s}_k|) \Big] \prod_k f(c_k)\mathrm{d}c_k \mathrm{d}^N x, \tag{2.66}$$

with the canonical partition function

$$Z(N) = \int \exp\Big[-\frac{1}{2} \sum_{1\le j\ne k\le N}\sum c_j c_k U(|\mathbf{s}_j - \mathbf{s}_k|) \Big] \prod_k f(c_k)\mathrm{d}c_k \mathrm{d}^N x. \tag{2.67}$$

The coupling constants $\{c_j\}_{j=1}^N$ are a sequence of i.i.d. (independent and identically distributed) real numbers, distributed according to a distribution density function $f(c)$. When $N \to \infty$, the weak limit points of the sequence are characterized by the minimizers of the free energy functional

$$\mathcal{F}(\rho) = \frac{1}{2} \int_{\Lambda^2} \int_{\mathbb{R}^2} c_1 c_2 U(x_1, x_2)\rho(x_1)\rho(x_2) f(c_1) f(c_2) \mathrm{d}^2 c \mathrm{d}^2 x + \int_\Lambda \rho(x) \ln(|\Lambda|\rho(x))\mathrm{d}x.$$

(2.68)

Besides, each weak limit point μ is a superposition of the typical canonical ensemble measures ρ, in the sense that

$$^{(n)}\mu = \int_{\mathfrak{P}(\Lambda)} \zeta^{\otimes n} \mathrm{d}\nu(\zeta|\mu) \tag{2.69}$$

where the decomposition measure ν concentrates on the set of minimizers ρ of $\mathcal{F}$. Moreover, any minimizer ρ satisfies the Euler-Lagrange equation, i.e., the fixed point problem,

$$\rho(x;c) = \frac{e^{-\int_\Lambda \int_\mathbb{R} cc' U(x,y)\rho(y) f(c')\mathrm{d}c'\mathrm{d}y}}{\int_\Lambda \int_\mathbb{R} e^{-\int_\Lambda \int_\mathbb{R} cc' U(x,y)\rho(y) f(c')\mathrm{d}c'\mathrm{d}y} f(c)\mathrm{d}c\mathrm{d}x} \tag{2.70}$$

Such a setup generalizes the Euler-Lagrange equation (1.43) with only two choices for the value of the constant γ to a broader type of equations. If we choose $f(c) = \delta_\gamma$, in particular, then the original (1.43) is recovered as a special case.

In the next chapter, an even broader type of equations with $\Lambda = \mathbb{S}^{\mathrm{D}}$ will be discussed.

Chapter 3

The Generalized Prescribed Q-Curvature Problem

Now we come to the statistical mechanics approach to the generalized prescribed Q-curvature problem, where $\Lambda = \mathbb{S}^{\mathrm{D}} \subset \mathbb{R}^{\mathrm{D}+1}$, and the interaction, denoted by U, is no longer continuous and bounded but has logarithmic singularities. We follow [KiWa12], where the 2-dim problem was studied, with an application to incompressible, inviscid fluid flows on $\mathbb{S}^2$.

Define the canonical ensemble measure as

$$\mathrm{d}\mu^{(N)} = \langle \mathfrak{Z}_N \rangle_f^{-1} e^{-\beta\left(\frac{1}{N-1} \sum\sum_{j<k} c_j c_k U(\mathbf{s}_j, \mathbf{s}_k) + \gamma \sum_k c_k V(\mathbf{s}_k) \right)} \mathrm{d}\varrho_f^N \tag{3.1}$$

and the partition function as

$$\langle \mathfrak{Z}_N \rangle_f(\beta,\gamma) \stackrel{\mathrm{def}}{=} \int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^N} e^{-\beta\left(\frac{1}{N-1} \sum\sum_{j<k} c_j c_k U(\mathbf{s}_j, \mathbf{s}_k) + \gamma \sum_k c_k V(\mathbf{s}_k) \right)} \mathrm{d}\varrho_f^N \tag{3.2}$$

where the abbreviation $\sum\sum_{j<k}$ means the double sum over $1 \le j < k \le N$, $\sum_k$ means the sum over $1 \le k \le N$, and $\mathrm{d}\varrho_f(\mathbf{s}, c) \equiv f(c)\mathrm{d}c\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s})$, $\mathrm{d}\varrho_f^N$ is the abbreviation of $\prod_{j=1}^N \mathrm{d}\varrho_f(\mathbf{s}_j, c_j)$, with f the probability distribution of the random variable c on $\mathbb{R}$. Here $\mathrm{d}^{\mathrm{D}}\underline{\alpha}$ is the normalized uniform measure on $\mathbb{S}^{\mathrm{D}}$, while $\mathrm{d}^{\mathrm{D}}\alpha$ is the standard uniform measure on $\mathbb{S}^{\mathrm{D}}$, so that

$$\mathrm{d}^{\mathrm{D}}\underline{\alpha} = \frac{1}{\alpha(\mathrm{D})}\mathrm{d}^{\mathrm{D}}\alpha \tag{3.3}$$

in which the constant $\alpha(\mathrm{D})$ stands for the area of the D-dim unit sphere, i.e.

$$\alpha(\mathrm{D}) = \mathrm{Area}(\mathbb{S}^{\mathrm{D}}) = \begin{cases} \dfrac{2}{k!}\pi^{k+1} & \text{if } \mathrm{D} = 2k+1 \\ \dfrac{2(2\pi)^k}{(2k-1)!!} & \text{if } \mathrm{D} = 2k \end{cases} \tag{3.4}$$

The integral (3.2) can be estimated from above by adapting the strategy from [CLMP92], [Kie93], and [Kie11], using either a multi-variable Hölder inequality, the inequality of arithmetic and geometric means, or simply Jensen's inequality w.r.t. $\frac{1}{N}\sum_{j=1}^{N}(\,\cdot\,)$, and noting that the resulting integral factors into an $N-1$ fold product:

$$\begin{aligned}
&\int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^N} e^{-\beta\left(\frac{1}{N-1}\sum\sum_{j<k} c_j c_k U(\mathbf{s}_j,\mathbf{s}_k)+\gamma\sum_k c_k V(\mathbf{s}_k)\right)} \mathrm{d}\varrho_f^N \\
= \;& \int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^N} \left(\prod_{k=1}^{N}\prod_{j\neq k} e^{-\beta\frac{1}{2(N-1)}c_j c_k U(\mathbf{s}_j,\mathbf{s}_k)}\right)\cdot e^{-\beta\gamma\sum_k c_k V(\mathbf{s}_k)} \mathrm{d}\varrho_f^N \\
= \;& \int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^N} \left(\prod_{k=1}^{N}\prod_{j\neq k} e^{-\beta\frac{N}{2(N-1)}c_j c_k U(\mathbf{s}_j,\mathbf{s}_k)}\right)^{\frac{1}{N}}\cdot e^{-\beta\gamma\sum_k c_k V(\mathbf{s}_k)} \mathrm{d}\varrho_f^N \\
\leq \;& \int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^N} \frac{1}{N}\left(\sum_{k=1}^{N}\prod_{j\neq k} e^{-\beta\frac{N}{2(N-1)}c_j c_k U(\mathbf{s}_j,\mathbf{s}_k)}\right)\cdot e^{-\beta\gamma\sum_k c_k V(\mathbf{s}_k)} \mathrm{d}\varrho_f^N \qquad (3.5)\\
= \;& \frac{1}{N}\sum_{k=1}^{N}\int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^N} \left(\prod_{j\neq k} e^{-\beta\frac{N}{2(N-1)}c_j c_k U(\mathbf{s}_j,\mathbf{s}_k)-\beta\gamma c_j V(s_j)}\right)\cdot e^{-\beta\gamma c_k V(\mathbf{s}_k)} \mathrm{d}\varrho_f^N \\
= \;& \int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^N} \left(\prod_{j\neq 1} e^{-\beta\frac{N}{2(N-1)}c_j c_1 U(\mathbf{s}_j,\mathbf{s}_1)-\beta\gamma c_j V(\mathbf{s}_j)}\right)\cdot e^{-\beta\gamma c_1 V(\mathbf{s}_1)} \mathrm{d}\varrho_f^N \\
= \;& \int_{\mathbb{S}^{\mathrm{D}}\times\mathbb{R}} \left[\int_{\mathbb{S}^{\mathrm{D}}\times\mathbb{R}} e^{-\frac{N}{2(N-1)}\beta c c' U(\mathbf{s},\mathbf{s}')} e^{-\beta\gamma c' V(\mathbf{s}')} \mathrm{d}\varrho_f'\right]^{N-1} e^{-\beta\gamma c V(\mathbf{s})} \mathrm{d}\varrho_f
\end{aligned}$$

where $\mathrm{d}\varrho_f = f(c)\mathrm{d}c\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s})$ and $\mathrm{d}\varrho_f' = f(c')\mathrm{d}c'\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s}')$. By Fubini-Tonelli, we can exchange the order of integration in the $(\mathbf{s}, c)$, respectively $(\mathbf{s}', c')$ variables.

Suppose first that the support of f is bounded (hence compact). Let $\underline{c} = \min \mathrm{supp}\,(f)$ and $\overline{c} = \max \mathrm{supp}\,(f)$. Denote $\max |V(\mathbf{s})|$ by M_V. Then $e^{-\beta\gamma c V(\mathbf{s})} < C(\beta, \gamma)$, and it suffices to address the $\mathrm{d}^{\mathrm{D}}\underline{\alpha}'$ integral. Now, suppose U is the Green's function of the GJMS operator in the form of

$$U(\mathbf{s}, \mathbf{s}') = C(\mathrm{D}) \ln \frac{1}{|\mathbf{s}-\mathbf{s}'|} + \text{constant term} \qquad (3.6)$$

with both the positive coefficient $C(\mathrm{D})$ and the constant term depending on D. More precisely, when the dimension D is even, $\mathrm{D} = 2k$, the constant

$$C(\mathrm{D}) = \frac{1}{2^{2k-2}[(k-1)!]^2\alpha(2k-1)} = \frac{1}{2^{2k-1}\pi^k(k-1)!} \qquad (3.7)$$

Besides, the constant term is bounded below. We note that the additive constant in U does not change the integrability of the $\mathrm{d}^{\mathrm{D}}\underline{\alpha}'$ integral. Thus, the $\mathrm{d}^{\mathrm{D}}\underline{\alpha}'$ integral on the right hand side of (3.5) behaves like $\int_0^\epsilon x^p dx$ with $p = (\mathrm{D}-1) + \frac{N}{2(N-1)}\beta c c' C(\mathrm{D})$, so it is finite if and only if $cc'\beta > a(N)$, with $a(N) = -\frac{2\mathrm{D}}{C(\mathrm{D})}(1-\frac{1}{N})$. Clearly, $\beta = 0$ is always allowed, but nonzero β values are restricted in an f-dependent manner. Namely, if f

is supported on both positive and negative c-values, then we have

$$-\frac{2\mathrm{D}}{C(\mathrm{D})}(1-1/N)/\underline{c}\bar{c} > \beta > -\frac{2\mathrm{D}}{C(\mathrm{D})}(1-1/N)/\max\{\underline{c}^2,\bar{c}^2\}, \tag{3.8}$$

whereas in case that $\operatorname{supp}(f) \subset \overline{\mathbb{R}}_+$ *or* $\operatorname{supp}(f) \subset \overline{\mathbb{R}}_-$, we just have

$$\beta > -\frac{2\mathrm{D}}{C(\mathrm{D})}(1-1/N)/\max\{\underline{c}^2,\bar{c}^2\} \tag{3.9}$$

as sufficient condition(s) for the existence of r.h.s.(3.5), and thus of l.h.s.(3.5).

Whether these strict bounds are also necessary depends on the shape of f. Take for instance the special case where $\operatorname{supp}(f) \subset \overline{\mathbb{R}}_+$. If we now set $\beta = -\frac{2\mathrm{D}}{C(\mathrm{D})}(1 - 1/N)/\bar{c}^2$ and $c = \bar{c}$ then, viewed as function of c', the $\mathrm{d}^{\mathrm{D}}\underline{\alpha}'$ integral will diverge when c' approaches $\bar{c}$, but if $f(c')$ appoaches zero fast enough when $c' \to \bar{c}$ then the c' integral will still be finite, and the strict inequality in (3.9) can be changed into a non-strict inequality. Similarly the other cases for $\operatorname{supp}(f)$ can be discussed. In any event, a simple calculus exercise shows that l.h.s.(3.5) diverges if $\beta < -\frac{2\mathrm{D}}{C(\mathrm{D})}(1-1/N)/\max\{\underline{c}^2,\bar{c}^2\}$ and, in case that $\operatorname{supp} f$ lives on both positive and negative values, also if $\beta > -\frac{2\mathrm{D}}{C(\mathrm{D})}(1 - 1/N)/\underline{c}\bar{c}$.

Next, suppose that $\operatorname{supp}(f)$ is unbounded. Then $\underline{c} = -\infty$ or $\bar{c} = +\infty$ (note that both can be true simultaneously). Now, if $\operatorname{supp}(f)$ lives on both positive and negative values, then $\beta = 0$ is the only allowed β value for l.h.s. (3.5) to be finite; this case will therefore not be discussed any further. Therefore, let $\operatorname{supp}(f) \subset \overline{\mathbb{R}}_+$ *or* $\operatorname{supp}(f) \subset \overline{\mathbb{R}}_-$; in the former case $0 \le \underline{c} < \bar{c} = \infty$, while in the latter case $0 \ge \bar{c} > \underline{c} = -\infty$. In either of these two cases, $\beta \ge 0$ is the necessary and sufficient condition for the $\mathrm{d}^{\mathrm{D}}\underline{\alpha}'$ integral in (3.5) to be finite. However, now that $cc' \ge 0$ can be arbitrarily large, when $\beta > 0$ there will be a $c_*(\beta,\gamma)$, no matter what γ is, such that the $\mathrm{d}c'$ integral will not exist for $c > c_*(\beta,\gamma)$ if $f(c')$ does not decay to zero faster than exponential. But even if f decays superexponentially fast to zero, it is not clear whether r.h.s. (3.5) is bounded by some C^N or not.

For this reason we henceforth assume that f has compact support, leaving the case of unbounded support (which includes the interesting Gauss distribution) for some future work. We are now ready to state and prove our main results.

3.1 The Main Results and Their Proofs

We first prove that $\ln\langle \mathfrak{Z}_N\rangle_f(\beta,\gamma) = N\mathfrak{f}_f(\beta,\gamma) + o(N)$.

Theorem 5. *Suppose that* $\mathrm{supp}\,(f)$ *is compact. If f is supported on both positive and negative c-values, let β satisfy*

$$-\frac{2\mathrm{D}}{C(\mathrm{D})}/\underline{c}\overline{c} > \beta > -\frac{2\mathrm{D}}{C(\mathrm{D})}/\max\{\underline{c}^2,\overline{c}^2\}, \tag{3.10}$$

whereas in case that $\mathrm{supp}\,(f) \subset \overline{\mathbb{R}}_+$ or $\mathrm{supp}\,(f) \subset \overline{\mathbb{R}}_-$, *suppose merely that*

$$\beta > -\frac{2\mathrm{D}}{C(\mathrm{D})}/\max\{\underline{c}^2,\overline{c}^2\}. \tag{3.11}$$

Then

$$\lim_{N\to\infty} \tfrac{1}{N}\ln\langle \mathfrak{Z}_N\rangle_f(\beta,\gamma) = \mathfrak{f}_f(\beta,\gamma) \quad \textit{exists}, \tag{3.12}$$

where $\mathfrak{f}_f(\beta,\gamma)$ is a non-negative, bi-convex real function, with $\mathfrak{f}_f(0,\gamma) = 0$.

Proof of Theorem 5:

We define the abbreviation $\ln\langle \mathfrak{Z}_N\rangle_f(\beta,\gamma) \stackrel{\mathrm{def}}{=} \mathfrak{F}_f^{(N)}(\beta,\gamma)$, explicitly

$$\mathfrak{F}_f^{(N)}(\beta,\gamma) = \ln\int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^N} e^{-\beta\left(\frac{1}{N-1}\sum\sum_{j<k} c_jc_kU(\mathbf{s}_j,\mathbf{s}_k)+\gamma\sum_k c_kV(\mathbf{s}_k)\right)}\mathrm{d}\varrho_f^N. \tag{3.13}$$

Note first that $\mathfrak{F}_f^{(N)}(0,\gamma) = 0\ \forall N$, so $\mathfrak{f}_f(0,\gamma)$ exists and $\mathfrak{f}_f(0,\gamma) = 0$, indeed.

Note next that Jensen's inequality w.r.t. $\mathrm{d}^{\mathrm{D}}\underline{\alpha}^N$ yields

$$\ln\int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^N} e^{-\beta\left(\frac{1}{N-1}\sum\sum_{j<k} c_jc_kU(\mathbf{s}_j,\mathbf{s}_k)+\gamma\sum_k c_kV(\mathbf{s}_k)\right)}\mathrm{d}\varrho_f^N \geq 0 \tag{3.14}$$

for all β satisfying (3.10), respectively (3.11), and arbitrary γ. To arrive at (3.14) we also used the integration condition

$$\int_{\mathbb{S}^{\mathrm{D}}} U(\mathbf{s},\mathbf{s}')\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s}') = 0\ \forall\ \mathbf{s}\in\mathbb{S}^{\mathrm{D}}, \tag{3.15}$$

and $\int_{\mathbb{S}^{\mathrm{D}}} V(\mathbf{s}_k)\mathrm{d}^{\mathrm{D}}\underline{\alpha} = 0$, and finally $\int_{\mathbb{R}} f(c)\mathrm{d}c = 1$. Thus,

$$\liminf_{N\to\infty} \tfrac{1}{N}\mathfrak{F}_f^{(N)}(\beta,\gamma) \geq 0. \tag{3.16}$$

Incidentally, a complementary upper bound to $N^{-1}\mathfrak{F}_f^{(N)}(\beta,\gamma)$ is obtained by noting that for each β satisfying the bounds pertinent to the support properties of f, eventually N will be large enough so that also (3.8), respectively (3.9) is satisfied. Now the upper bound r.h.s.(3.5) provides the upper bound

$$\limsup_{N\to\infty}\tfrac{1}{N}\mathfrak{F}_f^{(N)}(\beta,\gamma) \leq \ln\sup_{\mathbf{s},c}\int_{\mathbb{S}^{\mathrm{D}}\times\mathbb{R}} e^{-\frac{1}{2}\beta cc'U(\mathbf{s},\mathbf{s}')}e^{-\beta\gamma c'V(\mathbf{s}')}\mathrm{d}\varrho_f' \tag{3.17}$$

for all β satisfying (3.10), respectively (3.11), and arbitrary γ. The upper and lower bounds on $N^{-1}\mathfrak{F}_f^{(N)}(\beta,\gamma)$ guarantee the existence of limit points for the sequence $N\mapsto N^{-1}\mathfrak{F}_f^{(N)}(\beta,\gamma)$, but not yet a limit.

The existence of a non-negative limit (3.12) follows from (3.16) and:

Proposition 1. *Let β satisfy (3.10) or (3.11), pertinent to f. Also let $N = N_1 + N_2$ be big enough such that (3.8) or (3.9) hold irrespective of whether N_1 or N_2 replace N, there. Then $\mathfrak{F}_f^{(N)}(\beta,\gamma)$ is sub-additive in the sense that*

$$\mathfrak{F}_f^{(N)}(\beta,\gamma) \leq \mathfrak{F}_f^{(N_1)}(\beta,\gamma) + \mathfrak{F}_f^{(N_2)}(\beta,\gamma). \tag{3.18}$$

Proof of Proposition 1:

The proof follows closely the proof of proposition 1 in [Kie11], which has a precurser in [Kie93]. Namely, we note that (3.13) is the maximum for the *effective entropy of* $\varrho^{(N)}\in\mathfrak{P}^s((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^N)$, $N\geq 2$, given by

$$\mathcal{S}_{\beta,\gamma}^{(N)}\big(\varrho^{(N)}\big) \equiv \mathcal{R}^{(N)}\Big(\varrho^{(N)}|\varrho_f^N\Big) - \beta\varrho^{(N)}\Big[\tfrac{1}{N-1}\sum\sum_{1\leq j<k\leq N} c_jc_kU(\mathbf{s}_j,\mathbf{s}_k) + \gamma\sum_{1\leq k\leq N} c_kV(\mathbf{s}_k)\Big] \tag{3.19}$$

where the *entropy of* $\varrho^{(N)}$ *relative to* $\varrho_f^N\in\mathfrak{P}^s((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^N)$ is defined by

$$\mathcal{R}^{(N)}\Big(\varrho^{(N)}|\varrho_f^N\Big) = -\int_{\mathbb{S}^{\mathrm{D}}\times\mathbb{R}} \ln\Big[\tfrac{\mathrm{d}\varrho^{(N)}}{\mathrm{d}\varrho_f^N}\Big]\mathrm{d}\varrho^{(N)} \tag{3.20}$$

if $\varrho^{(N)}$ is absolutely continuous w.r.t. ϱ_f^N, and provided the integral in (3.20) exists; in all other cases, $\mathcal{R}^{(N)}\big(\varrho^{(N)}|\varrho_f^N\big) := -\infty$. Moreover, $\varrho^{(N)}(\,\cdot\,)$ denotes expected value $\int(\,\cdot\,)\varrho^{(N)}\big(\mathrm{d}^{\mathrm{D}}\underline{\alpha}^N\prod^N f\mathrm{d}c\big)$. For $N\geq 2$, when β satisfies (3.10), respectively (3.11), and for arbitrary γ, the effective entropy functional (3.19) achieves its supremum at the unique normalized measure

$$\varrho^{(N)}_{\beta,\gamma}(\mathrm{d}\varrho^N_f) = \frac{e^{-\beta\left(\frac{1}{N-1}\sum\sum_{j<k} c_jc_kU(\mathbf{s}_j,\mathbf{s}_k)+\gamma\sum_k c_kV(\mathbf{s}_k)\right)}\mathrm{d}\varrho^N_f}{\int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^N} e^{-\beta\left(\frac{1}{N-1}\sum\sum_{j<k} c_jc_kU(\mathbf{s}_j,\mathbf{s}_k)+\gamma\sum_k c_kV(\mathbf{s}_k)\right)}\mathrm{d}\varrho^N_f}; \tag{3.21}$$

here again, $\sum_k = \sum_{1\leq k\leq N}$, while $\sum\sum_{j<k} = \sum\sum_{1\leq j<k\leq N}$. Thus

$$\max_{\varrho^{(N)}\in\mathfrak{P}^s((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^N)} \mathcal{S}^{(N)}_{\beta,\gamma}\big(\varrho^{(N)}\big) = \mathcal{S}^{(N)}_{\beta,\gamma}\big(\varrho^{(N)}_{\beta,\gamma}\big). \tag{3.22}$$

Moreover,

$$\mathcal{S}^{(N)}_{\beta,\gamma}\big(\varrho^{(N)}_{\beta,\gamma}\big) = \mathfrak{F}^{(N)}_f(\beta,\gamma). \tag{3.23}$$

Now note that

$$\varrho^{(N)}_{\beta,\gamma}\Big(\sum_{1\leq k\leq N} c_kV(\mathbf{s}_k)\Big) = N\,{}^{(1)}\varrho^{(N)}_{\beta,\gamma}\big(cV(\mathbf{s})\big) \tag{3.24}$$

and

$$\varrho^{(N)}_{\beta,\gamma}\Big(\tfrac{1}{N-1}\sum\sum_{1\leq j<k\leq N} c_jc_kU(\mathbf{s}_j,\mathbf{s}_k)\Big) = N\,{}^{(2)}\varrho^{(N)}_{\beta,\gamma}\big(\tfrac{1}{2}cc'U(\mathbf{s},\mathbf{s}')\big), \tag{3.25}$$

where ${}^{(1)}\varrho^{(N)}_{\beta,\gamma}$ and ${}^{(2)}\varrho^{(N)}_{\beta,\gamma}$ are the first and second marginal measures of $\varrho^{(N)}_{\beta}$. So,

$$\begin{aligned}
\mathcal{S}^{(N)}_{\beta,\gamma}(\varrho^{(N)}_{\beta,\gamma}) \leq\ & \mathcal{R}^{(N_1)}\big({}^{(N_1)}\varrho^{(N)}_{\beta,\gamma}|\varrho^{N_1}_f\big) - N_1\beta\big[{}^{(2)}\varrho^{(N)}_{\beta,\gamma}\big(\tfrac{1}{2}cc'U(\mathbf{s},\mathbf{s}')\big) + {}^{(1)}\varrho^{(N)}_{\beta,\gamma}\big(\gamma cV(\mathbf{s})\big)\big] \\
& +\mathcal{R}^{(N_2)}\big({}^{(N_2)}\varrho^{(N)}_{\beta,\gamma}|\varrho^{N_2}_f\big) - N_2\beta\big[{}^{(2)}\varrho^{(N)}_{\beta,\gamma}\big(\tfrac{1}{2}cc'U(\mathbf{s},\mathbf{s}')\big) + {}^{(1)}\varrho^{(N)}_{\beta,\gamma}\big(\gamma cV(\mathbf{s})\big)\big] \\
\leq\ & \mathcal{R}^{(N_1)}\big(\varrho^{(N_1)}_{\beta,\gamma}|\varrho^{N_1}_f\big) - N_1\beta\big[{}^{(2)}\varrho^{(N_1)}_{\beta,\gamma}\big(\tfrac{1}{2}cc'U(\mathbf{s},\mathbf{s}')\big) + {}^{(1)}\varrho^{(N_1)}_{\beta,\gamma}\big(\gamma cV(\mathbf{s})\big)\big] \\
& +\mathcal{R}^{(N_2)}\big(\varrho^{(N_2)}_{\beta,\gamma}|\varrho^{N_2}_f\big) - N_2\beta\big[{}^{(2)}\varrho^{(N_2)}_{\beta,\gamma}\big(\tfrac{1}{2}cc'U(\mathbf{s},\mathbf{s}')\big) + {}^{(1)}\varrho^{(N_2)}_{\beta,\gamma}\big(\gamma cV(\mathbf{s})\big)\big] \\
=\ & \mathcal{S}^{(N_1)}_{\beta,\gamma}(\varrho^{(N_1)}_{\beta,\gamma}) + \mathcal{S}^{(N_2)}_{\beta,\gamma}(\varrho^{(N_2)}_{\beta,\gamma})
\end{aligned} \tag{3.26}$$

where the first inequality is the well-known sub-additivity of relative entropy together with setting $N = N_1 + N_2$ in (3.24) and (3.25), while the second inequality is just our maximum effective entropy variational principle.

This proves Proposition 1. $\square$

Proposition 1 and the lower bound (3.14) prove (3.12), and that $\mathfrak{f}_f(\beta,\gamma) \geq 0$.

Taking two β derivatives shows that the map $\beta \mapsto N^{-1}\mathfrak{F}_f^{(N)}(\beta,\gamma)$ is convex, and similarly two γ derivatives show that $\gamma \mapsto N^{-1}\mathfrak{F}_f^{(N)}(\beta,\gamma)$ is convex. So $\mathfrak{f}_f(\beta,\gamma) = \lim\limits_{N\to\infty} N^{-1}\mathfrak{F}_f^{(N)}(\beta,\gamma)$ is bi-convex.

This completes the proof of Theorem 5. □

Note that bi-convexity implies that $\mathfrak{f}_f(\beta,\gamma)$ is continuous in each variable.

To evaluate $\mathfrak{f}_f(\beta,\gamma)$ we now use a refinement of the strategy in [CLMP92], [Kie93] and [Kie11] to establish $\mathfrak{L}^\wp$ bounds uniformly in N for the N-sequence of each n-th marginal measure of (3.21), which reads

$$\mathrm{d}^{(n)}\varrho_{\beta,\gamma}^{(N)} = \frac{\displaystyle\int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^{N-n}} e^{-\beta\left(\frac{1}{N-1}\sum\sum_{j<k} c_jc_kU(\mathbf{s}_j,\mathbf{s}_k)+\gamma\sum_k c_kV(\mathbf{s}_k)\right)}\mathrm{d}\varrho_f^{N-n}}{\displaystyle\int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^{N}} e^{-\beta\left(\frac{1}{N-1}\sum\sum_{j<k} c_jc_kU(\mathbf{s}_j,\mathbf{s}_k)+\gamma\sum_k c_kV(\mathbf{s}_k)\right)}\mathrm{d}\varrho_f^{N}}\,\mathrm{d}\varrho_f^n; \tag{3.27}$$

here, the integral in the numerator runs over the variables $(\mathbf{s}_{n+1}, c_{n+1})$ to $(\mathbf{s}_N, c_N)$. Then we can extract an $\mathfrak{L}^\wp$-weakly convergent subsequence of each n-th marginal measure sequence. This information and the subadditivity of relative entropy finally allows us to extend the finite-N random-holodic variational principle to the limit $N\to\infty$, which characterizes $\mathfrak{f}_f(\beta,\gamma)$.

Lemma 1. *For each n and β satisfying (3.10), respectively (3.11), and for arbitrary γ, there exists a constant $C(n,\beta,\gamma)$ such that*

$$\mathrm{d}^{(n)}\varrho_{\beta,\gamma}^{(N)} \le C(n,\beta,\gamma)e^{-\frac{1}{N-1}\sum\sum_{j<k}\beta c_jc_kU(\mathbf{s}_j,\mathbf{s}_k)}\mathrm{d}\varrho_f^n. \tag{3.28}$$

Proof of Lemma 1:

We define a new a-priori measure $\mathrm{d}\tau_{\beta\gamma} = e^{-\beta\gamma cV(\mathbf{s})}\mathrm{d}\varrho_f$ and rewrite (3.27) as

$$\mathrm{d}^{(n)}\varrho_{\beta,\gamma}^{(N)} = \frac{\displaystyle\int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^{N-n}} e^{-\frac{1}{N-1}\sum\sum_{j<k}\beta c_jc_kU(\mathbf{s}_j,\mathbf{s}_k)}\mathrm{d}\tau_{\beta\gamma}^{N-n}}{\displaystyle\int_{(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^{N}} e^{-\frac{1}{N-1}\sum\sum_{j<k}\beta c_jc_kU(\mathbf{s}_j,\mathbf{s}_k)}\mathrm{d}\tau_{\beta\gamma}^{N}}\,\mathrm{d}\tau_{\beta\gamma}^n; \tag{3.29}$$

note that $\tau_{\beta\gamma}$ is generally not a probability measure. We now follow [Kie11].

Let $\mathbf{s}_1, ..., \mathbf{s}_n$ jointly be denoted by $S^{(n)}$, and $\mathbf{s}_{n+1}, ..., \mathbf{s}_N$ be denoted jointly by $S^{(N-n)}$. Then, for any $N\ge 2$ and $1\le n<N$ we set $S^{(N)}\equiv(S^{(n)},S^{(N-n)})$. Accordingly we write $\sum\sum_{1\le j<k\le N} c_jc_kU(\mathbf{s}_j,\mathbf{s}_k) = K^{(n)} + K^{(n,N-n)} + K^{(N-n)}$, where

the superscripts indicate, respectively, the dependence on $S^{(n)}$ alone, or on $S^{(n)}$ and $S^{(N-n)}$, or on $S^{(N-n)}$ alone.

Each K term has a number of logarithmic singularities, but $K^{(n)}$ has a fixed number of these and $(N-1)^{-1}K^{(n)}$ goes to zero pointwise a.e. when $N\to\infty$, so that eventually, when N is big enough, $\exp(-(N-1)^{-1}\beta K^{(n)})\in\mathfrak{L}^{\wp}((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^n,\mathrm{d}\varrho_f^n)\equiv\mathfrak{L}^{\wp}((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^n)$ for any $\wp<\infty$.

To estimate the remaining terms, for any $\wp<\infty$ we define the Lebesgue spaces $\mathfrak{L}^{\wp}_{\beta\gamma}((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^n)\equiv\mathfrak{L}^{\wp}((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^n,\mathrm{d}\tau^n_{\beta\gamma})$. Now, if f is supported on both positive and negative c-values, then all $\mathfrak{L}^{\wp}_{\beta\gamma}$-integrals below exist whenever

$$N\geq N_f(n,\beta)=\min_{N'>2n+1}\left\{N'\;\middle|\;\frac{2\mathrm{D}}{C(\mathrm{D})}/\underline{c}\overline{c}<-\beta\tfrac{N'-n-1}{N'-2n-1}<\frac{2\mathrm{D}}{C(\mathrm{D})}/\max\{\underline{c}^2,\overline{c}^2\}\right\};\tag{3.30}$$

in case that $\operatorname{supp}(f)\subset\overline{\mathbb{R}}_+$ *or* $\operatorname{supp}(f)\subset\overline{\mathbb{R}}_-$, all integrals below exist when

$$N\geq N_f(n,\beta)=\min_{N'>2n+1}\left\{N'\;\middle|\;-\beta\tfrac{N'-n-1}{N'-2n-1}<\frac{2\mathrm{D}}{C(\mathrm{D})}/\max\{\underline{c}^2,\overline{c}^2\}\right\}.\tag{3.31}$$

Set $q=(N-1)/2n$ and $q'=(N-1)/(N-2n-1)$.By Hölder's inequality,

$$\begin{aligned}&\left\|\exp\left(-\tfrac{1}{N-1}\beta[K^{(n,N-n)}+K^{(N-n)}]\right)\right\|_{\mathfrak{L}^1_{\beta\gamma}((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^{N-n})}\leq\\&\left\|\exp\left(-\tfrac{1}{N-1}\beta K^{(n,N-n)}\right)\right\|_{\mathfrak{L}^q_{\beta\gamma}((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^{N-n})}\left\|\exp\left(-\tfrac{1}{N-1}\beta K^{(N-n)}\right)\right\|_{\mathfrak{L}^{q'}_{\beta\gamma}((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^{N-n})}\end{aligned}\tag{3.32}$$

Notice that the norms involving $K^{(n,N-n)}$ are functions of n points in $\mathbb{S}^{\mathrm{D}}$. Now,

$$\left\|e^{-\frac{1}{N-1}\beta K^{(n,N-n)}}\right\|_{\mathfrak{L}^q_{\beta\gamma}((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^{N-n})}=\left\|e^{-\frac{1}{N-1}\sum_{k=1}^n\beta cc_kU(\mathbf{s}_k,\,\cdot\,)}\right\|^{N-n}_{\mathfrak{L}^q_{\beta\gamma}(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})},\tag{3.33}$$

by permutation symmetry. The right hand side of (3.33) can be estimated from above, uniformly in N, as follows. Since the constant term of $U(\mathbf{s},\mathbf{s}')$ is bounded below, we can modify it to be a nonnegative function $U^+(\mathbf{s},\mathbf{s}')$ by adding a positive constant big enough to $U(\mathbf{s},\mathbf{s}')$. Defining now

$$\mathcal{B}_f(\beta)\equiv\max_{cc'}\{-\beta cc'\}\qquad\text{and}\qquad\mathcal{B}^*_f(\beta)\equiv\max_{cc'}\{\beta cc'\},\tag{3.34}$$

we can first of all estimate the right hand side of (3.33) by

$$\left\|e^{-\frac{1}{N-1}\sum\limits_{k=1}^n\beta cc_kU(\mathbf{s}_k,\,\cdot\,)}\right\|^{N-n}_{\mathfrak{L}^q_{\beta\gamma}}\leq e^{n\frac{N-n}{N-1}\frac{\mathcal{B}^*_f(\beta)}{4\pi}}\left\|e^{-\frac{1}{N-1}\sum\limits_{k=1}^n\beta cc_kU^+(\mathbf{s}_k,\,\cdot\,)}\right\|^{N-n}_{\mathfrak{L}^q_{\beta\gamma}},\tag{3.35}$$

where we dropped the argument $(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})$ from $\mathfrak{L}^q_{\beta\gamma}(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})$, as no confusion could arise. Second, using (3.34) again, and then n-fold symmetric decreasing rearrangement [Ban80] (here: moving all $\mathbf{s}_k\to\mathbf{s}_0$), we estimate

$$\left\|e^{-\frac{1}{N-1}\sum_{k=1}^{n}\beta c c_k U^+(\mathbf{s}_k,\,\cdot\,)}\right\|^{N-n}_{\mathfrak{L}^q_{\beta\gamma}} \leq \left\|e^{\frac{1}{N-1}n\mathcal{B}_f(\beta)U^+(\mathbf{s}_0,\,\cdot\,)}\right\|^{N-n}_{\mathfrak{L}^q_{\beta\gamma}} \tag{3.36}$$

and note that the norm at the right hand side of (3.36) can be calculated exactly and equals

$$\left\|e^{\frac{1}{2}\mathcal{B}_f(\beta)U^+(\mathbf{s}_0,\,\cdot\,)}\right\|^{2n\frac{N-n}{N-1}}_{\mathfrak{L}^1_{\beta\gamma}} = \Big(\frac{\frac{2\mathrm{D}}{C(\mathrm{D})}}{\frac{2\mathrm{D}}{C(\mathrm{D})}-\mathcal{B}_f(\beta)}\int_{\mathbb{R}} e^{-\beta\gamma c V(\mathbf{s})}f(c)\mathrm{d}c\Big)^{2n\frac{N-n}{N-1}}, \tag{3.37}$$

which is $< C$ independently of N because $\frac{2\mathrm{D}}{C(\mathrm{D})}-\mathcal{B}_f(\beta)>0$, by hypothesis.

Next, the second norm at r.h.s. (3.32) can be rewritten thusly,

$$\left\|e^{-\frac{1}{N-1}\beta K^{(N-n)}}\right\|_{\mathfrak{L}^{q'}_{\beta\gamma}((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^{N-n})} = \langle\mathfrak{Z}_{N-n}\rangle_f\Big(\tfrac{N-n-1}{N-2n-1}\beta,\,\tfrac{N-2n-1}{N-n-1}\gamma\Big)^{1-2n/(N-1)}. \tag{3.38}$$

Since we already proved that the limit of the sequence

$$N\mapsto N^{-1}\mathfrak{F}^{(N)}_f(\beta,\gamma) = N^{-1}\ln\langle\mathfrak{Z}_N\rangle_f(\beta,\gamma)$$

exists for all $\mathcal{B}_f(\beta)<\frac{2\mathrm{D}}{C(\mathrm{D})}$, we see that

$$\langle\mathfrak{Z}_{N-n}\rangle_f\Big(\tfrac{N-n-1}{N-2n-1}\beta,\,\tfrac{N-2n-1}{N-n-1}\gamma\Big)^{-2n/(N-1)} \stackrel{N\to\infty}{\longrightarrow} e^{-2n\mathfrak{f}_f(\beta,\gamma)}, \tag{3.39}$$

which implies a bound uniformly w.r.t. N when $N\geq N_f$, because $\mathcal{B}_f(\beta)<\frac{2\mathrm{D}}{C(\mathrm{D})}$. It remains to estimate the term $\langle\mathfrak{Z}_{N-n}\rangle_f\Big(\frac{N-n-1}{N-2n-1}\beta,\,\frac{N-2n-1}{N-n-1}\gamma\Big)$.

Applying Jensen's inequality w.r.t. $\mathrm{d}^{\mathrm{D}}\underline{\alpha}^n$ to $\langle\mathfrak{Z}_N\rangle_f(\beta,\gamma)$ we find

$$\langle\mathfrak{Z}_N\rangle_f(\beta,\gamma)\geq\langle\mathfrak{Z}_{N-n}\rangle_f\Big(\tfrac{N-n-1}{N-1}\beta,\,\tfrac{N-1}{N-n-1}\gamma\Big), \tag{3.40}$$

where we used (3.15) and $\int_{\mathbb{S}^{\mathrm{D}}}V(\mathbf{s}_k)\mathrm{d}^{\mathrm{D}}\underline{\alpha}=0$, and finally $\int_{\mathbb{R}}f(c)\mathrm{d}c=1$. Next, define the expectation functional $\langle\,\cdot\,\rangle_N$ w.r.t. the probability measure

$$\langle\mathfrak{Z}_{N-n}\rangle_f\Big(\tfrac{N-n-1}{N-2n-1}\beta,\,\tfrac{N-2n-1}{N-n-1}\gamma\Big)^{-1}\exp\Big[-(N-2n-1)^{-1}\beta K^{(N-n)}\Big]\,\mathrm{d}\tau^{N-n}_{\beta\gamma}. \tag{3.41}$$

Then we have the identity

$$\frac{\langle\mathfrak{Z}_{N-n}\rangle_f\Big(\frac{N-n-1}{N-1}\beta,\,\frac{N-1}{N-n-1}\gamma\Big)}{\langle\mathfrak{Z}_{N-n}\rangle_f\Big(\frac{N-n-1}{N-2n-1}\beta,\,\frac{N-2n-1}{N-n-1}\gamma\Big)} = \Big\langle\exp\Big(\tfrac{2n}{(N-1)(N-2n-1)}\beta K^{(N-n)}\Big)\Big\rangle_N. \tag{3.42}$$

Now using Jensen's inequality w.r.t. $\langle \cdot \rangle_N$ yields

$$\left\langle \exp\left(\tfrac{2n}{(N-1)(N-2n-1)}\beta K^{(N-n)}\right)\right\rangle_N \geq \exp\left(\tfrac{2n}{(N-1)(N-2n-1)}\left\langle \beta K^{(N-n)}\right\rangle_N\right). \tag{3.43}$$

By elementary calculus,

$$-\partial_\beta\Big[\mathfrak{F}_f^{(N-n)}\Big(\tfrac{N-n-1}{N-2n-1}\beta,\, \tfrac{N-2n-1}{N-n-1}\gamma\Big)\Big] = \tfrac{1}{N-2n-1}\left\langle K^{(N-n)}\right\rangle_N + \gamma\left\langle \sum_{k=n+1}^{N} c_k V(s_k)\right\rangle_N . \tag{3.44}$$

Since the definition of $L^{(N)}$ implies that $|\gamma\left\langle \sum_{k=n+1}^{N} c_k V(s_k)\right\rangle_N| = O(N)$, we can right away turn our attention to l.h.s.(3.44).

Since $\beta \mapsto \mathfrak{F}_f^{(N)}(\beta,\gamma) \geq 0$ is convex and $\mathfrak{F}_f^{(N)}(0,\gamma) = 0$, its derivative $\partial_\beta\mathfrak{F}_f^{(N)}(\beta,\gamma) \leq 0$ when $\beta < 0$, and $\partial_\beta\mathfrak{F}_f^{(N)}(\beta,\gamma) \geq 0$ when $\beta > 0$, for each β satisfying $\mathcal{B}_f(\beta) < \frac{2\mathrm{D}}{C(\mathrm{D})}$ provided N is big enough for the integrals to exist. So $-\beta\partial_\beta\mathfrak{F}_f^{(N)}(\beta,\gamma) \leq 0$ for all β satisfying $\mathcal{B}_f(\beta) < \frac{2\mathrm{D}}{C(\mathrm{D})}$ and N big enough, and the same is true for l.h.s.(3.44). Therefore we need to show that $\beta\partial_\beta\mathfrak{F}_f^{(N)}(\beta,\gamma) \leq C_f(\beta,\gamma)N$.

For this we invoke the limit function $\mathfrak{f}_f(\beta,\gamma)$ which, by its bi-convexity, is β-differentiable almost everywhere. In particular, its right β-derivative $\partial_\beta^+\mathfrak{f}_f(\beta,\gamma)$ exists whenever $\mathcal{B}_f(\beta) < \frac{2\mathrm{D}}{C(\mathrm{D})}$, and by the β-convexity, for any two β values $\beta_1 < \beta_2$ satisfying $\mathcal{B}_f(\beta_k) < \frac{2\mathrm{D}}{C(\mathrm{D})}$, $k \in \{1,2\}$, we have the ordering

$$\partial_\beta^+\mathfrak{f}_f(\beta_1,\gamma) \leq \partial_\beta^+\mathfrak{f}_f(\beta_2,\gamma). \tag{3.45}$$

Moreover, since $\mathfrak{f}_f(0,\gamma) = 0$ as shown earlier, $\partial_\beta^+\mathfrak{f}_f(\beta,\gamma) \leq 0$ for $\beta < 0$, and $\partial_\beta^+\mathfrak{f}_f(\beta,\gamma) \geq 0$ for $\beta > 0$. Thus, for all β satisfying $\mathcal{B}_f(\beta) < \frac{2\mathrm{D}}{C(\mathrm{D})}$,

$$0 \leq \beta\partial_\beta^+\mathfrak{f}_f(\beta,\gamma) < \infty. \tag{3.46}$$

Now, for each β satisfying $\mathcal{B}_f(\beta) < \frac{2\mathrm{D}}{C(\mathrm{D})}$ there exists some $\epsilon > 0$ such that $(1+\epsilon)\beta \stackrel{\text{def}}{=} *\beta$ satisfies $\mathcal{B}_f(*\beta) < \frac{2\mathrm{D}}{C(\mathrm{D})}$, too. Note that $*\beta < \beta$ if $\beta < 0$ and $*\beta > \beta$ if $\beta > 0$. So by (3.45) and (3.46), for any β satisfying $\mathcal{B}_f(\beta) < \frac{2\mathrm{D}}{C(\mathrm{D})}$,

$$\beta\partial_\beta^+\mathfrak{f}_f(\beta,\gamma) \leq \beta\partial_\beta^+\mathfrak{f}_f(*\beta,\gamma). \tag{3.47}$$

Next, since $\frac{N-n-1}{N-2n-1} \stackrel{N\to\infty}{\longrightarrow} 1$, eventually $\frac{N-n-1}{N-2n-1}\beta \in [*\beta,\beta]$ if $\beta < 0$, respectively $\frac{N-n-1}{N-2n-1}\beta \in [\beta,*\beta]$ if $\beta > 0$. Therefore (cf. [Kie93]), eventually

$$\beta\partial_\beta\Big[\tfrac{1}{N-1}\mathfrak{F}_f^{(N-n)}\Big(\tfrac{N-n-1}{N-2n-1}\beta,\, \tfrac{N-2n-1}{N-n-1}\gamma\Big)\Big] \leq \beta\partial_\beta^+\mathfrak{f}_f(*\beta,\gamma). \tag{3.48}$$

And so, for some suitable $C > 0$, we conclude that uniformly in N,

$$\exp\Big(\tfrac{2n}{(N-1)(N-2n-1)}\Big\langle \beta K^{(N-n)}\Big\rangle_N\Big) \geq C\exp\Big(-2n\beta\partial_\beta^+ \mathfrak{f}_f(*\beta,\gamma)\Big). \qquad (3.49)$$

This proves Lemma 1. $\square$

By hypothesis, $f(c)$ has compact support, and $\mathbb{S}^{\mathrm{D}}$ is compact. So Lemma 1 guarantees that for each $n \in \mathbb{N}$ and $\wp < \infty$ the sequence $N \mapsto {}^{(n)}\!\varrho_{\beta,\gamma}^{(N)}$ is weakly compact in $\mathfrak{P}_\wp((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^n) \stackrel{\mathrm{def}}{=} (\mathfrak{P}\cap\mathfrak{L}^\wp)((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^n)$, which are the absolutely continuous (w.r.t. $\mathrm{d}\varrho_f^n$) probability measures on $(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^n$ whose density is in $\mathfrak{L}^\wp((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^n)$. (For non-compact domains, see [KiSp99, ChKi00].)

We next characterize the limit points in terms of the $N = \infty$ counterpart of the variational principle (3.22). We denote by $\mathfrak{P}^s((\mathbb{S}^{\mathrm{D}} \times \mathbb{R})^{\mathbb{N}})$ the permutation-symmetric probability measures on the set of infinite exchangeable sequences in $\mathbb{S}^{\mathrm{D}} \times \mathbb{R}$. Let $\{{}^{(n)}\!\varrho\}_{n\in\mathbb{N}}$ denote the sequence of marginals of any $\varrho \in \mathfrak{P}^s((\mathbb{S}^{\mathrm{D}} \times \mathbb{R})^{\mathbb{N}})$. The deFinetti-Dynkin-Hewitt-Savage decomposition theorem for $\mathfrak{P}^s((\mathbb{S}^{\mathrm{D}} \times \mathbb{R})^{\mathbb{N}})$ states that for each $\varrho \in \mathfrak{P}^s((\mathbb{S}^{\mathrm{D}} \times \mathbb{R})^{\mathbb{N}})$ there exists a unique probability measure $\nu(\mathrm{d}\varsigma|\varrho)$ on $\mathfrak{P}(\mathbb{S}^{\mathrm{D}} \times \mathbb{R})$, such that ${}^{(n)}\!\varrho$, the n-th marginal measure of ϱ, is given by

$$\mathrm{d}^{(n)}\!\varrho = \int_{\mathfrak{P}(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})} \varsigma^{\otimes n}(\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s}_1)\mathrm{d}c_1\cdots\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s}_n)\mathrm{d}c_n)\,\nu(\mathrm{d}\varsigma|\varrho) \quad \forall n\in\mathbb{N}; \qquad (3.50)$$

where $\varsigma^{\otimes n}(\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s}_1)\mathrm{d}c_1\cdots\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s}_n)\mathrm{d}c_n) \equiv \varsigma(\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s}_1)\mathrm{d}c_1)\otimes\cdots\otimes\varsigma(\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s}_n)\mathrm{d}c_n)$.

Theorem 6. *For any β satisfying $\mathcal{B}_f(\beta) < \frac{2\mathrm{D}}{C(\mathrm{D})}$ and $n\in\mathbb{N}$ the sequence $\{{}^{(n)}\varrho_{\beta,\gamma}^{(N)}\}_{N\in\mathbb{N}}$ is weakly $\mathfrak{L}^\wp$-compact for $1 \leq \wp < \infty$. So one can extract a subsequence $\{{}^{(n)}\varrho_{\beta,\gamma}^{(\dot{N}[N])}\}_{N\in\mathbb{N}}$ such that $\forall n\in\mathbb{N}$, weakly*

$$\lim_{N\to\infty} {}^{(n)}\!\varrho_{\beta,\gamma}^{(\dot{N}[N])} = {}^{(n)}\!\dot{\varrho}_{\beta,\gamma} \in \mathfrak{P}^s((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^n). \qquad (3.51)$$

The decomposition measure $\nu(\mathrm{d}\varsigma|\dot{\varrho}_{\beta,\gamma})$ of each limit point $\dot{\varrho}_{\beta,\gamma}$ is supported by the subset $(\mathfrak{P}\cap\mathfrak{L}^1\ln\mathfrak{L}^1)(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})$ of $\mathfrak{P}(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})$ which consists of measures $\varsigma_{\beta,\gamma}(\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s})\mathrm{d}c)$ which maximize the effective configurational entropy functional

$$\mathcal{S}_{\beta,\gamma}(\varsigma) \stackrel{\mathit{def}}{=} \mathcal{R}^{(1)}(\varsigma|\varrho_f) - \beta\tfrac{1}{2}\varsigma^{\otimes 2}\big(K^{(2)}\big) - \beta\gamma\varsigma\big(cV\big), \qquad (3.52)$$

and

$$\mathcal{S}_{\beta,\gamma}(\varsigma_{\beta,\gamma}) = \mathfrak{f}_f(\beta,\gamma) \qquad \forall\beta:\ \mathcal{B}_f(\beta) < \frac{2\mathrm{D}}{C(\mathrm{D})}. \qquad (3.53)$$

Proof of Theorem 6:

We introduce the subsets $\mathfrak{P}^s_\wp((\mathbb{S}^{\rm D}\times\mathbb{R})^{\mathbb{N}}) \subset \mathfrak{P}^s((\mathbb{S}^{\rm D}\times\mathbb{R})^{\mathbb{N}})$, with $\wp > 1$, as the probability measures on $(\mathbb{S}^{\rm D}\times\mathbb{R})^{\mathbb{N}}$ whose decomposition measure is concentrated on $\mathfrak{P}_\wp(\mathbb{S}^{\rm D}\times\mathbb{R}) \stackrel{\rm def}{=} (\mathfrak{P}\cap\mathfrak{L}^\wp)(\mathbb{S}^{\rm D}\times\mathbb{R})$, which are the absolutely continuous (w.r.t. $\mathrm{d}^{\rm D}\underline{\alpha}\mathrm{d}c$) probability measures on $\mathbb{S}^{\rm D}\times\mathbb{R}$ whose density is in $\mathfrak{L}^\wp(\mathbb{S}^{\rm D}\times\mathbb{R},\mathrm{d}^{\rm D}\underline{\alpha}\mathrm{d}c)$. Note that if $\varsigma\in\mathfrak{P}_\wp(\mathbb{S}^{\rm D}\times\mathbb{R})$ then also $\varsigma\in\mathfrak{L}^{\wp'}(\mathbb{S}^{\rm D}\times\mathbb{R})$ for all $\wp'\in[1,\wp]$, and so also $\varsigma\in(\mathfrak{L}^1\ln\mathfrak{L}^1)(\mathbb{S}^{\rm D}\times\mathbb{R})$.

By Jensen's inequality, any marginal measure of $\varrho\in\mathfrak{P}^s_\wp((\mathbb{S}^{\rm D}\times\mathbb{R})^{\mathbb{N}})$ is then in $(\mathfrak{P}\cap\mathfrak{L}^\wp)((\mathbb{S}^{\rm D}\times\mathbb{R})^n)$. The reverse can be shown also (cf. [HeSa55], [MeSp82]): if $\varrho\in\mathfrak{P}^s((\mathbb{S}^{\rm D}\times\mathbb{R})^{\mathbb{N}})$ has all its marginal measures in $(\mathfrak{P}\cap\mathfrak{L}^\wp)((\mathbb{S}^{\rm D}\times\mathbb{R})^n)$, then the decomposition measure $\nu(\mathrm{d}\varsigma|\varrho)$ is concentrated on $\mathfrak{P}_\wp(\mathbb{S}^{\rm D}\times\mathbb{R})$; i.e. $\varrho\in\mathfrak{P}^s_\wp((\mathbb{S}^{\rm D}\times\mathbb{R})^{\mathbb{N}})$.

The *mean energy of* $\varrho\in\mathfrak{P}^s_\wp((\mathbb{S}^{\rm D}\times\mathbb{R})^{\mathbb{N}})$ is now defined as

$$\underline{\mathcal{E}}(\varrho) \stackrel{\rm def}{=} \lim_{n\to\infty}\ \tfrac{1}{n}{}^{(n)}\varrho\Big(\tfrac{1}{n-1}\sum\sum_{1\le j<k\le n} c_jc_kU(\mathbf{s}_j,\mathbf{s}_k)\Big). \tag{3.54}$$

Clearly, the sequence at r.h.s.(3.54) is independent of n, and so

$$\underline{\mathcal{E}}(\varrho) \equiv \tfrac{1}{2}{}^{(2)}\varrho\big(K^{(2)}\big). \tag{3.55}$$

Moreover, by the linearity of $\varrho\mapsto\underline{\mathcal{E}}\big(\varrho\big)$ the presentation (3.50) yields

$$\underline{\mathcal{E}}(\varrho) = \int \tfrac{1}{2}\varsigma^{\otimes 2}\big(K^{(2)}\big)\,\nu(\mathrm{d}\varsigma|\varrho). \tag{3.56}$$

The *mean northern moment of* $\varrho\in\mathfrak{P}^s_\wp((\mathbb{S}^{\rm D}\times\mathbb{R})^{\mathbb{N}})$ is similarly defined as

$$\underline{\mathcal{N}}(\varrho) \stackrel{\rm def}{=} \lim_{n\to\infty}\ \tfrac{1}{n}{}^{(n)}\varrho\Big(\sum_{1\le k\le n} c_kV(\mathbf{s}_k)\Big), \tag{3.57}$$

Also the sequence at r.h.s.(3.57) is independent of n, and so

$$\underline{\mathcal{N}}(\varrho) \equiv {}^{(1)}\varrho\big(cV\big). \tag{3.58}$$

Again by the linearity of $\varrho\mapsto\underline{\mathcal{N}}\big(\varrho\big)$ the presentation (3.50) now yields

$$\underline{\mathcal{N}}(\varrho) = \int \varsigma\big(cV\big)\,\nu(\mathrm{d}\varsigma|\varrho). \tag{3.59}$$

The $N=\infty$ analogue of (3.20) is known as a *mean (relative) entropy of* $\varrho\in\mathfrak{P}^s((\mathbb{S}^{\rm D}\times\mathbb{R})^{\mathbb{N}})$, well-defined as limit

$$\underline{\mathcal{R}}(\varrho|\varrho_f) \equiv \lim_{n\to\infty}\ \tfrac{1}{n}\mathcal{R}^{(n)}\big({}^{(n)}\varrho|\varrho_f^n\big). \tag{3.60}$$

Here, $\mathcal{R}^{(n)}\big({}^{(n}\!\varrho|\varrho_f^n\big)$, $n \in \{1, ...\}$, is the relative entropy of ${}^{(n}\!\varrho$, as defined in (3.20); we also set $\sigma(k) = -1, 0, 1$ when $k < 0, = 0, > 0$, respectively. The limit (3.60) exists or is $-\infty$. This is a consequence of the next lemma [Kie93], [Kie11], adapted from [RoRu67] (section 2, proof of proposition 1; cf. also [Rue69]).

Lemma 2. *Relative entropy* $n \mapsto \mathcal{R}^{(n)}\big({}^{(n}\!\varrho|\varrho_f^n\big)$ *has the following properties:*

(A) Non-positivity*: For all* n,

$$\mathcal{R}^{(n)}\big({}^{(n}\!\varrho|\varrho_f^n\big) \leq 0; \tag{3.61}$$

(B) Monotonic decrease*: If* $n > m$ *then*

$$\mathcal{R}^{(n)}\big({}^{(n}\!\varrho|\varrho_f^n\big) \leq \mathcal{R}^{(m)}\big({}^{(m)}\!\varrho|\varrho_f^m\big); \tag{3.62}$$

(C) Strong sub-additivity*: For* m, $n \leq \ell$, *and* $k = \ell - m - n$,

$$\mathcal{R}^{(\ell)}\big({}^{(\ell)}\!\varrho|\varrho_f^\ell\big) \leq \mathcal{R}^{(m)}\big({}^{(m)}\!\varrho|\varrho_f^m\big) + \mathcal{R}^{(n)}\big({}^{(n}\!\varrho|\varrho_f^n\big) + \sigma(k)\mathcal{R}^{(|k|)}\big({}^{(|k|)}\!\varrho|\varrho_f^{|k|}\big). \tag{3.63}$$

Lemma 2 holds for $\varrho \in \mathfrak{P}^s((\mathbb{S}^{\mathrm{D}} \times \mathbb{R})^{\mathbb{N}})$ and $\varrho \in \mathfrak{P}^s((\mathbb{S}^{\mathrm{D}} \times \mathbb{R})^N)$ (then $k \leq N$ in ${}^{(k)}\!\varrho^{(N)}$).

Also adapted from [RoRu67], proof of proposition 3, is (cf. [Kie93, Kie11]):

Lemma 3. *The mean relative entropy functional (3.60) is affine linear.*

Lemma 3 paired with the deFinetti-Dynkin-Hewitt-Savage decomposition theorem for $\mathfrak{P}^s((\mathbb{S}^{\mathrm{D}} \times \mathbb{R})^{\mathbb{N}})$ yields the key formula

$$\underline{\mathcal{R}}(\varrho|\varrho_f) = \int \mathcal{R}(\varsigma|\varrho_f)\, \nu(\mathrm{d}\varsigma|\varrho), \tag{3.64}$$

where we also set $\mathcal{R}(\varsigma|\varrho_f) \equiv \mathcal{R}^{(1)}(\varsigma|\varrho_f)$.

Lastly, Lemma 4, also proved by adaptation of a proof in [RoRu67], their proposition 4, ends the listing of properties of mean relative entropy (3.60).

Lemma 4. *The mean entropy functional is weakly upper semi-continuous.*

Finally we define the *mean effective entropy of* $\varrho \in \mathfrak{P}^s_{\wp}((\mathbb{S}^{\mathrm{D}} \times \mathbb{R})^{\mathbb{N}})$ by

$$\underline{\mathcal{S}}_{\beta,\gamma}(\varrho) \equiv \underline{\mathcal{R}}(\varrho) - \beta\underline{\mathcal{E}}(\varrho) - \beta\gamma\underline{\mathcal{N}}(\varrho). \tag{3.65}$$

By (3.64), (3.56), and (3.59) we have

$$\underline{\mathcal{S}}_{\beta,\gamma}(\varrho) = \int_{\mathfrak{P}(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})} \mathcal{S}_{\beta,\gamma}(\varsigma)\,\nu(\mathrm{d}\varsigma|\varrho), \tag{3.66}$$

where $\mathcal{S}_{\beta,\gamma}(\varsigma)$ is the effective entropy functional introduced in (3.52). It is well-defined and finite for all β satisfying $\mathcal{B}_f(\beta) < \frac{2\mathrm{D}}{C(\mathrm{D})}$ whenever $\varsigma \in \mathfrak{P}_\wp(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})$, $\wp > 1$, because then $\varsigma \in (\mathfrak{L}^1 \cap \mathfrak{L}^1 \ln \mathfrak{L}^1)(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})$, and since U is in any $\mathfrak{L}^{\wp'}(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})$. In all other situations it is defined as $\mathcal{S}_{\beta,\gamma}(\varsigma) = -\infty$.

Now, for any β satisfying $\mathcal{B}_f(\beta) < \frac{2\mathrm{D}}{C(\mathrm{D})}$, and $1 < \wp < \infty$, we can extract a subsequence $\{{}^{(n)}\varrho_{\beta,\gamma}^{(\dot N[N])}\}_{N\in\mathbb{N}}$ such that $\forall n \in \mathbb{N}$,

$$\lim_{N\to\infty} \mathrm{d}^{(n)}\varrho_{\beta,\gamma}^{(\dot N[N])} = {}^{(n)}\dot\varrho_{\beta,\gamma}(\mathrm{d}\mu^n) \in \mathfrak{P}^s((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^n), \tag{3.67}$$

weakly in $\mathfrak{P}_\wp((\mathbb{S}^{\mathrm{D}}\times\mathbb{R})^n)$. Following [MeSp82] we next use sub-additivity (property (C) in Lemma 2) and then [Kie93, Kie11] negativity (property (A) in Lemma 2) of relative entropy, to obtain

$$\begin{aligned} \mathcal{R}^{(\dot N)}\big(\varrho_{\beta,\gamma}^{(\dot N)}|\varrho_f^{\dot N}\big) &\leq \left\lfloor \tfrac{\dot N}{n} \right\rfloor \mathcal{R}^{(n)}\big({}^{(n)}\varrho_{\beta,\gamma}^{(\dot N)}|\varrho_f^{n}\big) + \mathcal{R}^{(m)}\big({}^{(m)}\varrho_{\beta,\gamma}^{(\dot N)}|\varrho_f^{m}\big) \\ &\leq \left\lfloor \tfrac{\dot N}{n} \right\rfloor \mathcal{R}^{(n)}\big({}^{(n)}\varrho_{\beta,\gamma}^{(\dot N)}|\varrho_f^{n}\big), \end{aligned} \tag{3.68}$$

where $\lfloor a/b \rfloor$ is the integer part of a/b, and where $m < n$. Following [Kie93, Kie11], we use upper semi-continuity for the relative entropy to get

$$\limsup_{\dot N\to\infty} \mathcal{R}^{(n)}\big({}^{(n)}\varrho_{\beta,\gamma}^{(\dot N[N])}|\varrho_f^{n}\big) \leq \mathcal{R}^{(n)}\big({}^{(n)}\dot\varrho_{\beta,\gamma}|\varrho_f^{n}\big), \tag{3.69}$$

while $\frac{1}{\dot N}\left\lfloor \frac{\dot N}{n} \right\rfloor \to \frac{1}{n}$. Hence, dividing (3.68) by $\dot N[N]$ and letting $\dot N \to \infty$ gives

$$\limsup_{\dot N\to\infty} \tfrac{1}{\dot N}\mathcal{R}^{(\dot N)}\big(\varrho_{\beta,\gamma}^{(\dot N)}|\varrho_f^{\dot N}\big) \leq \tfrac{1}{n}\mathcal{R}^{(n)}\big({}^{(n)}\dot\varrho_{\beta,\gamma}|\varrho_f^{n}\big) \quad \forall n \in \mathbb{N}, \tag{3.70}$$

and now taking the infimum over n (equivalently: the limit $n \to \infty$) we get

$$\limsup_{\dot N\to\infty} \tfrac{1}{\dot N}\mathcal{R}^{(\dot N)}\big(\varrho_{\beta,\gamma}^{(\dot N)}|\varrho_f^{\dot N}\big) \leq \underline{\mathcal{R}}(\dot\varrho_{\beta,\gamma}). \tag{3.71}$$

Lastly, using (3.64) in (3.71) yields

$$\limsup_{\dot N\to\infty} \tfrac{1}{\dot N}\mathcal{R}^{(\dot N)}\big(\varrho_{\beta,\gamma}^{(\dot N)}|\varrho_f^{\dot N}\big) \leq \int \mathcal{R}(\varsigma|\varrho_f)\,\nu(\mathrm{d}\varsigma|\dot\varrho_{\beta,\gamma}), \tag{3.72}$$

where $\nu(\mathrm{d}\varsigma|\dot{\varrho}_{\beta,\gamma})$ is the Hewitt-Savage decomposition measure for $\dot{\varrho}_{\beta,\gamma}$.

Moreover, by weak $\mathfrak{L}^{\wp}$ convergence, for each $n \in \mathbb{N}$ we have

$$\lim_{\dot{N}\to\infty} {}^{(n)}\varrho_{\beta,\gamma}^{(\dot{N})}\Big(\tfrac{1}{n-1}\sum\sum_{1\leq j<k\leq n} c_j c_k U(\mathbf{s}_j,\mathbf{s}_k)\Big) = n\tfrac{1}{2}{}^{(2)}\dot{\varrho}_{\beta,\gamma}\big(K^{(2)}\big), \tag{3.73}$$

so division by n yields the mean energy of $\dot{\varrho}_{\beta,\gamma}$,

$$\lim_{\dot{N}\to\infty} \tfrac{1}{n}{}^{(n)}\varrho_{\beta,\gamma}^{(\dot{N})}\Big(\tfrac{1}{n-1}\sum\sum_{1\leq j<k\leq n} c_j c_k U(\mathbf{s}_j,\mathbf{s}_k)\Big) = \tfrac{1}{2}{}^{(2)}\dot{\varrho}_{\beta,\gamma}\big(K^{(2)}\big) \equiv \underline{\mathcal{E}}(\dot{\varrho}). \tag{3.74}$$

But of course, we also have

$$\varrho_{\beta,\gamma}^{(\dot{N})}\Big(\tfrac{1}{\dot{N}-1}\sum\sum_{1\leq j<k\leq \dot{N}} c_j c_k U(\mathbf{s}_j,\mathbf{s}_k)\Big) = \dot{N}\tfrac{1}{2}{}^{(2)}\varrho_{\beta,\gamma}^{(\dot{N})}\big(K^{(2)}\big), \tag{3.75}$$

so after division by $\dot{N}$, weak $\mathfrak{L}^{\wp}$ convergence again yields

$$\lim_{\dot{N}\to\infty} \tfrac{1}{\dot{N}}\varrho_{\beta,\gamma}^{(\dot{N})}\Big(\tfrac{1}{\dot{N}-1}\sum\sum_{1\leq j<k\leq \dot{N}} c_j c_k U(\mathbf{s}_j,\mathbf{s}_k)\Big) = \tfrac{1}{2}{}^{(2)}\dot{\varrho}_{\beta,\gamma}\big(K^{(2)}\big). \tag{3.76}$$

By (3.76) and (3.74), and recalling (3.56), we have

$$\lim_{\dot{N}\to\infty} \tfrac{1}{\dot{N}}\varrho_{\beta,\gamma}^{(\dot{N})}\Big(\tfrac{1}{\dot{N}-1}\sum\sum_{1\leq j<k\leq \dot{N}} c_j c_k U(\mathbf{s}_j,\mathbf{s}_k)\Big) = \int \tfrac{1}{2}\varsigma^{\otimes 2}\big(K^{(2)}\big)\,\nu(\mathrm{d}\varsigma|\dot{\varrho}_{\beta,\gamma}). \tag{3.77}$$

In a completely analogous manner we see that

$$\lim_{\dot{N}\to\infty} \tfrac{1}{\dot{N}}\varrho_{\beta,\gamma}^{(\dot{N})}\Big(\sum_{1\leq k\leq \dot{N}} c_k V(\mathbf{s}_k)\Big) = \int \varsigma\big(cV(\mathbf{s})\big)\,\nu(\mathrm{d}\varsigma|\dot{\varrho}_{\beta,\gamma}). \tag{3.78}$$

Estimate (3.72) and identities (3.77), (3.78) together with (3.66) now yield

$$\limsup_{\dot{N}\to\infty} \tfrac{1}{\dot{N}}\mathcal{S}_{\beta,\gamma}\big(\varrho_{\beta,\gamma}^{(\dot{N})}\big) \leq \int \mathcal{S}_{\beta,\gamma}(\varsigma)\,\nu(\mathrm{d}\varsigma|\dot{\varrho}_{\beta,\gamma}) \leq \sup_{\varsigma\in\mathfrak{P}_{\wp}} \mathcal{S}_{\beta,\gamma}(\varsigma) \tag{3.79}$$

for *any* subsequence $\dot{N}[N]$. Therefore,

$$\limsup_{N\to\infty} \tfrac{1}{N}\mathcal{S}_{\beta,\gamma}\big(\varrho_{\beta,\gamma}^{(N)}\big) \leq \sup_{\varsigma\in\mathfrak{P}_{\wp}} \mathcal{S}_{\beta,\gamma}(\varsigma). \tag{3.80}$$

On the other hand, for any $\varsigma \in \mathfrak{P}_{\wp}$ we have

$$\mathcal{S}_{\beta,\gamma}^{(N)}\big(\varrho_{\beta}^{(N)}\big) \geq \mathcal{R}^{(N)}\big(\varsigma^{\otimes N}|\varrho_f^N\big) \tag{3.81}$$

$$-\beta\varsigma^{\otimes N}\Big(\tfrac{1}{N-1}\sum\sum_{1\leq j<k\leq N} c_j c_k U(\mathbf{s}_j,\mathbf{s}_k) + \gamma\sum_{1\leq k\leq N} c_k V(\mathbf{s}_k)\Big)$$

$$= N\Big[\mathcal{R}^{(1)}\big(\varsigma|\underline{\mu}\big) - \beta\tfrac{1}{2}\varsigma^{\otimes 2}\big(K^{(2)}\big) - \beta\gamma\varsigma\big(cV(\mathbf{s})\big)\Big] \tag{3.82}$$

$$= N\mathcal{S}_{\beta,\gamma}(\varsigma), \tag{3.83}$$

by the variational principle for the effective N-body entropy (3.19). Taking a maximizing sequence $k \mapsto \varsigma_k \in \mathfrak{P}_\wp$ for $\mathcal{S}_{\beta,\gamma}(\varsigma)$, after division by N we find

$$\liminf_{N\to\infty} \tfrac{1}{N}\mathcal{S}_{\beta,\gamma}\big(\varrho^{(N)}_{\beta,\gamma}\big) \geq \sup_{\varsigma\in\mathfrak{P}_\wp} \mathcal{S}_{\beta,\gamma}(\varsigma). \tag{3.84}$$

The estimates (3.84) and (3.80) together prove that

$$\lim_{N\to\infty} \tfrac{1}{N}\mathcal{S}_{\beta,\gamma}\big(\varrho^{(N)}_{\beta,\gamma}\big) = \sup_{\varsigma\in\mathfrak{P}_\wp} \mathcal{S}_{\beta,\gamma}(\varsigma). \tag{3.85}$$

But then, by (3.79), we also have

$$\int \mathcal{S}_{\beta,\gamma}(\varsigma)\,\nu(\mathrm{d}\varsigma|\dot{\varrho}_{\beta,\gamma}) = \sup_{\varsigma\in\mathfrak{P}_\wp} \mathcal{S}_{\beta,\gamma}(\varsigma) \tag{3.86}$$

for *any* weak limit point $\dot{\varrho}$. Therefore the decomposition measure $\nu(\mathrm{d}\varsigma|\dot{\varrho}_{\beta,\gamma})$ is supported on those $\varsigma \in \mathfrak{P}_\wp$ which actually maximize $\mathcal{S}_{\beta,\gamma}(\varsigma)$; for suppose not, then the average $\int \mathcal{S}_{\beta,\gamma}(\varsigma)\,\nu(\mathrm{d}\varsigma|\dot{\varrho}_{\beta,\gamma}) < \sup_{\varsigma\in\mathfrak{P}_\wp} \mathcal{S}_{\beta,\gamma}(\varsigma)$ in contradiction to (3.86). Therefore, $\sup_{\varsigma\in\mathfrak{P}_\wp} \mathcal{S}_{\beta,\gamma}(\varsigma) = \max_{\varsigma\in\mathfrak{P}_\wp} \mathcal{S}_{\beta,\gamma}(\varsigma)$; furthermore, since $\dot{\varrho} \in \mathfrak{L}^\wp$, we can conclude that the maximizer is actually in $\mathfrak{L}^\wp$ for all $1 \leq \wp < \infty$.

This proves Theorem 6. $\square$

Corollary 1. *Any maximizer $\varsigma_{\beta,\gamma}$ of $\mathcal{S}_{\beta,\gamma}(\varsigma)$ over the set $\mathfrak{P}_\wp$ is of the form*

$$\varsigma_{\beta,\gamma}(\underline{\alpha}_0(\mathrm{d}\mathbf{s})\mathrm{d}c) = \rho_{\beta,\gamma}(\mathbf{s};c)f(c)\underline{\alpha}_0(\mathrm{d}\mathbf{s})\mathrm{d}c,$$

where $\rho_{\beta,\gamma}(\mathbf{s};c)$ is given by a solution to the following fixed point equation in $\mathfrak{P}(\mathbb{S}^{\mathrm{D}}\times\mathbb{R})$,

$$\rho(\mathbf{s};c) = \frac{e^{-\beta c\left(\int\!\int U(\mathbf{s},\tilde{\mathbf{s}})\tilde{c}\rho(\tilde{\mathbf{s}};\tilde{c})\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\tilde{\mathbf{s}})f(\tilde{c})\mathrm{d}\tilde{c}+\gamma V(\mathbf{s})\right)}}{\displaystyle\int_{\mathbb{R}}\int_{\mathbb{S}^{\mathrm{D}}} e^{-\beta\hat{c}\left(\int\!\int U(\hat{\mathbf{s}},\tilde{\mathbf{s}})\tilde{c}\rho(\tilde{\mathbf{s}};\tilde{c})\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\tilde{\mathbf{s}})f(\tilde{c})\mathrm{d}\tilde{c}+\gamma V(\mathbf{s})\right)}\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\hat{\mathbf{s}})f(\hat{c})\mathrm{d}\hat{c}}, \tag{3.87}$$

with β satisfying $\mathcal{B}_f(\beta) < \frac{2\mathrm{D}}{C(\mathrm{D})}$, and γ arbitrary.

3.2 Special Cases

We mention two choices of $f(c)$ which are of special interest.

3.2.1 $f(c) = \delta_{+1}(c)$

If we let the function f concentrate on the Dirac point measure δ_{+1}, i.e., c only takes the value $+1$, we arrive at the canonical ensemble measures

$$\mathrm{d}\mu^{(N)} = (\mathfrak{Z}_N)^{-1} e^{-\beta\left(\frac{1}{N-1}\sum\sum_{j<k} U(\mathbf{s}_j,\mathbf{s}_k)+\gamma\sum_k V(\mathbf{s}_k)\right)} \mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s}_1)\cdots \mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s}_N), \tag{3.88}$$

with the partition function

$$(\mathfrak{Z}_N)(\beta,\gamma) \stackrel{\text{def}}{=} \int_{(\mathbb{S}^{\mathrm{D}})^N} e^{-\beta\left(\frac{1}{N-1}\sum\sum_{j<k} U(\mathbf{s}_j,\mathbf{s}_k)+\gamma\sum_k V(\mathbf{s}_k)\right)} \mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s}_1)\cdots \mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s}_N). \tag{3.89}$$

Then the weak limit points of the sequence of canonical ensembles $\{\mu^{(N)}\}$ are superpositions of solutions to the following equation

$$\rho(\mathbf{s}) = \frac{e^{-\beta\left(\int U(\mathbf{s},\tilde{\mathbf{s}})\rho(\tilde{\mathbf{s}})\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\tilde{\mathbf{s}})+\gamma V(\mathbf{s})\right)}}{\int_{\mathbb{S}^{\mathrm{D}}} e^{-\beta\left(\int U(\hat{\mathbf{s}},\tilde{\mathbf{s}})\rho(\tilde{\mathbf{s}})\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\tilde{\mathbf{s}})+\gamma V(\hat{\mathbf{s}})\right)} \mathrm{d}^{\mathrm{D}}\underline{\alpha}(\hat{\mathbf{s}})}, \tag{3.90}$$

with β satisfying $-\beta < \frac{2\mathrm{D}}{C(\mathrm{D})}$, i.e., $\beta > -\frac{2\mathrm{D}}{C(\mathrm{D})}$, and γ arbitrary.

Now, apply the substitution $u(\mathbf{s}) = \int U(\mathbf{s},\tilde{\mathbf{s}})\rho(\tilde{\mathbf{s}})\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\tilde{\mathbf{s}}) - 1$ to the equation above, and recall that U is the Green's function of the operator P such that $PU = \delta - \frac{1}{\alpha(\mathrm{D})}$, then we get an equation for u as follows:

$$Pu(\mathbf{s}) = \frac{1}{\alpha(\mathrm{D})} \cdot \frac{e^{-\beta(u+\gamma V(\mathbf{s}))}}{\int_{\mathbb{S}^{\mathrm{D}}} e^{-\beta(u+\gamma V(\hat{\mathbf{s}}))}\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\hat{\mathbf{s}})} - \frac{1}{\alpha(\mathrm{D})} \tag{3.91}$$

where $\alpha(\mathrm{D})$ stands for the area of the sphere $\mathbb{S}^{\mathrm{D}}$.

The equation (3.91) is deceptively similar to the prescribed Q-curvature equation. However, we remind the readers that the constant β here must satisfy $\beta > -\frac{2\mathrm{D}}{C(\mathrm{D})}$, but not exactly equal to $-\frac{2\mathrm{D}}{C(\mathrm{D})}$. Hence the result is indeed an ϵ away from the true prescribed Q-curvature problem.[1]

---

[1]If we apply the formal substitution $Pu = -\frac{\beta}{\alpha(\mathrm{D})\mathrm{D}}\rho - (\mathrm{D}-1)!$ to the equation (3.90), then formally we get an equation for u as follows:

$$Pu(\mathbf{s}) = -\frac{\beta}{\alpha(\mathrm{D})\mathrm{D}} \frac{e^{\mathrm{D}u(\mathbf{s})+\mathrm{D}(\mathrm{D}-1)!-\beta\gamma V(\mathbf{s})}}{\int e^{\mathrm{D}u(\hat{\mathbf{s}})+\mathrm{D}(\mathrm{D}-1)!-\beta\gamma V(\hat{\mathbf{s}})}\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\hat{\mathbf{s}})} - (\mathrm{D}-1)!$$

Next, we let $Q(\mathbf{s}) = -\frac{\beta}{\alpha(\mathrm{D})\mathrm{D}} \frac{e^{\mathrm{D}(\mathrm{D}-1)!-\beta\gamma V(\mathbf{s})}}{\int e^{\mathrm{D}u(\hat{\mathbf{s}})+\mathrm{D}(\mathrm{D}-1)!-\beta\gamma V(\hat{\mathbf{s}})}\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\hat{\mathbf{s}})}$, then the equation above turns into

$$Pu(\mathbf{s}) = Q(\mathbf{s})e^{\mathrm{D}u(\mathbf{s})} - (\mathrm{D}-1)!.$$

This looks exactly the same as the prescribed Q-curvature equation. HOWEVER, such a substitution from ρ to u does not exist! Unless the parameter $\beta = -\frac{2\mathrm{D}}{C(\mathrm{D})}$, the requirement $Pu = -\frac{\beta}{\alpha(\mathrm{D})\mathrm{D}}\rho - (\mathrm{D}-1)!$ is inconsistent with the integration constraint $\int Pu = 0$.

However, the true prescribed Q-curvature equation can also be obtained using statistical mechanics techniques, namely, the treatment of the microcanonical ensemble will produce the desired result — for 2-dim, readers can refer to [Kie11].

3.2.2 $f(c) = \frac{1}{2}\delta_{+1}(c) + \frac{1}{2}\delta_{-1}(c)$

When $f(c) = \frac{1}{2}\delta_{+1}(c) + \frac{1}{2}\delta_{-1}(c)$, the fixed point equation (3.87) becomes:

$$\rho(\mathbf{s}; c) = \frac{\exp -\beta c\Big[\frac{1}{2}\int U(\mathbf{s},\tilde{\mathbf{s}})(\rho(\tilde{\mathbf{s}};1) - \rho(\tilde{\mathbf{s}};-1))\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\tilde{\mathbf{s}}) + \gamma V(\mathbf{s})\Big]}{\displaystyle\int \cosh\Big\{\beta\Big[\frac{1}{2}\int U(\mathbf{s},\tilde{\mathbf{s}})(\rho(\tilde{\mathbf{s}};1) - \rho(\tilde{\mathbf{s}};-1))\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\tilde{\mathbf{s}}) + \gamma V(\mathbf{s})\Big]\Big\}\,\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s})}, \tag{3.92}$$

and this leads to an equation for $\omega(\mathbf{s}) = \int_{\mathbb{R}} \rho(\mathbf{s}; c) f(c) dc = \frac{1}{2}[\rho(\mathbf{s}; 1) - \rho(\mathbf{s}; -1)]$ as follows

$$\omega(\mathbf{s}) = \frac{-\sinh\Big\{\beta\Big[\int U(\mathbf{s},\tilde{\mathbf{s}})\omega(\tilde{\mathbf{s}})\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\tilde{\mathbf{s}}) + \gamma V(\mathbf{s})\Big]\Big\}}{\displaystyle\int \cosh\Big\{\beta\Big[\int U(\mathbf{s},\tilde{\mathbf{s}})\omega(\tilde{\mathbf{s}})\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\tilde{\mathbf{s}}) + \gamma V(\mathbf{s})\Big]\Big\}\,\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s})} \tag{3.93}$$

Now suppose $u(\mathbf{s}) = \int U(\mathbf{s},\tilde{\mathbf{s}})\omega(\tilde{\mathbf{s}})\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\tilde{\mathbf{s}})$, then the equation above implies the following equation for u:

$$Pu = \frac{-\sinh\beta[u + \gamma V(\mathbf{s})]}{\int \cosh(\beta[u + \gamma V(\mathbf{s})])\mathrm{d}^{\mathrm{D}}\underline{\alpha}(\mathbf{s})} \tag{3.94}$$

In particular, when $\gamma = 0$ and $\mathrm{D} = 2$, the corresponding equation reads as

$$-\Delta u = \frac{-\sinh\beta u}{\int \cosh\beta u \mathrm{d}^2\underline{\alpha}(\mathbf{s})} \tag{3.95}$$

which would be the equation of immersed tori with constant mean curvature discussed in [Abr87, PiSt89], were the domain a flat torus. However, the domain in our discussion is the 2-dim sphere $\mathbb{S}^2$, not a flat torus; but nothing stops us from studying the same equation on different domains. Indeed, the Green's function U has logarithmic singularities on both $\mathbb{S}^2$ and the torus, but the periodicity involved in the torus case is not required by the $\mathbb{S}^2$ case.

Part II

A Generalization of Statistical Mechanics Techniques Applied to the Prescribed Sign-changing Q-curvature Problem

Chapter 4

Sign-changing Prescribed Curvature Problem

In this chapter, we will work on the prescribed Q-curvature problem in a bounded domain $\Lambda \subset \mathbb{R}^{\mathrm{D}}$, namely

$$Pu(x) = Q(x)e^{\mathrm{D}u(x)}, \tag{4.1}$$

where the function $Q(x)$ takes both positive and negative values. Yet, to focus on the technique itself, without loss of generality it suffices to let $\mathrm{D} = 2$ (for simplicity). Also, we write the equation in the form with a normalization constant, so that

$$-\Delta u(x) = \kappa \frac{K(x)e^{2u(x)}}{\int K(x)e^{2u(x)}\mathrm{d}x}; \tag{4.2}$$

here κ is a real parameter which can be interpreted as the integral Gaussian curvature whenever $\kappa = \int Ke^{2u}\mathrm{d}x \neq 0$. We remark here that the special case $\kappa = 0$ cannot be brought an equation into the form of (4.2), and therefore has to be discussed separately; but this $\kappa = 0$ case is not included in this thesis. We also remark that the substitution $\tilde{K} = -K$ into (4.2) will result in the same equation, so it suffices to assume that the integral $\int K(x)e^{2u}\mathrm{d}x > 0$. Note that $Q = K$ now, and the function K changes sign in its support. (4.2) is supplemented by the 0-Dirichlet boundary condition, since other boundary conditions can be absorbed to K as explained in Chapter 1.

As a warm up, let us imitate the procedure in Part I and derive the "formal variational principles" for u: First, notice that the Euler-Lagrange equation of the variational principle

$$H(u) = \frac{1}{2}\int |\nabla u(x)|^2\mathrm{d}x - \frac{\kappa}{2}\ln \int K(x)e^{2u(x)}\mathrm{d}x \tag{4.3}$$

is same as (4.2). Second, apply Legendre transform to the first term $\frac{1}{2}\int |\nabla u|^2\mathrm{d}x$ in (4.3), and get $-\frac{1}{2}\int\int Uv^{\otimes 2}\mathrm{d}^2x$ with $v = -\Delta u$ as the Euler-Lagrange equation. Indeed, an application of Legendre transform to the second term $-\frac{\kappa}{2}\ln\int K(x)e^{2u(x)}\mathrm{d}x$ of H results in $\frac{1}{2}\int v\ln\frac{v}{\kappa K}\mathrm{d}x$ with the Euler-Lagrange equation $v=\kappa\frac{K(x)e^{2u(x)}}{\int K(x)e^{2u(x)}\mathrm{d}x}$. Notice that by (4.2) the two Euler-Lagrange equations derived for the two terms coincide. Hence, putting the two terms together, and noticing that

$$H(u)=\left\{\frac{1}{2}\int|\nabla u(x)|^2\mathrm{d}x-\int uv\mathrm{d}x\right\}+\left\{\int uv\mathrm{d}x-\frac{\kappa}{2}\ln\int K(x)e^{2u(x)}\mathrm{d}x\right\},$$

the resulting functional of v is

$$F(v)=-\frac{1}{2}\int\int Uv^{\otimes 2}d^2x+\frac{1}{2}\int v\ln\frac{v}{\kappa K}\mathrm{d}x \tag{4.4}$$

where U is the Green's function for the operator $-\Delta$ with 0-Dirichlet boundary condition. Correspondingly, the Euler-Lagrange equation of F for a critical $\tilde{v}$ is then

$$\tilde{v}(x)=\kappa\frac{K(x)e^{2(U*\tilde{v})(x)}}{\int K(x)e^{2(U*\tilde{v})(x)}\mathrm{d}x} \tag{4.5}$$

We remind the readers that the notation "$*$" here means convolution, i.e.,

$$U*\tilde{v}=\int_\Lambda U(x_1,x_2)\tilde{v}(x_2)\mathrm{d}x_2=\int_\Lambda U(x_1-x_2)\tilde{v}(x_2)\mathrm{d}x_2,$$

with some obvious abuse of notation for U, because the Green's function $U(x_1,x_2)$ depends only on x_1-x_2.

Remark 4. *Notice that the entropy functional here is not the ordinary entropy containing "$v\ln v$", but the "entropy of a signed measure relative to κK". This is not only directly resulted from the Legendre transform, but also naturally required by the "$\ln$" in the functional. From the relation between u and v, we know that v is of the same sign as κK.*

Substitute (4.5) into its formal variational principle (4.4), and we get

$$\begin{aligned} F(\tilde{v}) &= -\tfrac{1}{2}\int_\Lambda\int_\Lambda G\tilde{v}^{\otimes 2}d^2x+\tfrac{1}{2}\int_\Lambda\tilde{v}(2G*\tilde{v})\mathrm{d}x-\tfrac{1}{2}\ln\int_\Lambda Ke^{2G*\tilde{v}}\mathrm{d}x \\ &= \tfrac{1}{2}\int_\Lambda\int_\Lambda G\tilde{v}^{\otimes 2}d^2x-\tfrac{1}{2}\ln\int_\Lambda Ke^{2G*\tilde{v}}\mathrm{d}x \end{aligned} \tag{4.6}$$

Now if the technique in Part I were applicable to sign-changing measures, then we could conclude that some critical points of F would be related to the weak limit points of the sequence of signed measures $\{\sigma^{(N)}\}_{N=1}^{\infty}$, where for any N, $\sigma^{(N)}$ is a critical point of the functional $G^{(N)}$ defined as

$$G^{(N)}(\sigma_N) = -\frac{1}{2(N-1)} \int_{\Lambda^N} \sum\sum_{k\neq l} G(x_k, x_l)\sigma'_N \mathrm{d}^N x + \frac{1}{2} \int_{\Lambda^N} \sigma'_N \ln \frac{\sigma'_N}{\kappa^N K^{\otimes N}} \mathrm{d}^N x. \quad (4.7)$$

Each critical point $\sigma^{(N)}$ is explicitly expressed as

$$\mathrm{d}\sigma^{(N)}(x_1, \cdots, x_N) = \frac{K^{\otimes N} \exp \frac{1}{N-1} \sum\sum_{k\neq l} G(x_k, x_l)}{\int_{\Lambda^N} K^{\otimes N} \exp \frac{1}{N-1} \sum\sum_{k\neq l} G(x_k, x_l) \mathrm{d}^N x} \mathrm{d}^N x. \quad (4.8)$$

Its weak limit points would be affine linear superpositions of infinite products of signed one-point measures, roughly in analogue of (2.12) and(2.13); and each one-point measure is a critical point of the functional F.

However, because K changes sign, the sequence $\sigma^{(N)}$ does not have an interpretation as canonical ensemble measures. Worse, $\sigma^{(N)}$ does not represent a statistical ensemble of systems in any known sense. This makes a direct application of our techniques of Chapter 3 impossible.

To circumvent this problem, we decompose the equation (4.2) into a system of two equations — each equation corresponds to a "no sign-changing" problem, so that a statistical mechanics interpretation exists for each equation conditioned on the solution of the other being given. Hence the technique of Messer and Spohn can work through for each equation separately. The problem thus reduces to finding a joint statistical treatment. We will modify Messer and Spohn's technique to find solutions to this joint system of equations, at the cost that we can not think of it as a mechanical system anymore. The mechanical interpretation will be lost.

4.1 Reformulation of the Prescribed Q-Curvature Problem

Let

$$K = ae^{\beta\psi} - be^{-\beta\psi}, \quad (4.9)$$

with both a and b positive constants, so that both $ae^{\beta\psi}$ and $be^{-\beta\psi}$ are positive.

Remark 5. *There is always some combination of* (a, b, β) *such that* $K \leftrightarrow \psi$. *In particular, let* $a = b = 1/2$, $\beta = 1$, *then* $K = \frac{e^{\psi}-e^{-\psi}}{2} = \sinh\psi$, *and hence* ψ *can be obtained by taking the inverse of the hyperbolic sine function.*

Let us decompose u into the linear combination of two functions ϕ_1 and ϕ_2, each of which satisfying a similar equation in the regime of Messer and Spohn's technique. Set $2u = \beta\phi_1 - \beta\phi_2$, and correspondingly, the equations for ϕ_1 and ϕ_2 are as follows:

$$-\Delta\phi_1 = \frac{2a\kappa}{\beta}\frac{e^{\beta(\psi-\phi_2+\phi_1)}}{Z} \tag{4.10}$$

$$-\Delta\phi_2 = \frac{2b\kappa}{\beta}\frac{e^{\beta(-\psi+\phi_1-\phi_2)}}{Z} \tag{4.11}$$

with $Z = \int_\Lambda K e^{\beta(\phi_1-\phi_2)}\mathrm{d}x$.

Lemma 5. *This system of the two equations (4.10) and (4.11) is equivalent to the original single equation (4.2), for any choice of* (a, b, β) *such that* $K = ae^{\beta\psi} - be^{-\beta\psi}$.

Proof of Lemma 5: On one hand, if ϕ_1 and ϕ_2 solve (4.10) and (4.11) respectively, then $u = \frac{\beta}{2}(\phi_1 - \phi_2)$ solves (4.2) trivially. On the other hand, if u is a solution to (4.2) (with 0-Dirichlet boundary condition), then by the representation $K = ae^{\beta\psi} - be^{-\beta\psi}$, the equation for u can be written as

$$-\Delta u = \kappa\frac{(ae^{\beta\psi} - be^{-\beta\psi})e^{2u}}{\int Ke^{2u}\mathrm{d}x} = \kappa a\frac{e^{\beta\psi+2u}}{\int Ke^{2u}\mathrm{d}x} - \kappa b\frac{e^{-\beta\psi+2u}}{\int Ke^{2u}\mathrm{d}x} \tag{4.12}$$

Let ϕ_1 be the unique solution to the equation (with 0-Dirichlet boundary condition)

$$-\Delta\phi_1 = \frac{2\kappa a}{\beta}\frac{e^{\beta\psi+2u}}{\int Ke^{2u}\mathrm{d}x}, \tag{4.13}$$

and ϕ_2 be the unique solution to the equation (with 0-Dirichlet boundary condition)

$$-\Delta\phi_2 = \frac{2\kappa b}{\beta}\frac{e^{-\beta\psi+2u}}{\int Ke^{2u}\mathrm{d}x}, \tag{4.14}$$

then their linear combination $\frac{\beta}{2}(\phi_1 - \phi_2)$ solves (4.2) and hence is equal to u. Now substitute $u = \frac{\beta}{2}(\phi_1 - \phi_2)$ back into (4.13) and (4.14) so that (4.10) and (4.11) are recovered.

This proves Lemma 5.

Because of (4.13) and(4.14), the freedom of choices for (a, b, β) allows us to choose $\beta = \kappa$.

In order to relate $-\Delta\phi_i$'s with probability measures, we set $-\Delta\bar{\phi}_1$ and $-\Delta\bar{\phi}_2$ to be the normalized measures $-\Delta\phi_1$ and $-\Delta\phi_2$, respectively, i.e. suppose that $\int -\Delta\phi_1 = A$, $\int -\Delta\phi_2 = B$, then by setting $\bar{\phi}_1 = \phi_1/A$, $\bar{\phi}_2 = \phi_2/B$, we have $\int -\Delta\bar{\phi}_i = 1$ for $i = 1, 2$. Correspondingly, equations (4.10) and (4.11) are turned into

$$-\Delta\bar{\phi}_1 = \frac{\exp\beta(\psi - B\bar{\phi}_2 + A\bar{\phi}_1)}{\int \exp\beta(\psi - B\bar{\phi}_2 + A\bar{\phi}_1)\mathrm{d}x} = \frac{\tilde{K}\exp\beta A\bar{\phi}_1}{\int \tilde{K}\exp\beta A\bar{\phi}_1\mathrm{d}x} \tag{4.15}$$

$$-\Delta\bar{\phi}_2 = \frac{\exp\beta(-\psi + A\bar{\phi}_1 - B\bar{\phi}_2)}{\int \exp\beta(-\psi + A\bar{\phi}_1 - B\bar{\phi}_2)\mathrm{d}x} = \frac{\hat{K}\exp\beta A\bar{\phi}_1}{\int \hat{K}\exp\beta A\bar{\phi}_1\mathrm{d}x} \tag{4.16}$$

where $\tilde{K} = \exp\beta(\psi - B\bar{\phi}_2)$ and $\hat{K} = \exp\beta(-\psi + A\bar{\phi}_1)$. Note: $A - B = 2\kappa/\beta = 2$ is a natural requirement from the original equation (4.2), and our choice is $\beta = \kappa$.

4.2 Existence of solutions to the continuum (fixed point) equations

Since $\int -\Delta\bar{\phi}_i = 1$ and $-\Delta\bar{\phi}_i \geq 0$ for $i = 1, 2$, we can define $-\Delta\bar{\phi}_i$ to be a probability measure ρ_i for $i = 1, 2$. The corresponding equations for ρ_i's are as follows:

$$\tilde{\rho}_1(x) = \frac{\exp\beta[AU * \tilde{\rho}_1(x) + \psi(x) - BU * \tilde{\rho}_2(x)]}{\int \exp\beta[AU * \tilde{\rho}_1(x) + \psi(x) - BU * \tilde{\rho}_2(x)]\mathrm{d}x}, \tag{4.17}$$

$$\tilde{\rho}_2(y) = \frac{\exp -\beta[BU * \tilde{\rho}_2(y) + \psi(y) - AU * \tilde{\rho}_1(y)]}{\int \exp -\beta[BU * \tilde{\rho}_2(y) + \psi(y) - AU * \tilde{\rho}_1(y)]dy}. \tag{4.18}$$

Note that we use the variable x for the first species, and the variable y for the second species, for convenience. We hope to get a pair $(\tilde{\rho}_1, \tilde{\rho}_2)$ solving the system of Euler-Lagrange equations (4.17) and (4.18).

For convenience, we will from now on replace the Green's function U by a bounded and Lipschitz continuous regularization of itself (like in [MeSp82]).

The contraction mapping technique is commonly used in fixed point problems. In our case, the Euler-Lagrange equations (4.17) and (4.18) can both be regarded as fixed point problems. Next, we show that under certain hypothesis, the equation (4.17) has a unique solution. Let $\tilde{T}_1$ be an operation from $\mathfrak{P}(\Lambda)$ to $\mathfrak{P}(\Lambda)$, defined by

$$\tilde{T}_1(\eta) = \frac{\exp\beta[AU * \eta(x) + \psi(x) - BU * \tilde{\rho}_2(x)]}{\int \exp\beta[AU * \eta(x) + \psi(x) - BU * \tilde{\rho}_2(x)]\mathrm{d}x} \tag{4.19}$$

where $\tilde{\rho}_2$ is given. For any two probability measures η_1, η_2 on the Borel sets of Λ, the $\mathfrak{L}^1$-distance between their images can be rewritten as a t-integral over $[0,1]$ and estimated as follows:

$$\begin{aligned}
& ||\tilde{T}_1(\eta_1) - \tilde{T}_1(\eta_2)||_{\mathfrak{L}^1(\Lambda)} \\
= \quad & || \exp [\beta AU * \eta_1(x) + \beta\psi(x) - \beta BU * \tilde{\rho}_2(x) - \ln Z_1] \\
& - \exp [\beta AU * \eta_2(x) + \beta\psi(x) - \beta BU * \tilde{\rho}_2(x) - \ln Z_2] ||_{\mathfrak{L}^1(\Lambda)} \\
= \quad & || \textstyle\int_0^1 \exp \Big\{ t[\beta AU * \eta_1(x) + \beta\psi(x) - \beta BU * \tilde{\rho}_2(x) - \ln Z_1] \\
& +(1-t)[\beta AU * \eta_2(x) + \beta\psi(x) - \beta BU * \tilde{\rho}_2(x) - \ln Z_2] \Big\} \\
& \cdot \beta AU * (\eta_1 - \eta_2) dt ||_{\mathfrak{L}^1(\Lambda)} \\
\leq \quad & || \exp \Big\{ t[\beta AU * \eta_1(x) + \beta\psi(x) - \beta BU * \tilde{\rho}_2(x) - \ln Z_1] \\
& +(1-t)[\beta AU * \eta_2(x) + \beta\psi(x) - \beta BU * \tilde{\rho}_2(x) - \ln Z_2] \Big\} ||_{\mathfrak{L}^1(\Lambda)} \\
& \cdot || \beta U * (A\eta_1 - B\eta_2) ||_{L^\infty(\Lambda)} \\
\leq \quad & || \exp t[\beta AU * \eta_1(x) + \beta\psi(x) - \beta BU * \tilde{\rho}_2(x) - \ln Z_1] ||_{L^{\frac{1}{t}}(\Lambda)} \\
& \cdot || \exp (1-t)[\beta AU * \eta_2(x) + \beta\psi(x) - \beta BU * \tilde{\rho}_2(x) - \ln Z_2] ||_{L^{\frac{1}{1-t}}(\Lambda)} \\
& \cdot || \beta AU * (\eta_1 - \eta_2) ||_{L^\infty(\Lambda)} \\
\leq \quad & |\beta| AM ||\eta_1 - \eta_2||_{\mathfrak{L}^1(\Lambda)}
\end{aligned} \tag{4.20}$$

where $M = \sup |U|$, under our earlier assumption that U is continuous and bounded. Thus, if $|\beta|AM < 1$, then $\tilde{T}_1$ is a contraction and hence a unique fixed point $\eta = \tilde{\rho}_1$ exists. Similarly, define another operator $\tilde{T}_2$ as

$$\tilde{T}_2(\eta) = \frac{\exp -\beta[BU * \eta(y) + \psi(y) - AU * \tilde{\rho}_1(y)]}{\int \exp -\beta[BU * \eta(y) + \psi(y) - AU * \tilde{\rho}_1(y)] dy} \tag{4.21}$$

with a given probability measure $\tilde{\rho}_1$. If $|\beta|BM < 1$, then $\tilde{T}_2$ is a contraction and hence a unique fixed point $\eta = \tilde{\rho}_2$ exists.

So when both $|\beta|AM$ and $|\beta|BM$ are less than 1, the system of continuum fixed point equations has a unique solution. Namely, with the help of contraction mappings, we can make a converging sequence of $(\rho_{1,k}, \rho_{2,l})$ and have $(\tilde{\rho}_1, \tilde{\rho}_2)$ as its limit. Start from any probability measure $\rho_{1,1}$, say the uniform distribution, on Λ, and solve (4.18) with $\rho_{1,1}$ in place for $\tilde{\rho}_1$ and the resulting $\rho_{2,1}$ is the continuum distribution of the second species particles conditioned on $\rho_{1,1}$. Then solve (4.17) with $\rho_{2,1}$ in place for $\tilde{\rho}_2$ and the obtained probability measure $\rho_{1,2}$ is the continuum distribution of the first species particles conditioned on $\rho_{2,1}$. Repeating this procedure, we can get a sequence as follows:

$$(\rho_{1,1},\rho_{2,1}),\ (\rho_{1,2},\rho_{2,1}),(\rho_{1,2},\rho_{2,2}),\cdots,(\rho_{1,k},\rho_{2,k}),(\rho_{1,k+1},\rho_{2,k}),(\rho_{1,k+1},\rho_{2,k+1}),\cdots$$

The $\mathfrak{L}^1$ distance between each adjacent pair has an estimate in the form of (4.20), and hence the sequence must converge to the unique solution pair $(\tilde{\rho}_1,\tilde{\rho}_2)$.

Remark 6. *The above fixed point calculation was done for the bounded continuous U, following the footsteps of Messer-Spohn [MeSp82]. A similar discussion can be carried out when U has logarithmic singularities, except that then one needs to replace the $\mathfrak{L}^1$ estimates by $\mathfrak{L}^p$ estimates, for $p>1$; compare with our treatment in Part I.*

4.2.1 The Continuum Variational Principles

The continuum variational principles of the ρ's are:

1) For Species 1,

$$\begin{aligned}\tilde{F}_1(\rho) &= -\tfrac{A}{2}\int\int U\rho^{\otimes 2}d^2x+\beta^{-1}\int\rho\ln(\rho/\tilde{K})\mathrm{d}x\\ &= -\tfrac{A}{2}\int\int U\rho^{\otimes 2}d^2x+\beta^{-1}\int\rho\ln\rho\mathrm{d}x-\int\rho(\psi-BU*\rho_2)\mathrm{d}x,\end{aligned}\tag{4.22}$$

with its Euler-Lagrange equation given by (4.17); and

2) for Species 2,

$$\begin{aligned}\tilde{F}_2(\rho) &= -\tfrac{B}{2}\int\int U\rho^{\otimes 2}d^2y-\beta^{-1}\int\rho\ln(\rho/\hat{K})\mathrm{d}y\\ &= -\tfrac{B}{2}\int\int U\rho^{\otimes 2}d^2y-\beta^{-1}\int\rho\ln\rho\mathrm{d}y-\int\rho(\psi-AU*\rho_1)\mathrm{d}y,\end{aligned}\tag{4.23}$$

with its Euler-Lagrange equation given by (4.18).

Remark 7. *Notice that the formal variational principle (4.4) is not a linear combination of the variational principles (4.22) and (4.23).*

Incidentally, there is a combined variational principle on the continuum level,

$$\begin{aligned}F_{1,2}(\rho_1,\rho_2) &= -\tfrac{A^2}{2}\int\int U\rho_1^{\otimes 2}d^2x-\tfrac{B^2}{2}\int\int U\rho_2^{\otimes 2}\mathrm{d}^2x\\ &\quad+\tfrac{A}{\beta}\int\rho_1\ln\rho_1 dx-\tfrac{B}{\beta}\int\rho_2\ln\rho_2\mathrm{d}x\\ &\quad-A\int\rho_1\psi\mathrm{d}x-B\int\rho_2\psi\mathrm{d}x+AB\int\int U\rho_1\otimes\rho_2\mathrm{d}^2x.\end{aligned}\tag{4.24}$$

By taking partial derivatives with respect to ρ_1 and ρ_2, equations (4.17) and (4.18) can be recovered respectively. Notice that the "critical points" of this combined variational principle do not provide local maxima or local minima, but saddle points.

4.3 Atomization

It is natural to atomize both species at the same time and try to find the weak limit points of the individual sequence of ensemble measures. An intuitive thought is to find a joint distribution for both species and hope to find its limit; but a calculation later tells us that this is impossible.

4.3.1 The Paired Variational Principles

Indeed, on the (N_1, N_2)-body level,

1) For Species 1, the variational principle is

$$\begin{aligned} G_1^{(N_1)}(\mu^{(N_1)}) &= -\tfrac{A}{2(N_1-1)}\int\sum\sum_{i\neq j} U_{ij}\mu^{(N_1)}d^{N_1}x + \beta^{-1}\int \mu^{(N_1)}\ln\mu^{(N_1)}d^{N_1}x \\ &\quad -\int \mu^{(N_1)}[\sum_{i=1}^{N_1}\psi(x_i) - \tfrac{B}{N_2}\sum_{i=1}^{N_1}\sum_{a=1}^{N_2} U(x_i, y_a)]d^{N_1}x, \end{aligned} \tag{4.25}$$

where U_{ij} is the abbreviation for $U(x_i, x_j)$, with its Euler-Lagrange equation

$$\mu_1^{(N_1|N_2)} = \frac{\exp\beta[\sum_{i=1}^{N_1}\psi(x_i) - \frac{B}{N_2}\sum_{i=1}^{N_1}\sum_{a=1}^{N_2} U(x_i, y_a) + \frac{A}{2(N_1-1)}\sum\sum_{i\neq j} U(x_i, x_j)]}{\int\exp\beta[\sum_{i=1}^{N_1}\psi(x_i) - \frac{B}{N_2}\sum_{i=1}^{N_1}\sum_{a=1}^{N_2} U(x_i, y_a) + \frac{A}{2(N_1-1)}\sum\sum_{i\neq j} U(x_i, x_j)]d^{N_1}x}, \tag{4.26}$$

and the value of the functional at the critical point(s) is

$$\begin{aligned} & G_1^{(N_1)}(\mu_1^{(N_1|N_2)}) \\ = & -\beta^{-1}\ln\int\exp\beta[\sum_{i=1}^{N_1}\psi(x_i) - \tfrac{B}{N_2}\sum_{i=1}^{N_1}\sum_{a=1}^{N_2} U(x_i, y_a) + \tfrac{A}{2(N_1-1)}\sum\sum_{i\neq j} U(x_i, x_j)]d^{N_1}x. \end{aligned} \tag{4.27}$$

By Messer-Spohn's technique, if we fix $N_2 > 0$ and let $N_1 \to \infty$, then

$$\lim_{N_1\to\infty}\frac{1}{N_1}G_1^{(N_1)}(\mu_1^{(N_1|N_2)}) = F_1(\rho_1), \tag{4.28}$$

where ρ_1 is a superposition of the solutions to the Euler-Lagrange equation

$$\rho_1(x) = \frac{\exp\beta[AU*\rho_1(x) + \psi(x) - \frac{B}{N_2}\sum_a U(x, y_a)]}{\int\exp\beta[AU*\rho_1(x) + \psi(x) - \frac{B}{N_2}\sum_a U(x, y_a)]\mathrm{d}x} \tag{4.29}$$

of the variational principle

$$F_1(\rho) = -\frac{A}{2}\int\int U\rho^{\otimes 2}d^2x + \beta^{-1}\int \rho\ln\rho \mathrm{d}x - \int \rho[\psi(x) - \frac{B}{N_2}\sum_a U(x, y_a)]dx. \quad (4.30)$$

2) For Species 2, similarly, the variational principle is

$$\begin{aligned} G_2^{(N_2)}(\mu^{(N_2)}) &= -\tfrac{B}{2(N_2-1)}\int\sum_{a\neq b}\sum U_{ab}\mu^{(N_2)}d^{N_2}y - \beta^{-1}\int \mu^{(N_2)}\ln\mu^{(N_2)}d^{N_2}y \\ &\quad -\int \mu^{(N_2)}[\sum_{a=1}^{N_2}\psi(y_a) - \tfrac{A}{N_1}\sum_{i=1}^{N_1}\sum_{a=1}^{N_2}U(x_i, y_a)]d^{N_2}y, \end{aligned} \quad (4.31)$$

where U_{ab} is the abbreviation for $U(y_a, y_b)$, with its Euler-Lagrange equation

$$\mu_2^{(N_2|N_1)} = \frac{\exp -\beta[\sum_{a=1}^{N_2}\psi(y_a) - \frac{A}{N_1}\sum_{i=1}^{N_1}\sum_{a=1}^{N_2}U(x_i, y_a) + \frac{B}{2(N_2-1)}\sum_{a\neq b}\sum U(y_a, y_b)]}{\int \exp -\beta[\sum_{a=1}^{N_2}\psi(y_a) - \frac{A}{N_1}\sum_{i=1}^{N_1}\sum_{a=1}^{N_2}U(x_i, y_a) + \frac{B}{2(N_2-1)}\sum_{a\neq b}\sum U(y_a, y_b)]d^{N_2}y}, \quad (4.32)$$

and value of the functional at the critical point(s) is

$$\begin{aligned} &G_2^{(N_2)}(\mu_2^{(N_2|N_1)}) \\ = &-\beta^{-1}\ln\int \exp -\beta[\sum_{a=1}^{N_2}\psi(y_a) - \tfrac{A}{N_1}\sum_{i=1}^{N_1}\sum_{a=1}^{N_2}U(x_i, y_a) + \tfrac{B}{2(N_2-1)}\sum_{a\neq b}\sum U(y_a, y_b)]d^{N_2}y \end{aligned} \quad (4.33)$$

By Messer-Spohn's technique, if we fix $N_1 > 0$ and let $N_2 \to \infty$, then

$$\lim_{N_2\to\infty}\frac{1}{N_2}G_2^{(N_2)}(\mu_2^{(N_2|N_1)}) = F_2(\rho_2) \quad (4.34)$$

where ρ_2 is a superposition of the solutions to the Euler-Lagrange equation

$$\rho_2(y) = \frac{\exp -\beta[BU*\rho_2(y) + \psi(y) - \frac{A}{N_1}\sum_i U(x_i, y)]}{\int \exp -\beta[BU*\rho_2(y) + \psi(y) - \frac{A}{N_1}\sum_i U(x_i, y)]dy} \quad (4.35)$$

of the variational principle

$$F_2(\rho) = -\frac{B}{2}\int\int U\rho^{\otimes 2}d^2y - \beta^{-1}\int \rho\ln\rho dy - \int \rho[\psi(y) - \frac{A}{N_1}\sum_i U(x_i, y)]dy \quad (4.36)$$

The fixed point equations (4.29) and (4.35) each depends on the particular choice of N_2, (resp. N_1) points in the domain Λ. But the pair of continuum equations (4.17) and (4.18) each depends only on the solution of the other, i.e. on the limit distribution of the N_2 (resp. N_1) points.

So, what we want to study is actually that without fixing N_1 or N_2 first, but let $(N_1, N_2) \to (\infty, \infty)$ simultaneously, whether the pair

$$\Big(\frac{1}{N_1} G_1^{(N_1)}(\mu_1^{(N_1|N_2)}), \frac{1}{N_2} G_2^{(N_2)}(\mu_2^{(N_2|N_1)})\Big)$$

still converges to some $\Big(\tilde{F}_1(\tilde{\rho}_1), \tilde{F}_2(\tilde{\rho}_2)\Big)$. Here, $\tilde{F}_i$ and $\tilde{\rho}_i$ are the same as those in the continuum case.

Hence, we ask the question: Does there exist a joint distribution $\mu_{1,2}^{(N_1,N_2)}$ for the particles of the two species on the (N_1, N_2)-body level? If it does, then all we need to do is to analyze the limit of $\mu_{1,2}^{(N_1,N_2)}$ as $N_1 \to \infty, N_2 \to \infty$. In particular, the expected joint variational principle should look like

$$\begin{aligned} & G_{1,2}^{(N_1,N_2)}(\mu_{1,2}^{(N_1,N_2)}) \\ = \quad & -\tfrac{A^2}{2} \int U(x_1,x_2)^{(2)}\mu_1^{(N_1)}(x_1,x_2)\mathrm{d}^2x - \tfrac{B^2}{2} \int G(y_1,y_2)^{(2)}\mu_2^{(N_2)}(y_1,y_2)\mathrm{d}^2y \\ & +\tfrac{A}{\beta} \int {}^{(1)}\mu_1^{(N_1)}(x) \ln {}^{(1)}\mu_1^{(N_1)}(x)\mathrm{d}x - \tfrac{B}{\beta} \int {}^{(1)}\mu_2^{(N_2)}(y) \ln {}^{(1)}\mu_2^{(N_2)}(y)\mathrm{d}y \\ & -A \int {}^{(1)}\mu_1^{(N_1)}(x)\psi(x)\mathrm{d}x - B \int {}^{(1)}\mu_2^{(N_2)}(y)\psi(y)\mathrm{d}y \\ & +AB \int\int U(x,y)^{(1,1)}\mu_{1,2}^{(N_1,N_2)}(x,y)\mathrm{d}x\mathrm{d}y \end{aligned} \tag{4.37}$$

where

$$\mu_1^{(N_1)} = \int_{\Lambda^{N_2}} \mu_{1,2}^{(N_1,N_2)}\mathrm{d}^{N_2}y, \text{ and } \mu_2^{(N_2)} = \int_{\Lambda^{N_1}} \mu_{1,2}^{(N_1,N_2)}\mathrm{d}^{N_1}x. \tag{4.38}$$

We here also remind the readers that the left superscripts "(1)" and "(2)" stand for the orders of the marginals of a single species, and similarly "(1, 1)" means the mixed second marginal of two species. But such a joint variational principle only exists when a joint distribution $\mu_{1,2}^{(N_1,N_2)}$ exists, and the following subsection shows that it does not!

4.3.2 Absence of a Joint Distribution

With the pair of variational principles, it is natural to ask for the existence of a joint distribution for particles of the two species altogether. That is to say, we regard $\mu_1^{(N_1|N_2)}$ as the conditional distribution $\mu_{1|2}^{(N_1|N_2)}$ of the particles of Species 1, given the location of the particles of Species 2; and similarly, we regard $\mu_2^{(N_2|N_1)}$ as the conditional distribution $\mu_{2|1}^{(N_2|N_1)}$ of the particles of Species 2, given the location of the particles of Species 1. For simplicity, set $N_1 = N_2 = N$, and assume that a joint distribution $\mu_{1,2}^{(N,N)}$ exists. Under these hypotheses, the following equations are true:

$$\mu_{1|2}^{(N|N)}(x|y) = \frac{\mu_{1,2}^{(N,N)}(x,y)}{\mu_2^{(N)}(y)}, \text{ and } \mu_{2|1}^{(N|N)}(y|x) = \frac{\mu_{1,2}^{(N,N)}(x,y)}{\mu_1^{(N)}(x)}. \tag{4.39}$$

The ratio of these two equations gives

$$\frac{\mu_{1|2}^{(N|N)}(x|y)}{\mu_{2|1}^{(N|N)}(y|x)} = \frac{\mu_1^{(N)}(x)}{\mu_2^{(N)}(y)}, \tag{4.40}$$

and thus

$$\int \frac{\mu_{1|2}^{(N|N)}(x|y)}{\mu_{2|1}^{(N|N)}(y|x)} d^N x = \int \frac{\mu_1^{(N)}(x)}{\mu_2^{(N)}(y)} d^N x = \frac{1}{\mu_2^{(N)}(y)}, \tag{4.41}$$

leading to

$$\mu_2^{(N)}(y) = \Big[\int \frac{\mu_{1|2}^{(N|N)}(x|y)}{\mu_{2|1}^{(N|N)}(y|x)} d^N x\Big]^{-1}. \tag{4.42}$$

Similarly, we also have

$$\mu_1^{(N)}(x) = \Big[\int \frac{\mu_{2|1}^{(N|N)}(y|x)}{\mu_{1|2}^{(N|N)}(x|y)} d^N y\Big]^{-1}. \tag{4.43}$$

Besides, as a quick check, the two different expressions of the joint distribution $\mu_{1,2}^{(N,N)}$ by $\mu_{1|2}^{(N|N)} \cdot \mu_2^{(N)}$ and $\mu_{2|1}^{(N|N)} \cdot \mu_1^{(N)}$ must coincide, i.e.

$$\mu_{1|2}^{(N|N)}(x|y) \cdot \Big[\int \frac{\mu_{1|2}^{(N|N)}(x|y)}{\mu_{2|1}^{(N|N)}(y|x)} d^N x\Big]^{-1} = \mu_{2|1}^{(N|N)}(y|x) \cdot \Big[\int \frac{\mu_{2|1}^{(N|N)}(y|x)}{\mu_{1|2}^{(N|N)}(x|y)} d^N y\Big]^{-1}. \tag{4.44}$$

That is to say, substituting in the explicit formulas of $\mu_{1|2}^{(N|N)}$ and $\mu_{2|1}^{(N|N)}$, the term

$$\frac{\exp \beta[\sum_i \psi(x_i) - \frac{B}{N}\sum_i\sum_a U(x_i,y_a) + \frac{A}{2(N-1)}\sum\sum_{i\neq j} U(x_i,x_j)]}{\int \exp \beta[\sum_i \psi(\tilde{x}_i) - \frac{B}{N}\sum_i\sum_a U(\tilde{x}_i,y_a) + \frac{A}{2(N-1)}\sum\sum_{i\neq j} U(\tilde{x}_i,\tilde{x}_j)]d^N\tilde{x}}$$
$$\cdot \Big[\int \frac{\exp \beta[\sum_i \psi(z_i) - \frac{B}{N}\sum_i\sum_a U(z_i,y_a) + \frac{A}{2(N-1)}\sum\sum_{i\neq j} U(z_i,z_j)]}{\exp -\beta[\sum_a \psi(y_a) - \frac{A}{N}\sum_i\sum_a U(z_i,y_a) + \frac{B}{2(N-1)}\sum\sum_{a\neq b} U(y_a,y_b)]}$$
$$\cdot\frac{\int \exp -\beta[\sum_a \psi(\tilde{y}_a) - \frac{A}{N}\sum_i\sum_a U(z_i,\tilde{y}_a) + \frac{B}{2(N-1)}\sum\sum_{a\neq b} U(\tilde{y}_a,\tilde{y}_b)]d^N\tilde{y}}{\int \exp \beta[\sum_i \psi(\tilde{x}_i) - \frac{B}{N}\sum_i\sum_a U(\tilde{x}_i,y_a) + \frac{A}{2(N-1)}\sum\sum_{i\neq j} U(\tilde{x}_i,\tilde{x}_j)]d^N\tilde{x}} d^N z\Big]^{-1}$$

$$(4.45)$$

must match with the term

$$\frac{\exp -\beta[\sum_a \psi(y_a) - \frac{A}{N}\sum_i\sum_a U(x_i,y_a) + \frac{B}{2(N-1)}\sum\sum_{a\neq b} U(y_a,y_b)]}{\int \exp -\beta[\sum_a \psi(\tilde{y}_a) - \frac{A}{N}\sum_i\sum_a U(x_i,\tilde{y}_a) + \frac{B}{2(N-1)}\sum\sum_{a\neq b} U(\tilde{y}_a,\tilde{y}_b)]d^N\tilde{y}}$$
$$\cdot \Bigg[\frac{\exp -\beta[\sum_a \psi(y_a) - \frac{A}{N}\sum_i\sum_a U(x_i,y_a) + \frac{B}{2(N-1)}\sum\sum_{a\neq b} U(y_a,y_b)]}{\exp \beta[\sum_i \psi(x_i) - \frac{B}{N}\sum_i\sum_a U(x_i,y_a) + \frac{A}{2(N-1)}\sum\sum_{i\neq j} U(x_i,x_j)]}$$
$$\cdot \int \frac{\int \exp \beta[\sum_i \psi(\tilde{x}_i) - \frac{B}{N}\sum_i\sum_a U(\tilde{x}_i,z_a) + \frac{A}{2(N-1)}\sum\sum_{i\neq j} U(\tilde{x}_i,\tilde{x}_j)]d^N\tilde{x}}{\int \exp -\beta[\sum_a \psi(\tilde{y}_a) - \frac{A}{N}\sum_i\sum_a U(x_i,\tilde{y}_a) + \frac{B}{2(N-1)}\sum\sum_{a\neq b} U(\tilde{y}_a,\tilde{y}_b)]d^N\tilde{y}} d^N z\Bigg]^{-1} \tag{4.46}$$

i.e. after simplification and rearrangement, the term

$$\exp \beta\Big\{ \sum_i \psi(x_i) - \sum_a \psi(y_a) - \frac{B}{N}\sum_i\sum_a U(x_i,y_a)$$
$$+\frac{A}{2(N-1)}\sum\sum_{i\neq j} U(x_i,x_j) - \frac{B}{2(N-1)}\sum\sum_{a\neq b} U(y_a,y_b)\Big\}$$
$$\cdot\Big[\int\int \exp \beta[\sum_i \psi(z_i) - \sum_a \psi(\tilde{y}_a) - \frac{A+B}{N}\sum_i\sum_a U(z_i,y_a) + \frac{A}{N}\sum_i\sum_a U(z_i,\tilde{y}_a)$$
$$+\frac{A}{2(N-1)}\sum\sum_{i\neq j} U(z_i,z_j) - \frac{B}{2(N-1)}\sum\sum_{a\neq b} U(\tilde{y}_a,\tilde{y}_b)]d^N\tilde{y}d^N z\Big]^{-1}$$

has to be the same as

$$\exp \beta\Big\{ \sum_i \psi(x_i) - \sum_a \psi(y_a) + \frac{A}{N}\sum_i\sum_a U(x_i,y_a)$$
$$+\frac{A}{2(N-1)}\sum\sum_{i\neq j} U(x_i,x_j) - \frac{B}{2(N-1)}\sum\sum_{a\neq b} U(y_a,y_b)\Big\}$$
$$\cdot\Big[\int\int \exp \beta[\sum_i \psi(\tilde{x}_i) - \sum_a \psi(t_a) + \frac{A+B}{N}\sum_i\sum_a U(x_i,t_a) - \frac{B}{N}\sum_i\sum_a U(\tilde{x}_i,t_a)$$
$$+\frac{A}{2(N-1)}\sum\sum_{i\neq j} U(\tilde{x}_i,\tilde{x}_j) - \frac{B}{2(N-1)}\sum\sum_{a\neq b} U(t_a,t_b)]d^N\tilde{x}d^N t\Big]^{-1}$$

The above equation implies that $A + B = 0$, but this contradicts the requirement $A, B > 0$. Consequently, a joint distribution on the (N_1, N_2)-level does not exist under the condition $A, B > 0$. This completes the proof.

So, instead of considering the combined variational principle, we still need to consider the paired Euler-Lagrange equations as a system. This suggests that a different way of "atomizing" should be considered.

4.4 Quasi-Atomization

In this section, we replace both variational principles (4.25) and (4.31) by two variational principles "conditioned" on the distribution (instead of the locations) of the particles of the other species.

Thus the corresponding variational principles are

1) For Species 1, on the N_1-body level,

$$\begin{aligned} \mathcal{G}_1^{(N_1)}(\mu^{(N_1)}) \quad = \quad & -\tfrac{A}{2(N_1-1)} \int \sum\sum_{i\neq j} U_{ij}\mu^{(N_1)} d^{N_1}x + \beta^{-1}\int \mu^{(N_1)} \ln \mu^{(N_1)} \mathrm{d}^{N_1}x \\ & - \int \mu^{(N_1)}[\sum_{i=1}^{N_1} \psi(x_i) - B\sum_{i=1}^{N_1}(U * {}^{(1)}\bar{\mu}_2^{(N_2)})(x_i)]\mathrm{d}^{N_1}x \end{aligned} \tag{4.47}$$

with its Euler-Lagrange equation

$$\bar{\mu}_1^{(N_1)} = \frac{\exp\beta[\sum_{i=1}^{N_1}\psi(x_i) - B\sum_{i=1}^{N_1}(U * {}^{(1)}\bar{\mu}_2^{(N_2)})(x_i) + \frac{A}{2(N_1-1)}\sum\sum_{i\neq j} U_{ij}]}{\int \exp\beta[\sum_{i=1}^{N_1}\psi(x_i) - B\sum_{i=1}^{N_1}(U * {}^{(1)}\bar{\mu}_2^{(N_2)})(x_i) + \frac{A}{2(N_1-1)}\sum\sum_{i\neq j} U_{ij}]\mathrm{d}^{N_1}x} \tag{4.48}$$

2) For Species 2, on the N_2-body level,

$$\begin{aligned} \mathcal{G}_2^{(N_2)}(\mu^{(N_2)}) \quad = \quad & -\tfrac{B}{2(N_2-1)} \int \sum\sum_{a\neq b} U_{ab}\mu^{(N_2)} d^{N_2}y - \beta^{-1}\int \mu^{(N_2)} \ln \mu^{(N_2)} \mathrm{d}^{N_2}y \\ & - \int \mu^{(N_2)}[\sum_{a=1}^{N_2} \psi(y_a) - A\sum_{a=1}^{N_2}(U * {}^{(1)}\bar{\mu}_1^{(N_1)})(y_a)]\mathrm{d}^{N_2}y \end{aligned} \tag{4.49}$$

with its Euler-Lagrange equation

$$\bar{\mu}_2^{(N_2)} = \frac{\exp-\beta[\sum_{a=1}^{N_2}\psi(y_a) - A\sum_{a=1}^{N_2}(U * {}^{(1)}\bar{\mu}_1^{(N_1)})(y_a) + \frac{B}{2(N_2-1)}\sum\sum_{a\neq b} U_{ab}]}{\int \exp-\beta[\sum_{a=1}^{N_2}\psi(y_a) - A\sum_{a=1}^{N_2}(U * {}^{(1)}\bar{\mu}_1^{(N_1)})(y_a) + \frac{B}{2(N_2-1)}\sum\sum_{a\neq b} U_{ab}]\mathrm{d}^{N_2}y} \tag{4.50}$$

Taking a closer look at the equations (4.25), (4.26), (4.31) and (4.32), we notice that the variational principles can be combined into a joint variational principle of

$(\mu_1^{(N_1)}, \mu_2^{(N_2)})$ as follows:

$$
\begin{aligned}
& G_{1,2}^{(N_1,N_2)}(\mu_1^{(N_1)}, \mu_2^{(N_2)}) \\
= \quad & -\tfrac{A^2}{2N_1(N_1-1)} \int \sum\sum_{i\neq j} U(x_i,x_j)\mu_1^{(N_1)} \mathrm{d}^{N_1}x - \tfrac{B^2}{2N_2(N_2-1)} \int \sum\sum_{a\neq b} U(y_a,y_b)\mu_2^{(N_2)} \mathrm{d}^{N_2}y \\
& +\tfrac{A}{\beta N_1} \int \mu_1^{(N_1)} \ln \mu_1^{(N_1)} \mathrm{d}^{N_1}x - \tfrac{B}{\beta N_2} \int \mu_2^{(N_2)} \ln \mu_2^{(N_2)} \mathrm{d}^{N_2}y \\
& -\tfrac{A}{N_1} \int \mu_1^{(N_1)} \sum_{i=1}^{N_1} \psi(x_i) \mathrm{d}^{N_1}x - \tfrac{B}{N_2} \int \mu_2^{(N_2)} \sum_{a=1}^{N_2} \psi(y_a) \mathrm{d}^{N_2}y \\
& +\tfrac{AB}{N_1N_2} \int\int \sum_{i=1}^{N_1}\sum_{a=1}^{N_2} U(x_i,y_a)\mu_1^{(N_1)}\mu_2^{(N_2)} \mathrm{d}^{N_1}x\mathrm{d}^{N_2}y \\
= \quad & -\tfrac{A^2}{2} \int U(x_1,x_2)^{(2)}\mu_1^{(N_1)}(x_1,x_2)\mathrm{d}^2x - \tfrac{B^2}{2} \int G(y_1,y_2)^{(2)}\mu_2^{(N_2)}(y_1,y_2)\mathrm{d}^2y \\
& +\tfrac{A}{\beta} \int {}^{(1)}\mu_1^{(N_1)}(x) \ln {}^{(1)}\mu_1^{(N_1)}(x)\mathrm{d}x - \tfrac{B}{\beta} \int {}^{(1)}\mu_2^{(N_2)}(y) \ln {}^{(1)}\mu_2^{(N_2)}(y)\mathrm{d}y \\
& -A \int {}^{(1)}\mu_1^{(N_1)}(x)\psi(x)\mathrm{d}x - B \int {}^{(1)}\mu_2^{(N_2)}(y)\psi(y)\mathrm{d}y \\
& +AB \int\int U(x,y)^{(1)}\mu_1^{(N_1)}(x)^{(1)}\mu_2^{(N_2)}(y)\mathrm{d}x\mathrm{d}y
\end{aligned} \tag{4.51}
$$

Partial differentiation with respect to μ_1 and μ_2 recovers equations (4.26) and (4.32), respectively.

4.4.1 Contraction Mappings: Control Non-uniform in N

In order to show that a solution $(\bar{\mu}_1, \bar{\mu}_2)$ exists, we consider the following two mappings and prove that they are contraction mappings:

1) For Species 2, on the N_2-body level, let $T_1^{(N_1)}$ be the mapping from the first marginal of an N_2-dim distribution measure to the first marginal of an N_1-dim distribution measure, defined by:

$$
\begin{aligned}
& T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}) \\
= \quad & \frac{\int_{\Lambda^{N_1-1}} \exp\ \beta[\sum_{i=1}^{N_1}\psi(x_i) - B\sum_{i=1}^{N_1}(U * {}^{(1)}\mu_2^{(N_2)})(x_i) + \frac{A}{2(N_1-1)}\sum\sum_{i\neq j} U_{ij}]\mathrm{d}^{N_1-1}x}{\int_{\Lambda^{N_1}} \exp\ \beta[\sum_{i=1}^{N_1}\psi(x_i) - B\sum_{i=1}^{N_1}(U * {}^{(1)}\mu_2^{(N_2)})(x_i) + \frac{A}{2(N_1-1)}\sum\sum_{i\neq j} U_{ij}]\mathrm{d}^{N_1}x},
\end{aligned} \tag{4.52}
$$

where U_{ij} stands for $U(x_i, x_j)$.

2) For Species 1, on the N_1-body level, let $T_2^{(N_2)}$ be the mapping from the first marginal

of an N_1-dim distribution measure to the first marginal of an N_2-dim distribution measure, defined by:

$$T_2^{(N_2)}({}^{(1)}\mu_1^{(N_1)}) = \frac{\int_{\Lambda^{N_2-1}} \exp -\beta[\sum_{a=1}^{N_2} \psi(y_a) - A\sum_{a=1}^{N_2}(U * {}^{(1)}\mu_1^{(N_1)})(y_a) + \frac{B}{2(N_2-1)}\sum\sum_{a\neq b} U_{ab}]\mathrm{d}^{N_2-1}y}{\int_{\Lambda^{N_2}} \exp -\beta[\sum_{a=1}^{N_2} \psi(y_a) - A\sum_{a=1}^{N_2}(U * {}^{(1)}\mu_1^{(N_1)})(y_a) + \frac{B}{2(N_2-1)}\sum\sum_{a\neq b} U_{ab}]\mathrm{d}^{N_2}y}, \tag{4.53}$$

where U_{ab} stands for $U(y_a, y_b)$.

With a coarse estimate similar to the one on the continuum level, we can conclude that when $|\beta|AMN_1 < 1$ and $|\beta|BMN_2 < 1$ with the natural requirement from decomposition $A - B = 2$, the operators $T_1^{(N_1)}$ and $T_2^{(N_2)}$ are contraction mappings, so that a unique pair of solutions $({}^{(1)}\mu_1^{(N_1)}, {}^{(1)}\mu_2^{(N_2)})$ exists. This shows that the mutual conditioning of these two ensemble measures, given by (4.48) and (4.50), is consistently formulated.

However, this estimate is not good enough to guarantee a contraction for arbitrarily large (but fixed) N_1 and N_2 with the same chosen constants A and B, and (small) $|\beta|$. Nevertheless, a refined approach, discussed next, will show that as N_1 and N_2 both approach ∞ with the same chosen constants A and B, and (small) $|\beta|$. The fixed point mappings (4.52) and (4.53) iterate into a fixed point of the continuum equations (4.17) and (4.18).

4.4.2 Contraction Mappings: with A, B, $|\beta|$ Independent of N

In this subsection, we will argue convincingly that it is possible to show that

$$||T_2^{(N_2)}({}^{(1)}\mu_1^{(N_1)}) - T_2^{(N_2)}({}^{(1)}\tilde{\mu}_1^{(N_1)})||_{\mathfrak{L}^1(\Lambda)} \leq C_1||{}^{(1)}\mu_1^{(N_1)} - {}^{(1)}\tilde{\mu}_1^{(N_1)}||_{\mathfrak{L}^1(\Lambda)} \tag{4.54}$$

for some constant $C_1 < 1/2$ if N_2 is large enough, and

$$||T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}) - T_1^{(N_1)}({}^{(1)}\tilde{\mu}_2^{(N_2)})||_{\mathfrak{L}^1(\Lambda)} \leq C_2||{}^{(1)}\mu_2^{(N_2)} - {}^{(1)}\tilde{\mu}_2^{(N_2)}||_{\mathfrak{L}^1(\Lambda)} \tag{4.55}$$

for some constant $C_2 < 1/2$ if N_1 is large enough. Then combining the inequalities above, we get

$$\begin{aligned} & ||T_2^{(\hat{N}_2)}({}^{(1)}\mu_1^{(N_1)}) - T_2^{(\hat{N}_2)}({}^{(1)}\tilde{\mu}_1^{(N_1)})||_{\mathfrak{L}^1(\Lambda)} + ||T_1^{(\hat{N}_1)}({}^{(1)}\mu_2^{(N_2)}) - T_1^{(\hat{N}_1)}({}^{(1)}\tilde{\mu}_2^{(N_2)})||_{\mathfrak{L}^1(\Lambda)} \\ \leq\ & (C_1 + C_2)\left(||{}^{(1)}\mu_1^{(N_1)} - {}^{(1)}\tilde{\mu}_1^{(N_1)}||_{\mathfrak{L}^1(\Lambda)} + ||{}^{(1)}\mu_2^{(N_2)} - {}^{(1)}\tilde{\mu}_2^{(N_2)}||_{\mathfrak{L}^1(\Lambda)}\right) \end{aligned} \tag{4.56}$$

if both $\hat{N}_1$ and $\hat{N}_2$ are large enough, with the constant $C_1 + C_2 < 1$ independent of N's.

Note that both images $T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)})$ and $T_2^{(N_2)}({}^{(1)}\mu_1^{(N_1)})$ are measures of a single variable. Observe that the combination of the first and second terms of the exponents in T_1 separates as follows:

$$\begin{aligned} & \sum_{i=1}^{N_1}\left[\psi(x_i) - B(U * {}^{(1)}\mu_2^{(N_2)})(x_i)\right] \\ =\ & \left[\psi(x_1) - B(U * {}^{(1)}\mu_2^{(N_2)})(x_1)\right] + \sum_{i=2}^{N_1}\left[\psi(x_i) - B(U * {}^{(1)}\mu_2^{(N_2)})(x_i)\right]. \end{aligned} \tag{4.57}$$

Now clearly the third term

$$\beta\frac{A}{2(N_1 - 1)}\sum\sum_{i \neq j} U(x_i, x_j)$$

does not separate into two parts — one concerned with x's with indices between 2 and N_1, the other concerned with x_1. However, if we can show that it separates approximately with a controllably small error, then the proof runs fluently in the same spirit of (4.20) in the continuum case. Fortunately, we know a priori from the technique of Messer-Spohn, the average of the single sum, $\frac{1}{N_1-1}\sum_{j=2}^{N_1} U(x_1, x_j)$, in (4.52) is approximately the same as the convolution

$$(U * T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}))(x_1) = \int_\Lambda U(x_1, z)T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)})(z)\mathrm{d}z,$$

when N_1 is large and the Law of Large Numbers holds. For any fixed constant $\varepsilon > 0$, on the subset of Λ^{N_1-1} that

$$(\Lambda^{N_1-1})_\varepsilon = \left\{ Dist\left(\frac{1}{N_1 - 1}\sum_{j=2}^{N_1}\delta_{x_j}, T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)})\right) < \varepsilon \right\},$$

we replace the single sum by the convolution, with an error bound

$$\left|\frac{1}{N_1 - 1}\sum_{j=2}^{N_1} U(x_1, x_j) - (U * T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}))(x_1)\right| < \varepsilon.$$

So that the exponent in (4.52) can be separated as:

$$\begin{aligned} &\beta\Big[\psi(x_1) - B(U * {}^{(1)}\mu_2^{(N_2)})(x_1) + A(U * T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}))(x_1)\Big] \\ + \quad &\beta\Big[\sum_{i=2}^{N_1}\psi(x_i) - B\sum_{i=2}^{N_1}(U * {}^{(1)}\mu_2^{(N_2)})(x_i) + \tfrac{A}{2(N_1-1)}\sum\sum_{2\le i\neq j\le N_1} U(x_i,x_j)\Big] \end{aligned} \tag{4.58}$$

and the error is bounded by $|\beta|\varepsilon$. The modified $T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)})$ is then simplified to

$$\frac{\exp\Big\{\beta\Big[\psi(x_1) - B(U * {}^{(1)}\mu_2^{(N_2)})(x_1) + A(U * T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}))(x_1)\Big]\Big\}}{\int_\Lambda \exp\Big\{\beta\Big[\psi(x_1 - B(U * {}^{(1)}\mu_2^{(N_2)})(x_1) + A(U * T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}))(x_1)\Big]\Big\}\,\mathrm{d}x_1} \tag{4.59}$$

The estimate for the difference between such single variate fractions is again similar to the one for the continuum case. More precisely, $||T_1({}^{(1)}\mu_1^{(N_2}) - T_1({}^{(1)}\tilde{\mu}_2^{(N_2)})||_{\mathfrak{L}^1(\Lambda)}$ is bounded by the greatest one among the following four differences, with $\sigma_1, \sigma_2 = \pm 1$:

$$\begin{aligned} &\Big|e^{2\sigma_1\beta\varepsilon}\frac{\exp\Big\{\beta\Big[\psi(x_1) - B(U * {}^{(1)}\mu_2^{(N_2)})(x_1) + A(U * T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}))(x_1)\Big]\Big\}}{\int_\Lambda \exp\Big\{\beta\Big[\psi(x_1 - B(U * {}^{(1)}\mu_2^{(N_2)})(x_1) + A(U * T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}))(x_1)\Big]\Big\}\,\mathrm{d}x_1} \\ - \quad &e^{2\sigma_2\beta\varepsilon}\frac{\exp\Big\{\beta\Big[\psi(x_1) - B(U * {}^{(1)}\tilde{\mu}_2^{(N_2)})(x_1) + A(U * T_1^{(N_1)}({}^{(1)}\tilde{\mu}_2^{(N_2)}))(x_1)\Big]\Big\}}{\int_\Lambda \exp\Big\{\beta\Big[\psi(x_1 - B(U * {}^{(1)}\tilde{\mu}_2^{(N_2)})(x_1) + A(U * T_1^{(N_1)}({}^{(1)}\tilde{\mu}_2^{(N_2)}))(x_1)\Big]\Big\}\,\mathrm{d}x_1}\Big| \end{aligned} \tag{4.60}$$

Case 1. When $\sigma_1 = \sigma_2 = \sigma$ then (4.60) is bounded from above by

$$\begin{aligned} &e^{2\sigma\beta\varepsilon}\Big(|\beta|BM||{}^{(1)}\mu_2^{(N_2)} - {}^{(1)}\tilde{\mu}_2^{(N_2)}||_{\mathfrak{L}^1(\Lambda)} \\ &+|\beta|AM||T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}) - T_1^{(N_1)}({}^{(1)}\tilde{\mu}_2^{(N_2)})||_{\mathfrak{L}^1(\Lambda)}\Big) \end{aligned} \tag{4.61}$$

Recall that the Taylor expansion of the function $e^x = \displaystyle\sum_{k=0}^{\infty}\frac{x^k}{k!}$, when $0 \le x \le 1/2$, we have the following estimates:

$$\begin{aligned} e^x &= 1 + x + \tfrac{x^2}{2!} + \tfrac{x^3}{3!} + \tfrac{x^4}{4!} + \cdots \\ &\le 1 + x + \tfrac{x^2}{2} + \tfrac{x^3}{2^2} + \tfrac{x^4}{2^3} + \cdots \\ &= 1 + \tfrac{x}{1-x/2} \\ &\le 1 + 2x, \end{aligned} \tag{4.62}$$

and

$$\begin{aligned} e^{-x} &= 1 - x + \tfrac{x^2}{2!} - \tfrac{x^3}{3!} + \tfrac{x^4}{4!} - \cdots \\ &\leq 1 - x + \tfrac{x^2}{2} + \tfrac{x^3}{2^2} + \tfrac{x^4}{2^3} + \cdots \\ &= 1 - x + \tfrac{x^2/2}{1-x/2} \\ &\leq 1 - x + x^2 \\ &\leq 1 - \tfrac{x}{2}, \end{aligned} \tag{4.63}$$

together with the inequalities $1+x \leq e^x$ and $1-x \leq e^{-x}$. Thus (4.61) is bounded from above by

$$C\left(|\beta|BM||^{(1)}\mu_2^{(N_2)} - {}^{(1)}\tilde{\mu}_2^{(N_2)}||_{\mathfrak{L}^1(\Lambda)} + |\beta|AM||T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}) - T_1^{(N_1)}({}^{(1)}\tilde{\mu}_2^{(N_2)})||_{\mathfrak{L}^1(\Lambda)}\right), \tag{4.64}$$

with $C = (1 + 4|\beta|\varepsilon)$ for $\sigma = 1$; and with $C = (1 - |\beta|\varepsilon)$ for $\sigma = -1$.

Hence, in Case 1, we have the estimate as

$$||T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}) - T_1^{(N_1)}({}^{(1)}\tilde{\mu}_2^{(N_2)})||_{\mathfrak{L}^1(\Lambda)} \leq C||^{(1)}\mu_2^{(N_2)} - {}^{(1)}\tilde{\mu}_2^{(N_2)}||_{\mathfrak{L}^1(\Lambda)}, \tag{4.65}$$

with the constant

$$C = \max\left\{\frac{(1+4|\beta|\varepsilon)|\beta|BM}{1-(1+4|\beta|\varepsilon)|\beta|AM}, \frac{(1-|\beta|\varepsilon)|\beta|BM}{1-(1-|\beta|\varepsilon)|\beta|AM}\right\}.$$

Case 2. When $\sigma_1 = -\sigma_2$ then (4.60) is bounded from above by

$$\begin{aligned} &5|\beta|\varepsilon + \Big(|\beta|BM||^{(1)}\mu_2^{(N_2)} - {}^{(1)}\tilde{\mu}_2^{(N_2)}||_{\mathfrak{L}^1(\Lambda)} \\ &+|\beta|AM||T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}) - T_1^{(N_1)}({}^{(1)}\tilde{\mu}_2^{(N_2)})||_{\mathfrak{L}^1(\Lambda)}\Big) \end{aligned} \tag{4.66}$$

Now if we linearly relate ε to $||^{(1)}\mu_2^{(N_2)} - {}^{(1)}\tilde{\mu}_2^{(N_2)}||_{\mathfrak{L}^1(\Lambda)}$, say

$$\varepsilon = \xi||^{(1)}\mu_2^{(N_2)} - {}^{(1)}\tilde{\mu}_2^{(N_2)}||_{\mathfrak{L}^1(\Lambda)},$$

where ξ is a constant independent of N, then the estimate for Case 2 is

$$||T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)}) - T_1^{(N_1)}({}^{(1)}\tilde{\mu}_2^{(N_2)})||_{\mathfrak{L}^1(\Lambda)} \leq C||^{(1)}\mu_2^{(N_2)} - {}^{(1)}\tilde{\mu}_2^{(N_2)}||_{\mathfrak{L}^1(\Lambda)} \tag{4.67}$$

with the constant

$$C = \frac{5|\beta|\xi + |\beta|BM}{1 - |\beta|AM}.$$

The size of the subset of Λ^{N_1-1} that

$$\Lambda^{N_1-1}\setminus(\Lambda^{N_1-1})_\varepsilon=\left\{Dist\left(\frac{1}{N_1-1}\sum_{j=2}^{N_1}\delta_{x_j},T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)})\right)\geq\varepsilon\right\},$$

can be estimated by the theory of large deviations to be exponentially small in N_1, with the rate function given by a relative entropy. We assume that this relative entropy is bounded below by $c\varepsilon^2$, which is true under certain plausible conditions that we hope to verify in the future. Now with the same choice $\varepsilon=\xi||{}^{(1)}\mu_2^{(N_2)}-{}^{(1)}\tilde{\mu}_2^{(N_2)}||_{\mathfrak{L}^1(\Lambda)}$, we have $e^{-cN_1\varepsilon^2}<\tilde{\delta}\varepsilon$ whenever $N_1>N_{crit}$ with $N_{crit}=\lceil\frac{1}{\varepsilon}\ln\frac{1}{\tilde{\delta}\varepsilon}\rceil$. By symmetry, this is also true for N_2.

Putting the inequalities on the two subsets $(\Lambda^{N_1-1})_\varepsilon$ and $\Lambda^{N_1-1}\setminus(\Lambda^{N_1-1})_\varepsilon$ together, we have the estimate on the whole Λ as

$$||T_1^{(N_1)}({}^{(1)}\mu_2^{(N_2)})-T_1^{(N_1)}({}^{(1)}\tilde{\mu}_2^{(N_2)})||_{\mathfrak{L}^1(\Lambda)}\leq(C+\tilde{\delta}\xi)||{}^{(1)}\mu_2^{(N_2)}-{}^{(1)}\tilde{\mu}_2^{(N_2)}||_{\mathfrak{L}^1(\Lambda)}\quad(4.68)$$

where C is the same constant as on the subset $(\Lambda^{N_1-1})_\varepsilon$ and $\tilde{\delta}$ can be as small as one wishes. Again, by symmetry, an analogous estimate is true for $T_2^{(N_2)}$. Hence, a combined estimate in the form of (4.56) is obtained. Now by iteration we can get a sequence of pairs of measures $({}^{(1)}\mu_1^{(N_1[k])},{}^{(1)}\mu_2^{(N_2[k])})$, where k stands for the times of iterations, and

$${}^{(1)}\mu_1^{(N_1[k+1])}=T_1^{(N_1[k+1])}({}^{(1)}\mu_2^{(N_2[k])}),\ {}^{(1)}\mu_2^{(N_2[k+1])}=T_2^{(N_2[k+1])}({}^{(1)}\mu_1^{(N_1[k])}).$$

In each step, an equality in the form of (4.56) holds. So that when the N's tend to ∞, weak limit points can be expected (but not necessary to be unique).

Remark 8. *We conjecture that the mapping*

$$({}^{(1)}\mu_1^{(N_1)},{}^{(1)}\mu_2^{(N_2)})\mapsto(T_2({}^{(1)}\mu_1^{(N_1)}),T_1({}^{(1)}\mu_2^{(N_2)}))$$

must in fact have a unique fixed point for all (N_1,N_2) with A, B fixed and $|\beta|$ sufficiently small but independent of N; in that case the sequence

$$({}^{(1)}\mu_1^1,{}^{(1)}\mu_2^1),(T_1^{(2)}({}^{(1)}\mu_2^{(1)}),T_2^{(2)}({}^{(1)}\mu_1^{(1)})),(T_1^{(3)}({}^{(1)}\mu_2^{(2)}),T_2^{(3)}({}^{(1)}\mu_1^{(2)})),\cdots,\quad(4.69)$$

with the reduction formulas ${}^{(1)}\mu_1^{(N)}=T_1^{(N)}({}^{(1)}\mu_2^{(N-1)})$ and ${}^{(1)}\mu_2^{(N)}=T_2^{(N)}({}^{(1)}\mu_1^{(N-1)})$, is weakly compact, and so it converges to a pair of limit points $({}^{(1)}\mu_1^{(\mathbb{N})},{}^{(1)}\mu_2^{(\mathbb{N})})$, after *extracting a subsequence. By the technique of Messer and Spohn, the limit points* ${}^{(1)}\mu_1^{(\mathbb{N})}$ *and* ${}^{(1)}\mu_2^{(\mathbb{N})}$ *are each a superposition of the solutions to the continuum equation (4.22) and (4.23), respectively. Thus the original function (4.5) and hence (4.2) has a solution.*

If $C_1 + C_2 < 1$ *implies that* $|\beta| AM < 1$ *and* $|\beta| BM < 1$*, then indeed the limit fixed point is unique.*

Remark 9. *The pair of equations studied here may not have an interpretation on the particle level, because particles don't distribute themselves based on the "expected" distribution of other species. However, animals in the real world do behave according to their knowledge on their preys or predators. This alternatively provides a biological insight of the model studied in this chapter.*

References

[Abr87] Abresch, U., *Constant mean curvature tori in terms of elliptic functions,* J. Reine Angew. Math. **374**, 169C192 (1987).

[Are79] Aref, H., *Motion of three vortices,* Phys. Fluids **22**, 393–400 (1979).

[Are10] Aref, H., (ed.), *150 years of vortex dynamics*, Proc. IUTAM Symp. (TU Denmark), Oct. 12-16, 2008; IUTAM bookseries **20**, Springer (2010).

[ArPo82] Aref, H., and Pomphrey, N., *Integrable and chaotic motions of four vortices. I. The case of identical vortices*, Proc. Roy. Soc. London A **380**, 359-387 (1982).

[Aub79] Aubin, T., *Meilleures constantes dans le théorème d'inclusion de Sobolev et un théorème de Fredholm non linéaire pour la transformation conforme de la courbure scalaire,* J. Funct. Anal. **32**, no. 2, 148–174 (1979).

[Avi86] Aviles, P., *Conformal complete metrics with prescribed nonnegative Gaussian curvature in* $\mathbb{R}^2$*,* Invent. Math. **83**, no. 3, 519–544 (1986).

[Ban80] Bandle, C., *Isoperimetric inequalities and applications,* Pitman, Boston, (1980).

[BaTi07] Bardos, C., and Titi, E., *Euler equations for incompressible ideal fluids*, Russian Math. Surveys **62**, 409–451 (2007).

[BeMa82] Beale, J.T., and Majda, A., *Vortex methods. II. Higher order accuracy in two and three dimensions*, Math. Comp. **39**, 29–52 (1982).

[Bec93] Beckner, W., *Sharp Sobolev inequalities on the sphere and the Moser-Trudinger inequality*, Ann. of Math. **138**, 213–242 (1993).

[Bil68] Billingsley, P., *Convergence of probability measures*, J. Wiley and Sons, New York (1968).

[BoKo08] Boatto, S., and Koiller, J., *Vortices on closed surfaces*, available as eprint arXiv:0802.4313v1 (2008).

[Bra87] Branson, T., *Group representations arising from Lorentz conformal geometry*, J. Funct. Anal. **74**, no. 2, 199–291 (1987).

[Bro24] Brodetzky, S., *Vortex motion*, in Proc. 1st. Int. Congr. Appl. Math. (Delft), 374–379 (1924).

[Bol96] Boltzmann, L., *Vorlesungen über Gastheorie*, J.A. Barth, Leipzig (1896); English translation: "Lectures on Gas theory" (S.G. Brush, transl.), Univ. California Press, Berkeley (1964).

[BoVe11] Bouchet, F., and Venaille, A., *Statistical mechanics of two-dimensional and geophysical flows*, Phys. Rep. **515**, 227-296 (2012).

[CLMP92] Caglioti, E., Lions, P. L., Marchioro, C., and Pulvirenti, M., *A special class of stationary flows for two-dimensional Euler equations: A statistical mechanics description*, Commun. Math. Phys. **143**, 501–525 (1992).

[CLMP95] Caglioti, E., Lions, P. L., Marchioro, C., and Pulvirenti, M., *A special class of stationary flows for two-dimensional Euler equations: A statistical mechanics description. II*, Commun. Math. Phys. **174**, 229–260 (1995).

[CaON91] Campbell, L. J., and O'Neil, K., *Statistics of two-dimensional point vortices and high energy vortex states*, J. Stat. Phys. **65**, 495–529 (1991).

[CaLo92] Carlen, E., and Loss, M., *Competing symmetries, the logarithmic HLS inequality, and Onofri's inequality on* $\mathbb{S}^n$, Geom. Funct. Anal. **2** 90–104 (1992).

[Cha96] Chang., S.Y.A., *On a Fourth-Order Partial Differential Equation in Conformal Geometry* Harmonic analysis and partial differential equations (Chicago, IL, 1996), 127–150, Chicago Lectures in Math., Univ. Chicago Press, Chicago, IL, 1999.

[Cha08] Chang., S.Y.A., Eastwood, M., Ørsted, B., Yang, P. *What is Q-curvature?* Acta Appl. Math. **102**, no. 2-3, 119–125 (2008).

[ChYa87] Chang., S.Y.A., and Yang, P., *Prescribing Gaussian curvature on* $\mathbb{S}^2$*,* Acta Math. **159**, 215–259 (1987).

[ChYa88] Chang., S.Y.A., and Yang, P., *Conformal deformation of metrics on* $\mathbb{S}^2$, J. Diff. Geom. **27**, 259–296 (1988).

[ChYa08] Chang., S.Y.A., and Yang, P., *The Q-curvature equation in conformal geometry,* Géométrie différentielle, physique mathématique, mathématiques et société. II. Astérisque **322**, 23–38 (2008).

[ChKi94] Chanillo, S., and Kiessling, M. K.-H., *Rotational symmetry of solutions of some nonlinear problems in statistical mechanics and in geometry,* Commun. Math. Phys. **160**, 217–238 (1994).

[ChKi95] Chanillo, S., and Kiessling, M. K.-H., *Conformally invariant systems of nonlinear PDE of Liouville type,* Geom. Funct. Anal. **5**, 924–947 (1995).

[ChKi00] Chanillo, S., and Kiessling, M. K.-H., *Surfaces with prescribed Gauss curvature*, Duke Math. J. **105**, 309–353 (2000).

[Cha10] Chavanis, P.H., *Kinetic theory of stellar systems, two-dimensional vortices and the HMF model*, Theor. Comput. Fluid Dyn **24**, 217–239 (2010).

[ChLi91] Chen, W., and Li, C., *Classification of solutions of some nonlinear elliptic equations,* Duke Math. J. **63**, 615–622 (1991).

[ChLi97] Cheng, K., and Lin, C., *On the asymptotic behavior of solutions of the conformal Gaussian curvature equations in* $\mathbb{R}^2$*,* Math. Ann. **308**, no. 1, 119–139 (1997).

[ChLi98A] Cheng, K., and Lin, C., *Compactness of conformal metrics with positive Gaussian curvature in* $\mathbb{R}^2$*,* Ann. Scuola Norm. Sup. Pisa Cl. Sci. (4) **26**, no. 1, 31–45 (1998).

[ChLi98B] Cheng, K., and Lin, C., *On the conformal Gaussian curvature equation in* $\mathbb{R}^2$*,* J. Differential Equations **146**, no. 1, 226–250 (1998).

[ChNi91A] Cheng, K., and Ni, W., *On the structure of the conformal Gaussian curvature equation on* $\mathbb{R}^2$*,* Duke Math. J. **62**, no. 3, 721–737 (1991).

[ChNi91B] Cheng, K., and Ni, W., *On the structure of the conformal Gaussian curvature equation on* $\mathbb{R}^2$*. II,* Math. Ann. **290**, no. 4, 671–680 (1991).

[ChMa90] Chorin, A.J., and Marsden, J.E., *A mathematical introduction to fluid mechanics*, Texts in Appl. Math. 4, Springer (1990).

[CETT05] Costeniuc, M., Ellis, R.S., Touchette, H., and Turkington, B., *The generalized canonical ensemble and its universal equivalence with the microcanonical ensemble,* J. Stat. Phys. **119**, 1283–1329 (2005).

[DeZe98] Dembo, A., and Zeitouni, O., *Large deviations techniques and applications*, Springer, New York (1998).

[DMT98] Dibattista, M.T., Majda, A.J., and Turkington, B., *Prototype geophysical vortex structures via large-scale statistical theory* Geophys. Astrophys. Fluid Dynam. **89**, 235-283 (1998).

[DJLW97] Ding, W., Jost, J., Li, J., and Wang, G., *The differential equation* $\Delta u = 8\pi - 8\pi h e^u$ *on a compact Riemann surface*, Asian J. Math. **1**, 230–248 (1997)

[Dri88] Dritschel, D.G., *Contour surgery: a topological reconnection scheme for extended integrations using contour dynamics*, J. Comp. Phys. **77**, 240–266 (1988).

[DrPo92] Dritschel, D.G., and Polvani, L., *The roll-up of vorticity strips on the surface of a sphere*, J. Fluid. Mech. **234**, 47–69 (1992).

[DüPu82] Dürr, D., and Pulvirenti, M., *On the vortex flow in bounded domains*, Commun. Math. Phys. **85**, 265–273 (1982).

[Dur95] Durrett, R., *Probability: Theory and Examples*, 2^{nd} ed., Duxbury Press (1995).

[Dyn53] Dynkin, E. B., *Klassy ekvivalentnyh slučaǐnyh veličin*, Uspeki Mat. Nauk. **6**, 125–134 (1953).

[EiSch02] Eichelsbacher, P., and Schmock, U., *Large deviations of U-empirical measures in strong topologies and applications*, Ann. Inst. Henri Poincaré – PR **38**, 779–797 (2002).

[Ell85] Ellis, R.S., *Entropy, large deviations, and statistical mechanics*, Springer, New York (1985).

[EHT00] Ellis, R.S., Haven, K., and Turkington, B., *Large deviation principles and complete equivalence and nonequivalence results for pure and mixed ensembles*, J. Stat. Phys. **101**, 999–1064 (2000).

[EySp93] Eyink, G., and Spohn, H., *Negative-temperature states and large-scale, long-lived vortices in two-dimensional turbulence*, J. Stat. Phys. **70**, 833–886 (1993).

[EySr06] Eyink, G., and Sreenivasan, K.R., *Onsager and the theory of hydrodynamic turbulence*, Rev. Mod. Phys. **78**, 87-135 (2006).

[deF37] de Finetti, B., *La prévision: ses lois logiques, ses sources subjectives*, *Annales Inst. Henri Poincaré* **7**, 1–68 (1937).

[FJM92] Forrester, P.J., Jancovici, B., and Madore, J., *The two-dimensional Coulomb gas on a sphere: exact results*, J. Stat. Phys. **69**, 179–192 (1992).

[FoJa96] Forrester, P.J., and Jancovici, B., *The two-dimensional two-component plasma plus background on a sphere: exact results*, J. Stat. Phys. **84**, 337–357 (1996).

[FrRu82] Fröhlich, J., and Ruelle, D., *Statistical mechanics of vortices in an inviscid two-dimensional fluid*, Commun. Math. Phys. **87**, 1–36 (1982).

[Gib02] Gibbs, J.W., *Elementary Principles in Statistical Mechanics*, Yale Univ. Press, New Haven (1902); reprinted by Dover, New York (1960).

[GHL90] Goodman, J., Hou T.Y., Lowengrub, J. *Convergence of the point vortex method for the 2-D Euler equations*, Commun. Pure Appl. Math. **43**, 415–430 (1990).

[GJMS92] Graham, C. Robin, Jenne, R., Mason, L. and Sparling, G. *Conformally Invariant Powers of the Laplacian, I: Existence*, J. London Math. Soc. **s2-46 (3)**: 557-565 (1992).

[Hal79] Hald, O.H., and delPrete, V.M., *Convergence of vortex methods for Euler's equations*, Math. Comp. **32** 791–809 (1978).

[Han90] Han, Z.C., *Prescribing Gaussian curvature on* $\mathbb{S}^2$, Duke Math. J. **61**, 679–703 (1990).

[HeSa55] Hewitt, E., and Savage, L. J., *Symmetric measures on Cartesian products*, Trans. Amer. Math. Soc. **80**, 470–501 (1955).

[JoMo73] Joyce, G., and Montgomery, D.C., *Negative temperature states for the two-dimensional guiding center plasma*, J. Plasma Phys. **10**, 107–121 (1973).

[Kat67] Kato, T., *On classical solutions of the two-dimensional nonstationary Euler equation*, Arch. Rat. Mech. Anal. **25**, 188-200 (1967).

[KaWa74] Kazdan, J., and Warner, F., *Curvature functions for compact 2-manifolds*, Ann. of Math. **99**, 14–47 (1974).

[Kel98] Keller, G., *Equilibrium States in Ergodic Theory*, London Mathematical Society Student Text **42**, Cambridge University Press

[Kie89] Kiessling, M. K.-H., *On the equilibrium statistical mechanics of isothermal classical self-gravitating matter*, J. Stat. Phys. **55**, 203–257 (1989).

[Kie93] Kiessling, M. K.-H., *Statistical mechanics of classical particles with logarithmic interactions,* Commun. Pure Appl. Math. **46**, 27–56 (1993).

[Kie95] Kiessling, M. K.-H., *Negative temperature bounds for 2D vorticity compounds*, Lett. Math. Phys. **34**, 49–57 (1995).

[Kie00] Kiessling, M.K.-H., *Statistical mechanics approach to some problems in conformal geometry*, Physica **A 279**, 353-368 (2000).

[Kie08] Kiessling, M.K.-H., *Statistical equilibrium dynamics,* pp.91-108 in *AIP Conf. Proc.* **970**, A. Campa, A. Giansanti, G. Morigi, and F. Sylos Labini (eds.), American Inst. Phys. (2008).

[Kie09b] Kiessling, M.K.-H., *The Vlasov continuum limit for the classical microcanonical ensemble,* Rev. Math. Phys. **21**, 1145–1195 (2009).

[Kie09c] Kiessling, M.K.-H., *A note on classical ground state energies,* J. Stat. Phys. **136**, 275–284 (2009).

[Kie11] Kiessling, M.K.-H. *Typicality analysis for the Newtonian N-body problem on $\mathbb{S}^2$ in the $N \to \infty$ limit*, J. Stat. Mech.: Th. Exp., P01028, 1–70 (2011).

[KiLe97] Kiessling, M.K.-H., and Lebowitz, J.L., *The micro-canonical point vortex ensemble: Beyond equivalence,* Lett. Math. Phys. **42**, 43–58 (1997).

[KiSp99] Kiessling, M.K.-H., and Spohn, H., *A note on the eigenvalue density of random matrices*, Comm. Math. Phys. **199**, 683–695 (1999).

[KiWa12] Kiessling, M.K.-H., and Wang, Y., *Onsagers Ensemble for Point Vortices with Random Circulations on the Sphere*, J. Stat. Phys **148**, 896-932 (2012).

[KiOk87] Kimura, Y., and Okamoto, H., *Vortex motion on a sphere*, J. Phys. Soc. Japan **56**, 4203–4206 (1987).

[Kir83] Kirchhoff, G. *Vorlesungen über mathematische Physik. Mechanik*, chpt. 20, 3rd ed., Teubner, Leipzig (1883).

[Lan73] Lanford, O.E.,III., *Entropy and equilibrium states in classical statistical physics*, pp.1–107 in: Lenard, A. (ed.), *Statistical mechanics and mathematical problems*, Conf. Proc. of the Battelle Seattle Recontres 1971, *Lect. Notes Phys.* **20** (J. Ehlers et al., eds.), Springer (1973).

[Li95A] Li, Y. *The Nirenberg problem in a domain with boundary,* Topol. Methods Nonlinear Anal. **6**, no. 2, 309C329 (1995).

[Li95B] Li, Y. *Prescribing scalar curvature on Sn and related problems. I,* J. Differential Equations **120**, no. 2, 319C410 (1995).

[Li96] Li, Y. *Prescribing scalar curvature on Sn and related problems. II. Existence and compactness,* Comm. Pure Appl. Math. **49**, no. 6, 541C597 (1996).

[LDN08] Lim, C.C., Ding, X., and Nebus, J. *Vortex dynamics, Statistical Mechanics and Planetary atmospheres,* World Scientific (2008).

[Lin43] Lin, C.C., *On the motion of vortices in two dimensions,* The University of Toronto Press, Toronto, Canada (1943).

[Lin00] Lin, C.-S., *Uniqueness of solutions to the mean field equations for the spherical Onsager vortex*, Arch. Ration. Mech. Anal. **153**, 153–176 (2000).

[Lio53] Liouville, J., *Sur l'équation aux différences partielles* $\partial^2 \log \lambda / \partial u \partial v \pm \lambda / 2a^2 = 0$, J. de Math. Pures Appl. **18**, 71–72 (1853).

[LuPo77] Lundgren, T. S., and Pointin, Y. B., *Statistical mechanics of two-dimensional vortices*, J. Stat. Phys. **17**, 323–355 (1977).

[Ma98] Ma, L., *Bifurcation in Nirenberg's problem,* C. R. Acad. Sci. Paris Sér. I Math. **326**, no. 5, 583–588 (1998).

[MaPu84] Marchioro, C., and Pulvirenti, M., *Vortex methods in two-dimensional fluid dynamics*, Lecture notes in physics 203, Springer, Berlin (1984).

[MaPu94] Marchioro, C., and Pulvirenti, M., *Mathematical theory of incompressible nonviscous fluids*, Springer-Verlag, New York (1994).

[McO85] McOwen, Robert C., *Conformal metrics in* $\mathbb{R}^2$ *with prescribed Gaussian curvature and positive total curvature,* Indiana Univ. Math. J. **34**, no. 1, 97–104 (1985).

[MON10] Meleshko, V.V., Ostrovskyi, V., Newton, P.K., *Stability of the configurations of point vortices on a sphere,* J. Math. Sci. **171**, 603–619 (2010).

[MeSp82] Messer, J., and Spohn, H., *Statistical mechanics of the isothermal Lane-Emden equation*, J. Stat. Phys. **29**, 561–578 (1982).

[Mil90] Miller, J. *Statistical mechanics of Euler equations in two dimensions*, Phys. Rev. Lett. **65**, 2137-2140 (1990).

[MoJo74] Montgomery, D.C., and Joyce, G., *Statistical mechanics of "negative temperature" states*, Phys. Fluids **17**, 1139–1145 (1974).

[MoMa11] Montgomery, D., and Matthaeus, W. H., *Oseen vortex as a maximum entropy state of a two dimensional fluid*, Phys. Fluids **23**, art. 075104 1-6 (2011).

[Metal91] Montgomery, D., Matthaeus, W. H., Stribling, W. T., Martinez, D., and Oughton, S., *Relaxation in two dimensions and the "sinh-Poisson" equation*, Phys. Fluids A **4**, 3–6 (1991).

[Mos71] Moser, J., *A sharp form of an inequality by N. Trudinger*, Indiana Univ. Math. J. **20**, 1077–1092 (1971).

[Mos73] Moser, J., *"On a nonlinear problem in differential geometry" in Dynamical systems (Proc. Sympos., Univ. Bahia, Salvador, 1971),* Academic Press, New York, 273–280 (1973).

[NeKi98] Newton, P.K., and Kidambi, R., *Motion of three point vortices on a sphere,* Physica D **116**, 143–175 (1998).

[Ni82] Ni, W., *On the elliptic equation* $\Delta u + K(x)e2u = 0$ *and conformal metrics with prescribed Gaussian curvatures,* Invent. Math. **66**, no. 2, 343–352 (1982).

[Oba71] Obata, M., *The conjectures on conformal transformations of Riemannian manifolds,* J. Differential Geometry **6**, 247–258 (1971/72).

[ONRe91] O'Neil, K., and Redner, R. A., *On the limiting distribution of pair-summable potential functions in many-particle systems*, J. Stat. Phys. **62**, 399–410 (1991).

[Ono82] Onofri, E., *On the positivity of the effective action in a theory of random surfaces*, Commun. Math. Phys. **86**, 321–326 (1982).

[Ons49] Onsager, L., *Statistical hydrodynamics*, Nuovo Cim. Suppl. **6**, 279–287 (1949).

[Pan08] Paneitz, S., *A Quartic Conformally Covariant Differential Operator for Arbitrary Pseudo-Riemannian Manifolds (Summary)*, SIGMA **4**, 036–038 (2008).

[PeCh02] Peng, J., Chen Q., *Differential Geometry*, (Written in Chinese), Advanced Education Press, China, (2002).

[PiSt89] Pinkall, U.; Sterling, I., *On the Classification of Constant Mean Curvature Tori*, Ann. of Math. (2) **130**, no. 2, 407C451 (1989).

[Poi93] Poincaré, H., *Théorie des Tourbillons,* Deslies Frères, Paris, (1893).

[PoLu76] Pointin, Y. B., and Lundgren, T. S., *Statistical mechanics of two-dimensional vortices in a bounded container*, Phys. Fluids **19**, 1459–1470 (1976).

[PoDr93] Polvani, L.M., and Dritschel, D.G., *Wave and vortex dynamics on the surface of a sphere*, J. Fluid Mech. **255**, 35-64 (1993).

[PrTa01] Prajapat, J., and Tarantello, G., *On a class of elliptic problems in* $\mathbb{R}^2$*: symmetry and uniqueness results,* Proc. Roy. Soc. Edinburgh **131**, 967–985 (2001).

[Rob90] Robert, R., C. R. Acad. Sci., Ser. I, **311**, 575-578 (1990).

[RoSo92] Robert, R., and Sommeria, J., *Relaxation towards a statistical equilibrium state in two-dimensional perfect fluid dynamics*, Phys. Rev. Lett. **69**, 2776-2779 (1992).

[RoRu67] Robinson, D. W., and Ruelle, D., *Mean entropy of states in classical statistical mechanics,* Commun. Math. Phys. **5**, 288–300 (1967).

[Rue69] Ruelle, D., *Statistical Mechanics: Rigorous Results*, Benjamin, New York (1969).

[SaTo97] Saff, E.B., and Totik, V., *Logarithmic potentials with external fields*, Grundlehren Math. Wiss. **316**, Springer, Berlin (1997).

[Sat72] Sattinger, D. H., *Conformal metrics in* $\mathbb{R}^2$ *with prescribed curvature,* Indiana Univ. Math. J. **22**, 1–4 (1972/73).

[SmON90] Smith, R. A., and O'Neil, T. M., *Nonaxisymmetric thermal equilibria of a cylindrically bounded guiding-center plasma or discrete vortex system*, Phys. Fluids B **2**, 2961–2975 (1990).

[Stu67] Stuart, J. T., *On finite amplitude oscillations in laminar mixing layers*, J. Fluid Mech. **29** 417–440 (1967).

[Tar97] Tarantello, G., *Vortex-condensations of a non-relativistic Maxwell-Chern-Simons theory,* J. Differential Equations **141**, no. 2, 295–309 (1997).

[Tou09] Touchette, H., *The large deviation approach to statistical mechanics*, Phys. Rep. **478**, 1–69 (2009).

[Tru67] Trudinger, N. S., *On imbeddings into Orlicz spaces and some applications*, J. Math. Mech. **17**, 473–483 (1967).

[Tur99] Turkington, B., *Statistical equilibrium measures and coherent states in two-dimensional turbulence*, Commun. Pure Appl. Math. **52**, 781-809 (1999).

[Var84] Varadhan, S.R.S., *Large deviations and applications*, CBMS-NSF Regional Conf. Ser. in Appl. Math. **46**, SIAM, Philadelphia (1984).

[WeMc91] Weiss, J. B., and McWilliams, J. C., *Nonergodicity of point vortices,* Phys. Fluids A **3**, 835–844 (1991).

[Zer02] Zermelo, E. *Hydrodynamische Untersuchungen über die Wirbelbewegungen in einer Kugelfläche*, Z. Math. Phys. **47**, 201–237 (1902).

Vita

Yu Wang

2006-2013 Ph. D. in Mathematics, Rutgers University

2004-2006 M. Sc. in Mathematics, Wuhan University

2001-2004 B. Sc. in Mathematics, Wuhan University

2006-13 Teaching/Graduate assistant, Department of Mathematics, Rutgers University