PROCEEDINGS OF THE
AMERICAN MATHEMATICAL SOCIETY
Volume 146, Number 7, July 2018, Pages 3127–3142
http://dx.doi.org/10.1090/proc/13875
Article electronically published on March 30, 2018

BOUNDS ON THE COMPLEXITY OF REPLICA SYMMETRY BREAKING FOR SPHERICAL SPIN GLASSES

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(Communicated by Zhen-Qing Chen)

ABSTRACT. In this paper, we study the Crisanti-Sommers variational problem, which is a variational formula for the free energy of spherical mixed p-spin glasses. We begin by computing the dual of this problem using a min-max argument. We find that the dual is a 1D problem of obstacle type, where the obstacle is related to the covariance structure of the underlying process. This approach yields an alternative way to understand Replica Symmetry Breaking at the level of the variational problem through topological properties of the coincidence set of the optimal dual variable. Using this duality, we give an algorithm to reduce this a priori infinite dimensional variational problem to a finite dimensional one, thereby confining all possible forms of Replica Symmetry Breaking in these models to a finite parameter family. These results complement the authors' related results for the low temperature Γ-limit of this variational problem. We briefly discuss the analysis of the Replica Symmetric phase using this approach.

1. INTRODUCTION

The analysis of variational formulas for free energies plays a central role in statistical physics. The phenomenological properties of their optimizers are of particular interest as they play the role of an order parameter, encoding physical properties of the system. In the study of mean field spin glasses, these formulas traditionally come in the form of a strictly convex minimization problem over the space of probability measures. Put briefly, the minimizers of these problems are related to the laws of relative positions of configurations drawn from a corresponding Gibbs measure. Changes in the topology of their support are related to the presence and nature of a spin glass phase. For more on this see [15, 18, 19].

Though there has been major progress in the mathematical study of variational problems arising from mean field spin glasses in recent years [1,2,14,15], many interesting questions remain open. In this paper, we present an alternative perspective on a class of these problems, specifically those coming from the spherical mixed p-spin glass models. In this class, the variational problem involves the *Crisanti-Sommers functional* which we define presently.

Let $\xi(t) = \beta^2 \sum_{p\geq 2} \beta_p^2 t^p$ satisfy $\xi(1+\epsilon) < \infty$ and let h be a non-negative real number. Call $\xi_0 = \beta^{-2}\xi$. The parameters ξ_0, β, and h are called the *model*,

Received by the editors April 17, 2017.
2010 *Mathematics Subject Classification.* Primary 60K35, 82B44, 82D30, 49S05, 49N15; Secondary 49K15, 49N60.

inverse temperature, and *external field* respectively. For $\mu \in \Pr([0,1])$, let $\phi_\mu(t) = \int_t^1 \mu([0,s])ds$. The Crisanti-Sommers functional is then defined as

$$P_{\xi,h}(\mu) = \frac{1}{2}\left(\int_0^1 \xi'' \phi_\mu \, ds + \int_0^1 \left(\frac{1}{\phi_\mu} - \frac{1}{1-s}\right) ds + h^2 \phi_\mu(0)\right).$$

As $\phi_\mu(s) \leq 1 - s$, the second term is non-negative so that this functional is well defined. Observe that the functional is strictly convex by the strict convexity of the function $x \mapsto \frac{1}{x}$, and is lower semi-continuous in the weak-$*$ topology. (For experts: this is a lower semi-continuous extension of the functional originally defined by Crisanti and Sommers [12]. See [14, Section 6.1] for more details.)

The Crisanti-Sommers variational problem is given by

$$F(\xi, h) = \min_{\mu \in \Pr([0,1])} P_{\xi,h}(\mu). \tag{1.0.1}$$

This gives a variational formula for the free energy in spherical mixed p-spin glasses. In particular, for $\sigma \in S^{N-1}(\sqrt{N})$, if we define the Hamiltonian

$$H_N(\sigma) = \beta \sum_{p=2}^{\infty} \frac{\beta_p}{N^{\frac{p-1}{2}}} \sum_{i_1,\ldots,i_p=1}^{N} g_{i_1,\ldots,i_p} \sigma_{i_1} \cdots \sigma_{i_p} + h \sum_{i=1}^{N} \sigma_i, \tag{1.0.2}$$

where $g_{i_1 \ldots i_p}$ are i.i.d. standard normal random variables, then

$$F(\xi, h) = \lim_{N \to \infty} \frac{1}{N} \log \int_{S^{N-1}(\sqrt{N})} e^{H_N(\sigma)} dvol_{N-1} \quad a.s.$$

where $dvol_{N-1}$ is the normalized volume form on $S^{N-1}(\sqrt{N})$. This was first established by Crisanti and Sommers [12] non-rigorously using the Replica method. It was proved by Talagrand [22] in the case that ξ is even and Chen [6] for general ξ.

Of particular interest in the analysis of the variational problem (1.0.1) is the development of its phase diagram. In particular, one is interested in characterizing the regions in (ξ, h)-space where the minimizer, μ, has

- 1 atom, called Replica Symmetry (RS),
- $k + 1$ atoms, called k-step Replica Symmetry Breaking (kRSB),
- an absolutely continuous part, called full Replica Symmetry Breaking (fRSB).

One is also interested in the nature of the fRSB phase, e.g., whether there are many absolutely continuous components in the support of μ, and whether there are atoms in between.

The notion of Replica Symmetry Breaking (RSB) was introduced by Parisi in his groundbreaking papers [21]. The physical interpretation and mathematical foundations of RSB has been a subject of great research for several decades in both communities. In many models, and in particular (1.0.2), there is a rigorous mathematical interpretation of RSB that depends on the form of the optimizer of (1.0.1). For a physically minded discussion of this see [18], and for a mathematically minded discussion of this see [19].

With this picture in mind, it then becomes of paramount interest to determine which models have what forms of RSB. Until now, this question has been studied by either: proposing an ansatz — perhaps through some deep physical insight — and analytically testing its validity [1,22]; numerically optimizing the problem [18]; or performing some combination of the two [10,11,17]. Ideally, however, one would be able to simply look at a Hamiltonian and provide a simple a priori bound on the nature and complexity of RSB that can arise (perhaps after a back of the envelope calculation).

In this paper, we provide such a technique. We give a simple test which, given the form of the Hamiltonian, reduces the nature and form of the RSB to a simple finite parameter family. This family is given explicitly in terms of the model in Corollary 1.6.

We now turn to a more precise discussion of the methods introduced in this paper and their relation to the previous literature. Previously, the mathematical analysis of the Crisanti-Sommers problem focused on the study of the variational inequality

$$(\eta(s) - \xi(s), \nu - \mu) \geq 0 \quad \forall\, \nu \in \Pr([0,1]) \tag{1.0.3}$$

which arises from its first order optimality conditions. Here, η depends on the measure μ. The focus of this analysis is generally to test and rule out ansatzes. As P is strictly convex, one can prove that an ansatz is optimal by checking that (1.0.3) is satisfied. The non-locality of the map $\mu \mapsto \eta_\mu$ is a major technical difficulty in the study of RSB: the more complex the ansatz, the more unwieldy this approach becomes.

In this paper, we take a different approach. It is a classical observation that variational inequalities such as (1.0.3) can be encoded in an *obstacle problem*, that is, a problem of the form

$$\max_{\eta \geq \psi} D(\eta).$$

(See, e.g., [3, 4, 16].) Here, ψ is called the obstacle and D is a local functional (for this in our setting, see Section 1.1). This obstacle problem will be dual to (1.0.1), which we call the *primal problem*, and the dual variable will be η. The relation between the optimizers of the primal and dual problems is given by the case of equality in a certain Legendre transform.

Two new approaches emerge by allowing η to vary. First, one can analyze the dual problem in and of itself. Alternatively, one can simultaneously analyze pairs (μ, η) searching for a pair that satisfies a saddle-type condition. Furthermore, this new perspective permits methods and techniques which are natural for the dual problem and have no apparent analogues for the primal one. (See, e.g., the proof of Theorem 1.4 and Remark 3.1.)

As the dual is an obstacle problem, its first order optimality conditions will generate a measure that is supported on the *coincidence set,* $\{s : \eta = \psi\}$. Through the relation between the primal and dual variables, this measure will solve the primal problem (1.0.1).

This duality yields an alternative perspective on the study of Replica Symmetry Breaking. The nature and form of the RSB in a given system can be analyzed by studying the fine topological properties of the coincidence set of the dual, thereby connecting a question of pure spin glass theory to a question naturally arising in the study of free boundary problems in classical physics such as the shape of a constrained elastic beam [9]. Furthermore, this gives a natural interpretation for ξ — which describes the covariance structure of H_N — at the level of the dual: it is the obstacle, $\psi = \xi$.

This duality approach was introduced by the authors in [14] in the low temperature (large β) limit. There, after developing the low temperature $\Gamma-$limit of the Crisanti-Sommers problem, we obtained its dual problem. By analyzing the two problems simultaneously, we were able to unify independent conjectures in the mathematics and physics literatures regarding 1RSB at zero temperature. Furthermore, we obtained a simple functional form for the optimizer depending on only finitely many parameters, similar to the one given below in Corollary 1.6.

In this paper, we find that this duality approach can in fact be applied at all temperatures and external magnetic fields, and for all models. As foreshadowed by the form of the low temperature duality, the dual of the Crisanti-Sommers variational problem is a 1D problem of obstacle type. Although the structure of the proof at finite temperature resembles that of the limiting case, new subtitles emerge which alter the precise form of the dual problem: in particular, the principle value term in the Crisanti-Sommers functional must be handled carefully as one expects the natural dual variable to explode at a boundary point. Though this can still be treated via an abstract minimax argument as in [14], we choose instead to present a simpler, direct proof through the construction of a saddle point.

After obtaining the duality result, we turn to study its consequences for spherical spin glasses. A natural question in the study of obstacle problems is to analyze the coincidence set; in higher dimensions this has received much attention and one usually asks to characterize the nature of the resulting free boundaries (see, e.g., [3, 4]). Here, the dual problem is a 1D obstacle problem, so to characterize the coincidence set one immediately turns to questions regarding its topology. In fact, such a question has physical ramifications for spherical spin glasses. Through the duality, constraints on the topology of the coincidence set are constraints on the Replica Symmetry Breaking (RSB). As our main application, we present a method to confine the topology of the coincidence set, thereby reducing the nature of the RSB to an explicit finite parameter family. As an example of this application in practice, we note a recent observation of Chen and Panchenko [8] that this result, combined with [8, Theorem 2], yields a simple numerical method for finding models that have chaotic temperature dependence. Finally, we discuss some simple observations regarding RS in these systems.

1.1. **Duality.** The first step in our approach to the Crisanti-Sommers variational problem (1.0.1) is to obtain its dual. To state the dual problem we need the following notation. Define the vector space

$$X = \{\eta : \eta \in C^1([0,1)), \eta' \in Lip_{\mathrm{loc}}([0,1))\}.$$

Here we allow η to blow up at the point 1. Observe that for $\eta \in X$, the second distributional derivative, η'', can be identified with a measurable function on $[0,1]$ which is a.e. unique, and which is essentially bounded on subintervals of the form $[0, 1-\delta]$ where $\delta > 0$.

Let

$$\Lambda_{\xi,h} = \left\{\eta \in X : \eta \geq \xi, \eta'(0) = -h^2, \eta'' \geq 0 \text{ Leb.-a.e.}\right\}$$

and define the functional $D_{\xi,h} : \Lambda_{\xi,h} \to [-\infty, \infty)$ by

$$D_{\xi,h}(\eta) = \frac{1}{2}\left(\int_0^1 2\sqrt{\eta''(s)} - \eta''(s)\cdot(1-s) - \frac{1}{1-s}\, ds - \eta(0) + h^2 + \xi(1)\right).$$

The integrand is measurable and, by the arithmetic-geometric inequality, it is nonpositive so that its integral is well defined.

Finally, we define the *coincidence set*,

$$\{s \in [0,1) : \eta(s) = \xi(s)\}.$$

Theorem 1.1. *(Duality) We have that*

$$\min_{\mu \in \Pr([0,1])} P_{\xi,h}(\mu) = \max_{\eta \in \Lambda_{\xi,h}} D_{\xi,h}(\eta).$$

Furthermore, there is a unique optimal pair $(\mu,\eta) \in \Pr([0,1]) \times \Lambda_{\xi,h}$, *which is characterized by the relations*

$$\begin{cases} \mu(\{\eta = \xi\}) = 1, \\ \eta'' \phi_\mu^2 = 1, \qquad Leb - a.e. \end{cases} \tag{1.1.1}$$

One can consider the optimality conditions (1.1.1) in various ways. For example, one can take μ as the variable to be optimized while constraining η to be given by

$$\eta_\mu = c - h^2 t + \int_0^t \int_0^s \frac{1}{\phi_\mu^2} d\tau ds,$$

where c is the number such that $\inf\{\eta_\mu - \xi\} = 0$. Then, the optimal μ is the probability measure which gives full mass to the coincidence set. This is equivalent to the primal approach to (1.0.1), i.e., the study of the variational inequality (1.0.3), and is also equivalent to Talagrand's characterization of the optimal μ from [22, Proposition 2.1].

A fundamentally different approach to (1.0.1) is to analyze its dual:

$$F(\xi,h) = \max_{\eta \in \Lambda_{\xi,h}} D_{\xi,h}(\eta). \tag{1.1.2}$$

The next result is regarding optimality and regularity for the dual variable, η.

Proposition 1.2. *Let η be optimal for* (1.1.2). *Then,*

- *Optimality:*

$$\left(\frac{1}{\sqrt{\eta''}}\right)'' = -\mu \tag{1.1.3}$$

  in the sense of distributions where μ solves (1.0.1). *Moreover, the support of μ is contained in the coincidence set.*
- *Regularity:*
  (1) $\eta \in C^2([0,1))$, $\eta''' \in BV((0,1-\delta)) \cap L^\infty((0,1-\delta))$ *for all* $\delta \in (0,1)$.
  (2) $\frac{1}{(1-s)^2} \leq \eta'' \leq \frac{C(\xi,h)}{(1-s)^2}$ *for some positive constant C.*
  (3) $\eta'' = \frac{1}{(1-s)^2}$ *sufficiently close to* 1.
- *Consistency: if* $\eta(s) = \xi(s)$, *then*

$$\eta'(s) = \xi'(s) \quad and \quad \eta''(s) \geq \xi''(s). \tag{1.1.4}$$

Proof. We begin with optimality. Observe that by the previous theorem, in particular by (1.1.1), we have that

$$\frac{1}{\sqrt{\eta''}} = \phi_\mu$$

a.e. where μ solves (1.0.1). Differentiating twice we see that (1.1.3) holds. The desired condition on the support of μ also follows from (1.1.1).

Now we prove regularity. We begin with claim (1). Observe that

$$\eta'' = \frac{1}{\phi_\mu^2}$$

a.e. Since ϕ_μ is continuous and strictly positive away from 1, it follows that $\eta \in C^2([0,1))$. Differentiating again, we find that

$$\eta''' = -\frac{\mu([0,s])}{\phi_\mu^2}$$

in the sense of distributions. Note that the right hand side belongs to

$$L^\infty((0,1-\delta)) \cap BV((0,1-\delta))$$

for all $\delta \in (0,1)$. Therefore, so does η'''. To prove the remaining claims, we will use that the optimal μ is supported away from 1 (cf. Lemma 4.1). This implies that $\phi_\mu = 1-s$ on a neighborhood of 1, so that claim (3) holds. Since η'' is continuous on $[0,1)$, it is bounded on each sub-interval of the form $[0,1-\delta]$ where $\delta \in (0,1)$. Combining this with claim (3) we deduce the upper bound part of claim (2); the lower bound part follows since in general $\phi_\mu \leq 1-s$.

Finally, we prove the consistency conditions. By its definition, the coincidence set consists of minimizers of $g = \eta - \xi$ on $[0,1)$. Since $g \in C^2([0,1))$, it follows that $g' = 0$ and $g'' \geq 0$ at such points. This proves (1.1.4). □

This result shows how to recover the optimal measure μ from the optimal dual variable η. Evidently, atoms in μ correspond to points in the coincidence set and intervals in the support of μ correspond to intervals in the coincidence set. Thus, one can bound the complexity of RSB by controlling the topology of the coincidence set. We explore this idea in the next section.

We note here that the next corollary is an immediate consequence of (1.1.4). In the cases of RS and 1RSB, this was observed by Chen and Panchenko in [8].

Corollary 1.3. *Suppose that $h = 0$. The point 0 is in the support of μ if and only if $\xi(t)$ is not identically $\beta t^2/2$ for some $\beta \leq 1$.*

Proof. Suppose that c is the smallest point in the support. Then, by an application of (1.1.3) and re-arranging (1.1.4), we immediately obtain the inequality

$$\xi'(c) \geq \xi''(c)c.$$

As ξ is a power series with non-negative coefficients, this is possible for $c > 0$ only when ξ is of the form at^2 for some a. Thus if ξ is not of this form, then $c = 0$. On the other hand, when ξ is of this form it is an elementary and well-known observation [20] that the minimizer of (1.0.1) is an atom at zero for $a < 1$ and some q_* for $a > 1$. □

1.2. **A finite dimensional reduction of RSB.** We now turn to the main result of this paper, namely the reduction of all possible RSB in spherical mixed p-spin glasses to a finite parameter family. To this end, define

$$\mathfrak{d} = \left(\frac{1}{\sqrt{\xi''}}\right)''.$$

Then we have the following theorem which controls the topology of the coincidence set.

Theorem 1.4. *(Rule of Signs) Let η be optimal for* (1.1.2) *and let* $0 \le a < b < 1$. *We have the following cases:*

(1) *If* $\mathfrak{d} > 0$ *on* (a,b), *then* $card(\{\eta = \xi\} \cap [a,b]) \le 2$.
(2) *If* $\mathfrak{d} \le 0$ *on* $[a,b]$ *and* $a, b \in \{\eta = \xi\}$, *then* $[a,b] \subset \{\eta = \xi\}$.

Remark 1.5. The first case can be seen on the primal side in the work of Talagrand [22, Proposition 2.2], and also in [12]. The second case is new and is the crux of our reduction of RSB.

Combining this result with the duality theory from the previous section gives a bound on the complexity of RSB. Observe that $\mathfrak{d}$ is either identically zero or has finitely many roots in $[0,1]$ by the analyticity of $\frac{3}{2}(\xi''')^2 - \xi''\xi''''$ in the unit disc $B(0,1) \subset \mathbb{C}$.

Corollary 1.6. *Let* $\{\mathfrak{d} > 0\} = \bigcup_{i=1}^{N_p}(a_i, b_i)$ *be the decomposition into connected components and similarly let* $\{\mathfrak{d} \le 0\} = \bigcup_{i=1}^{N_n}[a_i', b_i']$. *Then,* μ *must be of the form*

$$\mu = \sum_{i=1}^{N_p} m_{i_1}\delta_{q_{i_1}} + m_{i_2}\delta_{q_{i_2}} + \sum_{i=1}^{N_n} -\mathfrak{d}\mathbb{1}_{[r_{i_1}, r_{i_2}]}ds + n_{i_1}\delta_{r_{i_1}} + n_{i_2}\delta_{r_{i_2}}$$

where the points $q_{i_1}, q_{i_2} \in [a_i, b_i]$ *and* $r_{i_1}, r_{i_2} \in [a_i', b_i']$.

Remark 1.7. See [14, Section 1.2] for several examples of this reduction at zero-temperature (without the constraint that $\mu \in \Pr([0,1])$).

Proof. This follows by combining the optimality part of Proposition 1.2 with Theorem 1.4. In particular, the first sum comes from the first part of the rule of signs. The second sum follows from the second part of the rule of signs, combined with (1.1.3) and, in particular, the fact that if $(a,b) \subset \operatorname{supp}\mu \subset \{\eta = \xi\}$, then μ has density $-\mathfrak{d}$ on that interval. □

As a first application of Corollary 1.6, we demonstrate how one can ascertain the nature of μ in the case that $\xi''(0) = 0$. In this case, one has that $\mathfrak{d} > 0$ on a neighborhood of 0. (See the proof of Theorem 1.4 on page 3138.) Thus, on that same neighborhood, there can be at most two atoms in the support of μ. A similar result was shown in [1].

As a further application of Corollary 1.6, we note the recent work of Chen and Panchenko [8] regarding chaotic temperature dependence. In [8], Chen and Panchenko observed that this result can be used to numerically check chaotic temperature dependence. Evidently, the conditions of [8, Theorem 2] reduce to showing that if μ_1 optimizes (1.0.1) for $\xi = \alpha\xi_0$ and μ_2 optimizes (1.0.1) for $\xi = \gamma\xi_0$, then

$$\alpha\mu_1\{0\} \ne \gamma\mu_2\{0\}.$$

On the primal side this is of course a non-trival question. However, as observed by Chen and Panchenko in [8] one can easily check this condition numerically as a result of Corollary 1.6.

1.3. **Some remarks on replica symmetry.** We now comment briefly on the analysis of the RS region of the Crisanti-Sommers problem. It is an important and natural question to determine the region in (ξ, h)-space where the optimal measure is a single Dirac mass. On the dual side, the RS region contains the region where the coincidence set is a single point (given a positive solution of Question 1.8, these sets would coincide).

The standard method used to analyze RS is the ansatz-driven approach which we recap now briefly. Assume that the coincidence set consists of a single point q. Then by the optimality and consistency conditions (1.1.3) and (1.1.4), this point must satisfy

$$q = (\xi'(q) + h^2)(1-q)^2, \tag{1.3.1}$$

$$1 \geq \xi''(q)(1-q)^2. \tag{1.3.2}$$

If one proposes q which satisfies these relations, the question reduces to that of determining whether or not the corresponding ansatz, η, lies above the obstacle. For example at $h = 0$, this is equivalent to the condition of Talagrand [22, Proposition 2.3].

An important observation in these approaches is that the condition of strict inequality in (1.3.2) corresponds to the positivity of what is called the "replicon eigenvalue" in the physics literature (cf. [12, equation (4.9)]). It is an important and non-trivial question to determine for which parameters this positivity is also sufficient. This is the question of whether or not the de Almeida-Thouless line for the spherical model is the boundary between the RS and RSB phases [12]. The analogous question for the Ising-spin models, where $\sigma \in \{-1,1\}^N$, has been the subject of much research (see, e.g., [7, 15, 23, 24]).

For an example of how the duality method can be used to study this problem, consider the following. If q solves the fixed point equation, then for $t \leq q$, we have $\eta \geq \xi$ by positivity of the replicon eigenvalue. It remains to show that this positivity implies the result for $t \geq q$. Note that it suffices to prove that in fact

$$\eta''(t) \geq \xi''(t) \quad \forall t \geq q.$$

Observe that this condition is implied by the inequality

$$1 \geq \xi''(1)(1-q)^2.$$

A straightforward manipulation of (1.3.1) and (1.3.2) shows that this holds provided that $h^2 \geq \xi''(1)$. This argument is the dual version of those in [15, 23, 24].

One can also give ansatz-free arguments for RS. Consider the following proof of RS for $\xi''(1)$ sufficiently small. (An identical result is known for the Ising-spin models [7, 15].) Observe that by (1.1.4), if there are two coincidence points, a, b, then they must satisfy

$$\frac{1}{b-a}\int_a^b \eta'' = \frac{\xi'(b) - \xi'(a)}{b-a}.$$

The right hand side is upper bounded by $\xi''(1)$ by monotonicity and the left hand side is strictly lower bounded by 1 by the regularity part of Proposition 1.2. Thus for $\xi''(1) \leq 1$ there must be exactly one coincidence point and one atom in the support of μ. A similar proof can be given for the Ising-spin models using the fixed point equation and the maximum principle for the Parisi PDE.

A discrepancy between scalings of spherical and Ising-spin models. A natural question is to study the asymptotics of the Crisanti-Sommers variational problem in various limits where $\beta \to \infty$ (see, e.g., [5, 13–15]). Taking the limit $\beta \to \infty$ along the curve $\{\beta, h : \eta''(q) - \beta^2\xi_0''(q) = \Lambda\}$, one finds, after manipulating (1.3.1) and (1.3.2), that $\beta(1-q) \to c > 0$. This scaling, however, is different in the Ising-spin version of this model, i.e., when we restrict H_N to $\{-1,1\}^N$. In particular, it was shown by the authors in [14] that along the equivalent positive replicon eigenvalue curve for the Ising-spin models, one has that $\beta^2(1-q) \to c > 0$ for some c. Thus, the large β asymptotics in the two models appear to be fundamentally different, at least in the RS regime.

1.4. **Some open questions.** Before turning to the body of this paper, let us first point out the following natural questions which we leave for future research. A major obstruction in the analysis of (1.0.1) and similar problems (see, e.g., [1, 15, 23]) on the primal side is the existence of points at which the variational derivative G_μ (in the notation of [15]) achieves its minimum value, but which are not in the support of μ. In the language of this paper, this is the question of whether or not the set containment $\operatorname{supp}\mu \subseteq \{\eta = \xi\}$ is strict. Thus, an important question for future study in this field is:

Question 1.8. For which ξ and h are the coincidence set and the support of μ the same?

As a first step toward the resolution of this question, we note the following proposition.

Proposition 1.9. *If $\mathfrak{d}$ is not identically zero, then the elements of $\{\eta = \xi\}\setminus\operatorname{supp}\mu$ are isolated points. If $\mathfrak{d}$ is identically zero, then $\mu = m\delta_{r_1} + (1-m)\delta_{r_2}$ for $m \in [0,1]$ and $r_1, r_2 \in [0,1]$, and $\{\eta = \xi\} = [r_1, r_2]$.*

Proof. Assume that $\mathfrak{d}$ is not identically zero. By the rule of signs, the coincidence set is at most a union of isolated points and non-trivial intervals. Thus it remains to show that any interval in the coincidence set must be in the support of μ. To this end, observe that on any interval in the contact set, μ has density $-\mathfrak{d}$ by (1.1.3). By assumption, $\mathfrak{d}$ has only finitely many zeros so the interval must be in the support.

Now assume that $\mathfrak{d}$ is identically zero. The result then follows from Corollary 1.6. $\square$

Another natural question is the following:

Question 1.10. Find a probabilistic interpretation for the dual variable, η.

2. Proof of duality

In this section we prove Theorem 1.1. For readability, we neglect to write the subscripts ξ, h here and throughout the remainder of the paper. We also abbreviate $\mathrm{Pr} = \mathrm{Pr}([0,1])$.

Define the set $Q = \{\mu \in \mathrm{Pr} : \sup\operatorname{supp}\mu < 1\}$ and recall by [22] that the minimizer of (1.0.1) lies in Q. (For an alternative proof see Lemma 4.1.) Define the quantities

$$\tilde{D}(\eta) = \int_0^1 2\sqrt{\eta''} - \eta''(s)\cdot(1-s) - \frac{1}{1-s}ds - \eta(0) + \inf_{t\in[0,1)}\{\eta(t) - \xi(t)\} + h^2 + \xi(1),$$
$$\tilde{P}(\mu) = 2P(\mu).$$

First, we observe the following integration by parts lemma, whose proof we defer to the end of this section.

Lemma 2.1. *Let $\mu, \nu \in Q$ and $\eta \in X$. Then*

$$\int (\eta'' - \xi'')(\phi_\nu\text{-}\phi_\mu)\,dt = -\eta'(0)\cdot(\phi_\nu(0) - \phi_\mu(0)) - \int (\eta - \xi)\,d(\nu - \mu).$$

We now begin the proof of Theorem 1.1. First, we prove a preliminary duality result:

Lemma 2.2. *We have that*

$$\min_{\mu\in Q}\tilde{P}(\mu)=\max_{\substack{\eta\in X\\ \eta'(0)=-h^2}}\tilde{D}(\eta).$$

Furthermore an optimal pair (μ,η) *satisfies*

$$\eta''\phi_\mu^2=1\quad Leb-a.e.$$

$$\mu\left(\left\{\eta(s)-\xi(s)=\inf_t\left(\eta(t)-\xi(t)\right)\right\}\right)=1.$$

Finally if a pair (μ,η) *satisfies these relations, then it is optimal.*

Proof. We begin by proving the first part. Recall that for all $a,\lambda\in(0,\infty)$ we have

$$2\sqrt{\lambda}\le\lambda a+\frac{1}{a}\tag{2.0.1}$$

with equality if and only if $\lambda a^2=1$. With this in mind, we have for all $\mu\in Q$ and $\eta\in\Lambda$ that

$$\begin{aligned}\tilde{P}(\mu)&\ge\int_0^1\xi''(s)\phi_\mu(s)+2\sqrt{\eta''}-\phi_\mu\eta''-\frac{1}{1-s}ds+h^2\phi_\mu(0)\\&=\int_0^1(\eta''(s)-\xi''(s))(1-s-\phi_\mu(s))+\int_0^1 2\sqrt{\eta''}-\eta''(s)\cdot(1-s)-\frac{1}{1-s}\\&\quad+\int_0^1\xi''(s)\cdot(1-s)ds+h^2\phi_\mu(0).\end{aligned}$$

Applying Lemma 2.1 with $\nu=\delta_0$, we may integrate by parts to find that the last line is equal to

$$K(\mu,\eta)=\int_0^1(\eta-\xi)d\mu+\int_0^1 2\sqrt{\eta''}-\eta''(s)\cdot(1-s)-\frac{1}{1-s}ds-\eta(0)+h^2+\xi(1).$$

That is,

$$\tilde{P}(\mu)\ge K(\mu,\eta).$$

Observe that if we define η_μ by

$$\eta_\mu=-h^2t+\int_0^t\int_0^s\frac{1}{\phi_\mu^2}d\tau ds,\tag{2.0.2}$$

then it satisfies $\eta\in X$ and $\eta'(0)=-h^2$. By the case of equality in (2.0.1), we see that (up to the addition of a constant) it uniquely achieves the equality

$$\tilde{P}(\mu)=K(\mu,\eta_\mu).$$

Hence,

$$\tilde{P}(\mu)=\sup_{\substack{\eta\in X\\ \eta'(0)=-h^2}}K(\mu,\eta).$$

Evidently,

$$\inf_{\mu\in Q}K(\mu,\eta)=\tilde{D}(\eta).$$

This implies that

$$\inf_{\mu\in Q}\tilde{P}(\mu)=\inf_{\mu\in Q}\sup_{\substack{\eta\in X\\ \eta'(0)=-h^2}}K(\mu,\eta)\geq\sup_{\substack{\eta\in X\\ \eta'(0)=-h^2}}\inf_{\mu\in Q}K(\mu,\eta)=\sup_{\substack{\eta\in X\\ \eta'(0)=-h^2}}\tilde{D}(\eta).$$

The first part of the result then follows provided we can find a pair (μ,η) that achieves the equality

$$\tilde{P}(\mu)=K(\mu,\eta)=\tilde{D}(\eta).$$

Let μ be the optimizer of P and define $\eta=\eta_\mu$ as in (2.0.2). The result then follows provided

$$K(\mu,\eta)=\tilde{D}(\eta).$$

Observe that this will happen if and only if

$$\int\eta-\xi\,d\mu=\inf\{\eta-\xi\}\tag{2.0.3}$$

so it suffices to show this equality. To see (2.0.3), note that the first order optimality conditions for (1.0.1) are that μ satisfies

$$\int\left(\xi''-\frac{1}{\phi_\mu^2}\right)(\phi_\nu-\phi_\mu)dt+h^2(\phi_\nu(0)-\phi_\mu(0))\geq 0\quad\forall\,\nu\in Q.$$

Identifying the integrand, we see that this is

$$h^2(\phi_\nu(0)-\phi_\mu(0))-\int(\eta''-\xi'')(\phi_\nu-\phi_\mu)dt\geq 0.\tag{2.0.4}$$

Integrating by parts (see Lemma 2.1), we see that

$$\int(\eta''-\xi'')(\phi_\nu\text{-}\phi_\mu)\,dt=h^2(\phi_\nu(0)-\phi_\mu(0))-\int(\eta-\xi)\,d(\nu-\mu).$$

Combining this with (2.0.4) yields

$$\int\eta-\xi d\nu\geq\int\eta-\xi d\mu$$

for all $\nu\in Q$. The first result is then immediate.

Observe by the construction of η_μ and the preceding discussion that the optimal pair constructed satisfies the above relations. Since the two conditions (2.0.3) and that $\eta''\phi^2=1$ were necessary and sufficient for the equalities to hold, we see that the optimality conditions characterize optimal pairs as desired. □

We can now give the proof of the duality.

Proof of Theorem 1.1. Observe that by Lemma 2.2, and the fact that the minimizer of (1.0.1) belongs to Q (see Lemma 4.1), we have that

$$\min_{\mu\in\mathrm{Pr}}P(\mu)=\max_{\substack{\eta\in X\\ \eta'(0)=-h^2}}\frac{1}{2}\tilde{D}(\eta).$$

So, it suffices to show that

$$\max_{\substack{\eta\in X\\ \eta'(0)=-h^2}}\frac{1}{2}\tilde{D}(\eta)=\max_{\eta\in\Lambda}D(\eta).$$

To prove this, we begin by observing that $\tilde{D}$ is invariant under shifts $\eta \mapsto \eta + k$. Choose an optimal η for $\frac{1}{2}\tilde{D}$ (we know an optimizer exists from the proof of Lemma 2.2 above). Then if we set $\tilde{\eta} = \eta - \inf\{\eta - \xi\}$, it follows that

$$\frac{1}{2}\tilde{D}(\eta) = \frac{1}{2}\tilde{D}(\tilde{\eta}) = D(\tilde{\eta}).$$

Indeed, $\tilde{\eta} \geq \xi$ and $\inf\{\tilde{\eta} - \xi\} = 0$.

That the pair is unique can be seen as follows. Observe first that P is strictly convex so that the minimizing μ is unique. For D, note that although it is concave, it is not strictly concave. Nevertheless, if η_1 and η_2 were maximizers, then they would have the same second derivative by strict convexity of the square root function. As their derivative at 0 would be prescribed in the definition of Λ, we see that they could differ only by a constant. If this constant is non-zero, then this would change the value of the term $\eta(0)$ appearing in the definition of D, which would be a contradiction. Thus, the maximizing η is unique. That the pair is uniquely determined by the relations (1.1.1) follows from Lemma 2.2. ☐

Finally, we prove the integration by parts lemma that was used above.

Proof of Lemma 2.1. By an approximation argument, it suffices to prove Lemma 2.1 assuming that $\mu = f ds$ and $\nu = g ds$ where $f, g \in C_c^\infty((0,1))$, and that $\eta \in C_c^\infty([0,1))$. Given these, it follows that $\phi_\mu - \phi_\nu \in C_c^\infty([0,1))$. Hence, integrating by parts gives that

$$\begin{aligned}
&\int_0^1 (\eta'' - \xi'')(\phi_\nu - \phi_\mu)\, ds \\
&\quad = \int_0^1 -(\eta - \xi)'(\phi_\nu' - \phi_\mu')\, ds - \eta'(0)(\phi_\nu(0) - \phi_\mu(0)) \\
&\quad = \int_0^1 (\eta - \xi)(\phi_\nu'' - \phi_\mu'')\, ds - \eta'(0)(\phi_\nu(0) - \phi_\mu(0)) + \eta(0)(\phi_\nu'(0) - \phi_\mu'(0)).
\end{aligned}$$

Note we used that $\xi(0) = \xi'(0) = 0$. Given our assumptions on μ and ν,

$$\int_0^1 (\eta - \xi)(\phi_\nu'' - \phi_\mu'')\, ds = -\int_0^1 (\eta - \xi)\, d(\nu - \mu)$$

and $\phi_\nu'(0) = \phi_\mu'(0) = 0$. Plugging these into the above gives the result. ☐

3. Proof of the rule of signs

Throughout this section, we assume that $\eta \in \Lambda$ is optimal, i.e., that

$$D(\eta) = \max_{\eta \in \Lambda} D(\eta).$$

Our goal is to prove Theorem 1.4.

Proof of Theorem 1.4. We begin by proving (1), which we do by contradiction. Suppose that there are three coincidence points, t_1, t_2, and t_3, which satisfy $a \leq t_1 < t_2 < t_3 \leq b$. By (1.1.4), $\eta'(t_i) = \xi'(t_i)$ for each i, and $\eta''(t_3) \geq \xi''(t_3)$. By the mean value theorem, there exist points s_1, s_2 with $t_1 < s_1 < t_3 < s_2 < t_2$ such that $\eta''(s_i) = \xi''(s_i)$ for $i = 1, 2$. By (1.1.3), the function $t \to \frac{1}{\sqrt{\eta''(t)}}$ is concave. Hence, by the assumption on $\mathfrak{d}$, $t \to \frac{1}{\sqrt{\eta''(t)}} - \frac{1}{\sqrt{\xi''(t)}}$ is strictly concave on (t_1, t_2).

As this function vanishes at the points s_1, s_2, it must be strictly positive between. Thus, $\xi''(t_2) > \eta''(t_2)$ and this is a contradiction.

Now we prove (2). We proceed by a first variation argument. Introduce the path

$$[0,1] \to \Lambda, \quad \tau \to \eta_\tau = \eta + \tau(\tilde{\eta} - \eta)$$

where

$$\tilde{\eta}(t) = \begin{cases} \eta(t) & t \notin [a,b], \\ \xi(t) & t \in [a,b]. \end{cases} \tag{3.0.1}$$

That $\eta_\tau \in \Lambda$ for all τ, and in particular that $\eta_\tau \in X$, follows from our assumption that η is optimal and that $a, b \in \{\eta = \xi\}$. In particular, we have that $\eta' = \xi'$ at a, b by (1.1.4).

Now we note that D is concave and that the path η_τ is linear in τ, so that $\tau \to D(\eta_\tau)$ is concave. Thus, to conclude that $[a,b] \subset \{\eta = \xi\}$, we need only to prove that

$$\frac{d}{d\tau}^{-}|_{\tau=1} D(\eta_\tau) \geq 0, \tag{3.0.2}$$

since it then follows that

$$D(\tilde{\eta}) = D(\eta_1) \geq D(\eta_0) = D(\eta)$$

so that $\tilde{\eta}$ is also a maximizer of D. Since maximizers of D are unique (as shown in the proof of Theorem 1.1 on page 3137), we conclude that $\tilde{\eta} = \eta$ and hence that $[a,b] \subset \{\eta = \xi\}$.

Now we perform the required differentiation. First, note that

$$\eta_\tau(0) = \eta(0) \quad \forall \tau.$$

Also, note that

$$\int_a^b (\eta_\tau'' - \eta'')(1-s)\, ds = (\eta_\tau' - \eta')(1-s)|_a^b + (\eta_\tau - \eta)|_a^b = 0 \quad \forall \tau$$

by (1.1.4). It follows that

$$D(\eta_\tau) - D(\eta) = \int_a^b \sqrt{\eta_\tau''} - \sqrt{\eta''}\, ds \quad \forall \tau$$

so that

$$D(\eta_1) - D(\eta_\tau) = \int_a^b \sqrt{\eta_1''} - \sqrt{\eta_\tau''} = \int_a^b \sqrt{\xi''} - \sqrt{\xi'' + (1-\tau)(\eta'' - \xi'')}.$$

Hence,

$$\frac{d}{d\tau}^{-}|_{\tau=1} D(\eta_\tau) = \lim_{\tau \to 1^-} \frac{D(\eta_1) - D(\eta_\tau)}{1-\tau} = \int_a^b -\frac{1}{2}\frac{1}{\sqrt{\xi''}}(\eta'' - \xi'').$$

Here we used the monotone convergence theorem to pass to the limit, which we may do since $\eta'' - \xi''$ changes sign only finitely many times.

Now we claim that

$$\frac{d}{d\tau}^{-}|_{\tau=1} D(\eta_\tau) = \frac{1}{2}\int_a^b -\mathfrak{d}(\eta - \xi). \tag{3.0.3}$$

We prove this by case analysis. Suppose first that $a > 0$. This then follows by an integration by parts along with (1.1.4).

Now suppose that $a = 0$. We claim that when $\mathfrak{d} \leq 0$ on this interval, that (3.0.3) still holds by an integration by parts. Indeed, we claim that under this assumption that $\xi''(0) > 0$. With this claim in hand, integration by parts and (1.1.4) gives that

$$\int_\epsilon^b \frac{1}{\sqrt{\xi''}}(\eta'' - \xi'') = \int_\epsilon^b -\mathfrak{d}(\eta - \xi) - \frac{1}{\sqrt{\xi''}}(\eta' - \xi')(\epsilon) + (\frac{1}{\sqrt{\xi''}})'(\eta - \xi)(\epsilon)$$

for all $\epsilon \in (0, b)$. Since $\xi''(0) > 0$, $\frac{1}{\sqrt{\xi''}} \in L^1([0, b])$ and also $\frac{1}{\sqrt{\xi''}} \vee |(\frac{1}{\sqrt{\xi''}})'| \leq C$. Since $\eta \in C^2([0, 1))$ by Proposition 1.2, we can take $\epsilon \to 0$ to deduce (3.0.3).

We now prove the claim. Suppose, for contradiction, that $\xi''(0) = 0$. By direct manipulation, $\mathfrak{d}$ has the same sign as

$$s(t) = 3(\xi''')^2 - 2\xi'' \cdot \xi''''$$

for $t \in (0, 1)$. Let $k = \min\{p : \beta_p > 0\}$; then

$$s(t) = \beta_k^4 k^3 (k-1)^2 (k-2) t^{2k-6} + O(t^{2k-5}).$$

This is positive in a neighborhood of zero, contradicting the assumption that $\mathfrak{d} \leq 0$.

To complete the proof, observe that the integrand in (3.0.2) is non-negative by our assumption on $\mathfrak{d}$ and since $\eta \geq \xi$. Hence, (3.0.2) follows and therefore $[a, b] \subset \{\eta = \xi\}$. □

We conclude with the following remark.

Remark 3.1. This proof is an example of the observation alluded to in the introduction that there are methods available to the study of the dual problem that do not have apparent analogues for the primal one. In particular, the variation used above defined through (3.0.1) does not obviously have an associated path on the primal side, as it only becomes apparent that $\left(\frac{1}{\sqrt{\tilde{\eta}''}}\right)''$ is a probability measure a posteriori!

4. Appendix

To make this presentation self-contained we present an alternative proof of the following statement.

Lemma 4.1. *The minimizer of* (1.0.1) *belongs to* $Q = \{\mu \in \Pr : \sup \mathit{supp}\, \mu < 1\}$.

Proof. It suffices to prove the following claim: given $\mu \in \Pr \setminus Q$, there exists $\tilde{\mu} \in Q$ with $P(\tilde{\mu}) < P(\mu)$. We prove this by a first variation argument. Given $\mu \in \Pr$, consider the variation $[0, 1] \to \Pr$, $\epsilon \to \mu_\epsilon$ defined by

$$\mu_\epsilon([0, t]) = \begin{cases} \mu([0, t]) & 0 \leq t < 1 - \epsilon, \\ 1 & 1 - \epsilon \leq t \leq 1. \end{cases}$$

Note that $\mu_\epsilon \in Q$ if $\epsilon > 0$. Evidently

$$\phi_\epsilon = \phi_{\mu_\epsilon} = \begin{cases} \phi_\mu(t) - \phi_\mu(1 - \epsilon) + \epsilon & 0 \leq t < 1 - \epsilon, \\ 1 - t & 1 - \epsilon \leq t \leq 1, \end{cases}$$

so that

$$\phi_\epsilon - \phi = \begin{cases} \epsilon - \phi_\mu(1 - \epsilon) & 0 \leq t < 1 - \epsilon, \\ 1 - t - \phi_\mu(t) & 1 - \epsilon \leq t \leq 1. \end{cases}$$

Hence,

$$
\begin{aligned}
&P(\mu_\epsilon) - P(\mu) \\
&\quad = \int_0^1 (\xi'' - \frac{1}{\phi_\epsilon \phi})(\phi_\epsilon - \phi)\, ds + h^2(\phi_\epsilon(0) - \phi(0)) \\
&\quad = (\epsilon - \phi_\mu(1-\epsilon)) \left[\xi'(1-\epsilon) + h^2 - \int_0^{1-\epsilon} \frac{1}{\phi_\epsilon \phi} \right] + \int_{1-\epsilon}^1 (\xi'' - \frac{1}{\phi_\epsilon \phi})(1 - t - \phi)\, ds \\
&\quad = (i) + (ii).
\end{aligned}
$$

Now suppose that $\mu \in \Pr \setminus Q$, so that $\phi_\mu(1-\epsilon) < \epsilon$ for all $\epsilon > 0$. Using the upper bound $\phi_\epsilon \vee \phi \leq 1 - t$ and that ξ' is non-decreasing, we see that

$$
\xi'(1-\epsilon) + h^2 - \int_0^{1-\epsilon} \frac{1}{\phi_\epsilon \phi} \leq \xi'(1) + h^2 - \int_0^{1-\epsilon} \frac{1}{(1-t)^2} = \xi'(1) + h^2 - \frac{1-\epsilon}{\epsilon}.
$$

The right hand side is strictly negative for small enough ϵ, so (i) is strictly negative for small enough ϵ. Similarly, we see that (ii) is strictly negative for sufficiently small $\epsilon > 0$. It follows that $P(\mu_\epsilon) - P(\mu) < 0$ for small enough ϵ. □

Acknowledgments

We would like to thank R.V. Kohn for helpful discussions. We would like to thank A. Auffinger for encouraging the preparation of this paper. We would like to thank D. Panchenko for helpful comments regarding the presentation of this work. This research was conducted while the first author was supported by a National Science Foundation Graduate Research Fellowship DGE-0813964; and National Science Foundation grants DMS-1209165, OISE-0730136, and OISE-1604232, and while the second author was supported by a National Science Foundation Graduate Research Fellowship DGE-0813964; and National Science Foundation grants OISE-0967140 and DMS-1311833.

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