Global minimisers of energies related to dislocations

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We consider a nonlocal energy

$$I_\alpha(\mu) = \frac{1}{2} \iint_{\mathbb{R}^2\times\mathbb{R}^2} W_\alpha(x-y)\, d\mu(x)\, d\mu(y) + \frac{1}{2}\int_{\mathbb{R}^2} |x|^2\, d\mu(x)$$

defined on probability measures $\mu \in \mathcal{P}(\mathbb{R}^2)$, where the interaction potential W_α is given by

$$W_\alpha(x_1,x_2) = -\frac{1}{2}\log(x_1^2+x_2^2)+\alpha\frac{x_1^2}{x_1^2+x_2^2}, \qquad x=(x_1,x_2)\in\mathbb{R}^2\,.$$

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Dislocations

The kernel is obtained by adding to the Coulomb potential an anisotropic term weighted by a parameter $\alpha \in \mathbb{R}$.

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Dislocations: The planar case

Frostman

When the anisotrophy is switched off, $\alpha = 0$, there exists a unique probability measure that minimises the energy $I(\mu)$, namely, the normalised characteristic function of the unit disc D, $\frac{1}{\pi}\chi_D(z)$

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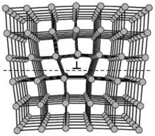


IDEALISED DISLOCATIONS

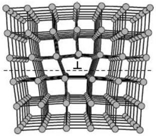
- Straight & parallel; edge
- Single slip, and single sign (all positive)

INTERACTION STRESS

- generated by a dislocation at 0

  and acting on a dislocation at x
- $F(x) = -\kappa \nabla V(x)$
- $V(x) = -\log|x| + \frac{x_1^2}{|x|^2}$

Conjecture: positive dislocations prefer to form vertical walls. Can we prove it ?



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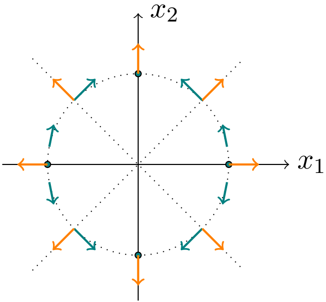

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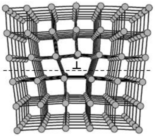

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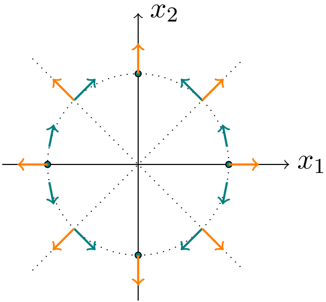

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Aim: Characterise the minimiser (equilibrium measure)

- Does the minimiser exist? Is it compactly supported?
- Is the minimiser unique?
- Does the minimiser possess any symmetries?
- What is the dimension of its support?
- Can we find the minimiser explicitly?

Some available results

In general one can consider the above problem for a variety of interaction potentials and confinements

- Huge literature on existence, confinement, regularity of minimisers for a variety of potentials and for a variety of applications.

  (e.g. Cañizo, Carrillo, Castorina, Chipot, Choksi, Delgadino, Fetecau, Figalli, Hittmeir, Huang, Kolokolnikov, Mainini, Mellet, Patacchini, Simione, Slepčev, Sugiyama, Topaloglu, Volzone, Yao, etc...)

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Dislocations: The planar case

Coming back to our dislocation potential

$$W_\alpha(x) = -\frac{1}{2}\log(x_1^2 + x_2^2) + \alpha\frac{x_1^2}{x_1^2 + x_2^2}.$$

In the case $\alpha = 1$, The minimisers of I_1 were since long conjectured to be vertical walls of dislocations, and this has been confirmed by [Mora, Rondi, Scardia (2016)]. They proved that the only minimiser of I_1 is the semi-circle law.

$$\mu_1 := \frac{1}{\pi}\delta_0 \otimes \sqrt{2 - x_2^2}\,\mathcal{H}^1 \llcorner (-\sqrt{2}, \sqrt{2}) \tag{1}$$

on the vertical axis.

It is not difficult to prove that μ_1, that is the semicircle law, is the only minimiser of I_α for $\alpha \geq 1$, since
$I_\alpha(\mu_1) = I_1(\mu_1) < I_1(\mu) \leq I_\alpha(\mu) \ \forall \mu \neq \mu_1$.

The case $\alpha < 0$ can be recovered from the knowledge of the case $\alpha > 0$ by switching x_1 and x_2, so we can limit our analysis to $\alpha \in (0, 1)$.

Can we characterise the minimiser of I_α for every $0 < \alpha < 1$?

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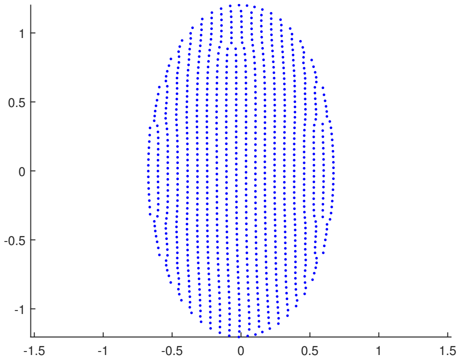

Dislocations: The planar case

Theorem (Carrillo, Mora, M. Rondi, Scardia, Verdera)

Let $0 \leq \alpha < 1$. The measure

$$\mu_\alpha := \frac{1}{\sqrt{1-\alpha^2}\pi} \chi_{\Omega(\sqrt{1-\alpha}, \sqrt{1+\alpha})}, \tag{2}$$

where

$$\Omega(\sqrt{1-\alpha}, \sqrt{1+\alpha}) := \left\{ x = (x_1, x_2) \in \mathbb{R}^2 : \; \frac{x_1^2}{1-\alpha} + \frac{x_2^2}{1+\alpha} < 1 \right\},$$

is the unique minimiser of the functional I_α among probability measures $\mathcal{P}(\mathbb{R}^2)$.

Dislocations: The planar case

What is surprising is that techniques developed in the context of fluid mechanics turn out to be crucial for the characterisation of the minimisers of the anisotropic energy I_α.

In particular the minimality of the semi-circle law for the dislocation energy I_1 can be deduced from our result by a limiting argument based on Γ-convergence.

That is, we obtain again the result of [Mora, Rondi, Scardia], but with a different proof based on methods from fluid mechanics and complex analysis

Moreover the case $\alpha = 1$ is in the context of edge dislocations of metals.

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Proof of the Theorem

In relation with the existence and uniqueness we have

Proposition

Let $\alpha \in [0,1]$. Then the energy I_α is well defined on $\mathcal{P}(\mathbb{R}^2)$, is strictly convex on the class of measures with compact support and finite interaction energy, and has a unique minimiser in $\mathcal{P}(\mathbb{R}^2)$. Moreover, the minimiser has compact support and finite energy.

In fact the key point for the uniqueness is that the Fourier transform of our kernel never vanishes

$$\langle \hat{W}_\alpha, \varphi \rangle = \frac{1}{2\pi} \int_{\mathbb{R}^2} \frac{(1-\alpha)\xi_1^2 + (1+\alpha)\xi_2^2}{|\xi|^4} \varphi(\xi)\, d\xi$$

for every φ in the Schwarz class.

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To obtain the characterisation of the mimimisers we use that standard computations in potential theory shows that any minimiser μ of I_α must satisfy the following Euler-Lagrange conditions.

If

$$P_\mu(x) = (W_\alpha * \mu(x)) + \frac{|x|^2}{2}$$

Then, one has

$$P_\mu(x) = C_\alpha \quad \text{for every } x \in \Omega(\sqrt{1-\alpha}, \sqrt{1+\alpha}),$$

and

$$P_\mu(x) \geq C_\alpha \quad \text{for every } x \in \mathbb{R}^2,$$

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In fact, we compute *explicitly* the gradient of $W_\alpha * \mu$, where $\mu = \frac{\chi_{\Omega(a,b)}}{|\Omega(a,b)|}$, both inside and outside $\Omega(a,b)$. This is enough to check the Euler-Lagrange equations and to conclude the proof of Theorem.

$$\nabla(W_\alpha * \mu)(x) + x = 0 \quad \text{for every } x \in \Omega(\sqrt{1-\alpha}, \sqrt{1+\alpha}),$$

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$$\nabla(W_\alpha * \mu)(x) + x \text{ does not vanish for every } x \in \mathbb{C} \setminus \Omega.$$

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Proof of the Theorem

In order to evaluate the convolution $\nabla W_\alpha * \mu$, it is convenient to work in complex variables.

In complex variables the potential W_α reads as

$$W_\alpha(x) \equiv W_\alpha(z) = -\frac{1}{2}\log(z\bar{z}) + \frac{\alpha}{2}\left(1 + \frac{z}{2\bar{z}} + \frac{\bar{z}}{2z}\right),$$

and its gradient

$$\nabla W_\alpha(x) = -\frac{x}{|x|^2} + 2\alpha\frac{x_1x_2}{|x|^4}x^\perp \equiv 2\bar{\partial}W_\alpha(z) = -\frac{1}{\bar{z}} + \frac{\alpha}{2}\frac{1}{z} - \frac{\alpha}{2}\frac{z}{\bar{z}^2}, \tag{3}$$

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Proof of the Theorem

We compute

$$\frac{1}{z} * \mu = \bar{z} - \lambda z \text{ inside } \Omega, \text{ being } \lambda = \frac{a-b}{a+b}$$

By taking the conjugate we obtain directly

$$\frac{1}{\bar{z}} * \mu = z - \lambda \bar{z} \text{ inside } \Omega.$$

One can also get

$$\frac{z}{\bar{z}^2} * \mu = \lambda(z - \lambda \bar{z}) \text{ inside } \Omega.$$

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Proof of the Theorem

Using the above computations inside and the fact that all the potential are linear inside one obtains

$$\begin{cases} -1-\alpha\lambda+ab=0, \\ \lambda+\dfrac{\alpha}{2}+\lambda^2\dfrac{\alpha}{2}=0, \end{cases}$$

Now, it is easy to check that $a=\sqrt{1-\alpha}$ and $b=\sqrt{1+\alpha}$ are the unique solution of the system.

To verify the second Euler-Lagrange condition one has to compute all the potentials outside.

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Proof of the Theorem

If E is the candidate ellipse, then one has to prove that

$$P_\mu(z) \geq C_\alpha, \;\; z \in \mathbb{C} \setminus \Omega$$

This requires a precise computation of ∇P_μ on $\mathbb{C} \setminus \Omega$

$$\nabla P_\mu(z) = -\frac{1}{z} * \mu + \frac{\alpha}{2}\left(\frac{1}{z} * \mu - \frac{z}{\bar{z}^2} * \right) + z$$

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$$\big(-\frac{1}{z} * \mu \big)(z) = 2h(\bar{z}), \quad z \notin \Omega$$

where

$$h(z) = \frac{1}{z + \sqrt{z^2 + c^2}}, \quad c^2 = b^2 - a^2$$

and

$$\big(-\frac{z}{\bar{z}^2} * \mu \big)(z) = 2\lambda h(\bar{z}) - 2h'(\bar{z})(z - \lambda \bar{z} - 2ab h(\bar{z}))$$

where

$$h'(\bar{z}) = -\frac{h(\bar{z})}{N(\bar{z})}, \quad N(z) = \sqrt{z^2 + c^2}$$

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So, we obtain

$$\nabla P_\mu(z) N(\bar{z}) = t, \qquad \frac{x^2}{a^2+t} + \frac{y^2}{b^2+t} = 1, \ t \geq 0$$

and

$$\langle \nabla P_\mu(z) \cdot N(z) \rangle = t, \quad \langle \nabla P_\mu(z) \cdot iN(z) \rangle = 0$$

Dislocations: The 3-D case

We consider a nonlocal energy

$$I_\alpha(\mu) = \frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} W_\alpha(x-y)\,d\mu(x)\,d\mu(y) + \frac{1}{2}\int_{\mathbb{R}^3} |x|^2\,d\mu(x) \quad (4)$$

defined on probability measures $\mu \in \mathcal{P}(\mathbb{R}^3)$, where the interaction potential W_α is given by

$$W_\alpha(x_1,x_2,x_3) = \frac{1}{|x|} + \alpha\frac{x_1^2}{|x|^3}, \qquad x = (x_1,x_2,x_3) \in \mathbb{R}^3, \quad (5)$$

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$$W_\alpha(x_1,x_2,x_3) = \frac{1}{|x|} + \alpha\frac{x_1^2}{|x|^3}, \qquad x = (x_1,x_2,x_3) \in \mathbb{R}^3, \quad (5)$$

Dislocations: The 3-D case

We consider a nonlocal energy

$$I_\alpha(\mu) = \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} W_\alpha(x-y)\, d\mu(x)\, d\mu(y) + \frac{1}{2} \int_{\mathbb{R}^3} |x|^2\, d\mu(x) \quad (4)$$

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Again the problem is to describe the minimisers of the above energy.

The kernel is obtained by adding to the 3 dimensional Coulomb potential an anisotropic term weighted by a parameter $\alpha \in \mathbb{R}$.

In the particular case where $\alpha = 0$, the minimiser is radial, and is given by $\mu_0 := \frac{3}{4\pi}\chi_{B_1(0)}$, the normalised characteristic function of the unit ball.

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Dislocations: The 3-D case

Theorem (Carrillo, Mora, M. Rondi, Scardia, Verdera)

Let $-1 < \alpha < 1$. There exist constants $a(\alpha)$ and $b(\alpha)$ such that the measure

$$\mu_\alpha := \frac{3}{ab^2 4\pi} \chi_{\Omega(a,b,b)}, \tag{6}$$

where

$$\Omega(a,b,b) := \left\{ x = (x_1, x_2, x_3) \in \mathbb{R}^3 : \ \frac{x_1^2}{a^2} + \frac{x_2^2}{b^2} + \frac{x_3^2}{b^2} < 1 \right\},$$

is the unique minimiser of the functional I_α among probability measures $\mathcal{P}(\mathbb{R}^3)$.

Dislocations: 3D

The minimizer is given by the probability measure of the characteristic functions of an oblate ellipsoid $(0 < \alpha < 1)$, the characteristic function of a ball ($\alpha = 0)$ or the characteristic function of a prolate ellipsoid $(-1 < \alpha < 0)$.

The computations are much more involved and we can not use some of the advantages of the complex numbers.

The idea is again to check the Euler-Lagrage Equations:

$$(W_\alpha * \mu_\alpha)(x) + \frac{|x|^2}{2} = C_\alpha \quad \text{for every } x \in \Omega(a,b,b), \tag{7}$$

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To do that, one has to compute explicitly the kernel associated to this energy inside and outside our ellipsoid.

Then it is better to use apropiate coordenates, that is the oblate espheroidal coordinates or the prolate spheroidal coordinates.

This solution, when α goes to 1 or to -1, converges to the characteristic function of an oblate or a prolate ellipsoid (It is different from the planar case).

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More general kernels

The next purpose is to study the problem of minimisers for more general kernels.

We consider energy functionals I^κ defined on probability measures in the plane, μ, as

$$I^\kappa(\mu) = \int_{\mathbb{C}}\int_{\mathbb{C}} W^\kappa(z-w)d\mu(z)d\mu(w) + \int_{\mathbb{C}} |z|^2 d\mu(z). \quad (9)$$

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where κ is an even kernel of homogeneity *zero*.

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$W^{\kappa}(0) = +\infty$ and is an even real-valued function, homogeneous of degree 0 and of class $C^3(\mathbb{C} \setminus \{0\})$

The question would be to give conditions on the kernel $\kappa(z)$ such that the minimisers of the above energy are ellipses.

Conjecture. If we have an smooth even kernel such that the Fourier transform is positive, then minimisers should be ellipses.

That is, the uniqueness will be a consequence of the positivity of the Fourier transform of the kernel.

The first Euler-Lagrange condition will determine the ellipse and it should be enough. It means that in some sense the second Euler-Lagrange condition is for free.

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We can not prove the conjecture in general and we can do it if the anisotrophic potential has small norm.

Theorem

There exists $\varepsilon_0 > 0$ such that if κ is an even real function, homogeneous of degree 0, of class C^3 off the origin, and satisfies the smallness condition.

$$|\nabla^j \kappa(z)| \leq \varepsilon_0 \quad for\, |z| = 1 \qquad and\, j \in \{0, 1, 2, 3\}.$$

Then there exists a triple (a, b, φ) such that the probability measure $\frac{\chi_E}{|E|}$,is the unique minimiser of the above energy, where

$$E = E(a, b, \varphi) = e^{i\varphi}\Big\{(x, y) \in \mathbb{R}^2 : \frac{x^2}{a^2} + \frac{y^2}{b^2} \leq 1\Big\}.$$

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In this result we get: Existence; Uniqueness and characterization of minimisers of energy.

For the higher dimensional case we have the corresponding result. Let's consider the energy

$$I^{\kappa}(\mu) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} W^{\kappa}(z-w)d\mu(z)d\mu(w) + \int_{\mathbb{R}^d} |z|^2 d\mu(z).$$

Here the interaction potential W^{κ} is given in higher dimensions by

$$W^{\kappa}(z) = -\frac{1}{|x|^{d-2}} + \kappa(x),$$

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Theorem

Let $d \geq 3$. There exists $\varepsilon_0 > 0$ such that if κ is real valued function, homogeneous of degree $2-d$, even in each variable, of class $\mathcal{C}^3$ off the origin, and satisfies the smallness condition

$$|\nabla^j \kappa(x)| \leq \varepsilon_0 \quad for\, |x| = 1 \qquad and\, j \in \{0, 1, 2, 3\}.$$

and $\hat{W}^k > 0$ outside the origin, then there exists an ellipsoid such that the probability measure $\frac{\chi_E}{|E|}$ is the unique minimiser of the above energy.

Here the ellipsoid is given by

$$E = \Big\{(x_1, x_2, \cdots x_d) \in \mathbb{R}^d : \frac{x_1^2}{a_1^2} + \frac{x_2^2}{a_2^2} + \cdots + \frac{x_d^2}{a_d^2} \leq 1\Big\}.$$

More general kernels

This result can be seen as the stability of ellipsoids as energy minimisers, since the minimiser of the Coulomb energy is the normalised characteristic function of a ball.

The idea of the proof is an approximation argument.

Uniqueness: We show that the energy I^κ is strictly convex on a class of measures that are relevant for the minimisers. We achieve this by showing that the Fourier transform of the potential W^k is positive outside the origin.

To get the characterisation we use Euler-Lagrange conditions. EL1 gives us a precise ellipsoid which is candidate to be the minimiser. In this point we use again that $\partial_{i,j}\kappa$ is constant on the ellipsoid.

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More general kernels

For the second Euler-Lagrange condition we adopt a purely perturbative argument, which exploit the “closeness” of every term of the equation. for κ small, to the corresponding term of the corresponding Euler-Lagrange condition for the case $\kappa = 0$.

A very recent result

In a very recent result Carrillo and Ruiwen Shu prove the following:

Theorem

If we take the family of planar kernels in (9) and the Fourier transform of the kernel is positive. Then one of the following holds:

- *There exists a unique triple* (a, b, φ) *such that* $\frac{\chi_E}{|E|}$ *is the unique minimiser, being* E *the ellipse* $E(a, b, \varphi)$.
- *There exits a unique pair* (b, φ) *such that* $Ce^{i\varphi}\sqrt{b^2 - x^2}\chi_L$ *is the unique minimiser. Here* L *is the interval* $L = (-b, b)$.

Open problems

In higher dimensions the arguments of Carrillo and Shu do not work in an easy way. More work is need for this case.

In higher dimensions for $|\alpha| > 1$ nothing is known. In this case we lost uniqueness and it means that more mathematics are needed. Moreover, Baremblat functions should appear at some place.

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Thank you for your attention