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# Mini-Workshop: Mathematics of Crystallisation

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Abstract. Crystallisation, by which we mean the formation of solids precipitating from a solution, is the central theme of the present mini-workshop. Participants discussed different approaches towards a rigorous mathematical understanding of crystallisation as well as detecting, modelling and establishing properties of crystalline and quasicrystalline structures.

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## Introduction by the Organizers

The mini-workshop *Mathematics of Crystallisation* was attended by 17 participants from different mathematical disciplines. Understanding the structure formation of crystals was the overarching theme of this week-long program. Even though this question is rather classical, a rigorous picture is still missing. However, the field currently undergoes a phase of renewed interest and activity, and the workshop brought together senior and junior mathematicians with a keen interest in crystallisation. Apart from presentations of current and classical results, the workshop aimed at identifying tractable and challenging questions for future research.

We had fifteen one-hour talks throughout the week, targeting a wide range of perspectives on the crystal problem. These talks were completed by four half-hour lectures on additional aspects on Friday afternoon, as well as a summary by one of the organisers. Furthermore, we had scheduled informal discussions every evening after dinner, which led to a lively interaction between the participants.

For a rough mathematical description of crystallisation, we consider a point process in $d$-dimensional space (representing the atoms in the crystal) equipped

with a pair or multi-body interaction that is given through a potential function and the desire is to study structural properties of the resulting configuration. In broad terms, the research presented at the workshop can be categorised in four themes.

The first theme summarises results on the energy minimising configurations. Laurent Bétermin studied the case when the point process is a Bravais lattice, and derived correspondences between the potential function and the resulting lattice. Lucia Scardia took a slightly different angle and studied the equilibrium measures for anisotropic energies, which allowed her to identify grain boundaries. Michael Baake gave a more algebraic view on the classification of large-angle grain boundaries by linking them with coincidence site lattices and algebraic number theory.

The second theme studied resulting configurations under a thermal measure at low but positive temperature. In contrast to the first theme (which would correspond to the particular case of temperature zero), the challenge is that defects and impurities arise at all scales. Physicists distinguish between two kinds of defects: Dislocations (such as missing atoms, line defects or screw defects) as well as disclinations. Uniform energy bound on these defects appears currently out of reach even for arbitrarily small temperatures; in particular, the energetic cost of disclinations, albeit seemingly costly, is not yet found. However, there is exciting new progress in restricted settings. The one-dimensional case is special because the possibility of defects is minimal on the line. Sabine Jansen and Bernd Schmidt presented novel results for the one-dimensional case at positive temperature, which give a somewhat detailed description of the statistical properties of one-dimensional crystals.

The two-dimensional case is highly challenging. A delicate artefact of the two-dimensional case is the absence of *positional* order (by Mermin–Wagner type arguments) so that only long-range *orientational* order appears possible. Alessandro Giuliani gave an overview talk about orientational order of two-dimensional crystals, outlining possible approaches for rigorous proofs. Florian Theil reported on joint work with Luke Williams on a two-dimensional model, where the chemical potential of defects is so large that the thermal measure excludes them statistically.

Modelling crystals in three dimensions was an important theme during the week. Two new models were proposed to demonstrate the breaking of linearised rotations. Diana Conache and Franz Merkl described a mesoscopic model of a three-dimensional crystal that is inspired by the classical Kosterlitz–Thouless model. The setting is a mixed discrete/continuum model: while the actual atoms are modelled on a microscopic scale (described in a continuum approximation), the relevant dislocations are described on a mesoscopic lattice. Florian Theil proposed a different route, where he models dislocations microscopically following a model by Ariza and Ortiz. It is a future challenge to prove the breaking of rotations (rather than linearised rotations) in a physically meaningful model.

A third theme of the workshop is the theory of quasicrystals. Uwe Grimm gave an overview talk about the construction of aperiodic tilings and their properties.

The notion of *order* is fundamental in establishing crystals, and crystallographers use diffraction experiments to distinguish order from disorder. Michael Baake presented a mathematical theory of diffraction, with a particular emphasis on quasicrystals. Holger Kösters extended this by calculating diffraction spectra for various point configurations. Franz Gähler completed the theme with a computational perspective by demonstrating molecular dynamics simulations.

Under the fourth theme, we gather results on related problems and techniques, whose solution presumably sheds light on crystallisation questions. Franz Gähler discussed the construction of tiling spaces. Alastair Rucklidge explained the link between pattern formation and the field of non-linear dynamics and discussed Fourier spectra of quasi-patterns. Alexander Magazinov explained his recent proof that Poisson hard disks percolate in sufficiently high density. Stefan Adams reported on results about gradient fields for non-linear elasticity. The underlying renormalisation scheme appears universal and might be of use in the crystallisation context as well.

The perfect scientific environment provided by the institute supported numerous mathematical discussion among the participants. The fact that most of the participants left the institute only on Saturday morning demonstrates this active attitude. We trust that the workshop was seed and fertiliser for exciting new results on the mathematics of crystallisation.

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## Mini-Workshop: Mathematics of Crystallisation

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# Abstracts

## Orientational order of 2D crystal at low temperatures: an overview, open problems and possible approaches

Alessandro Giuliani

In this talk, I will review the problem of understanding whether interacting particle systems at low temperature exhibit crystalline orientational order in two dimensions. The basic understanding comes from the harmonic (also known as gaussian, or 'spin wave') approximation, which predicts: positional and orientational order in three dimensions; orientational order without positional order in two dimensions. Absence of positional order for particle systems in two dimensions is well understood, on the basis of the Mermin-Wagner theorem [8], and of various quantitative extensions thereof [3, 10]. On the contrary, existence of orientational order has been proved so far only in toy models of interacting particles that either do not support dislocations [5, 7], or allow them but with an associated astronomical (i.e., box size dependent) energy cost [2]. It remains to be seen whether orientational ordering is possible in models supporting dislocations, with finite energy cost associated to each dislocation core. A possible toy model with this features is a statistical mechanics version of the Ariza–Ortiz model [1], which has features reminiscent of the Villain model for 2D rotators; in particular, the energy can be split exactly into an elastic plus 'vortex' part, the vortices representing now the dislocation cores. It is likely that the model can be treated by the methods used in 1981 by Fröhlich–Spencer [4] for understanding the Kosterlitz–Thouless phase in the 2D Villain model. However, it must be taken into account that energy of non-neutral clusters of vortices in the Ariza–Ortiz model scale very differently from the case of the Villain model: in particular, there are regular, non-neutral, arrangements of vortices that have an energy linear in the number of vortices ('Read-Shockley law' for the grain boundaries [6, 9]). I will argue that these configuration have the potential of changing qualitatively the predictions of spin-wave theory, possibly destroying orientational order in two dimensions.

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## Aperiodic tilings: construction and properties

Uwe Grimm

Non-crystallographic symmetries have intrigued artists and scientists for centuries. For instance, in the early 17th century, Johannes Kepler attempted to construct a fivefold tiling of the plane, a feat that was eventually completed successfully by Roger Penrose in 1974 [10]. Today, the Penrose tiling is still one of the paradigms of aperiodic order.

The field of aperiodic order developed rapidly after the surprising discovery of aperiodically ordered materials, now known as quasicrystals, in the early 1980s by Dan Shechtman [12], who was awarded the 2011 Nobel Prize in Chemistry. However, it builds on earlier work, in particular the theory of almost periodic functions developed by Harald Bohr in the early 20th century [5], and work on Wang tiles related to the undecidability of the domino problem [6]. A key contribution comes from Yves Meyer's work in harmonic analysis [8], although this was only fully recognised much later. For a general mathematical introduction to aperiodic order, see [1], and [9, 4, 11, 7, 2] for more details.

The talk introduced the notions of tilings of space and point sets in space, and two important equivalence concepts: *local indistinguishability* (LI) and *mutual local derivability* (MLD). The latter can be used to switch between tiling and point set pictures, in order to use a description of a given spatial structure that is most convenient for the purpose at hand.

There are three main approaches to construct aperiodic tilings, which are *local rules* (also known as matching rules), *inflation rules* (which in the symbolic context are usually referred to as substitution rules) and *cut and project sets* (or model sets, under mild extra assumptions). In the talk, examples for all these approaches were discussed. It was emphasised that local rules generally do *not* constitute local growth rules. While there are examples of aperiodic tilings that allow for all three constructions (for instance the Penrose tilings), this is not generally the case. For example, the pinwheel tiling of the plane arises from an inflation description but clearly cannot be embedded into a higher-dimensional periodic lattice, because it exhibits circular rotational symmetry. Several properties of certain classes of aperiodic tilings, such as repetitivity and pure point diffractivity, were introduced.

Model sets obtained from Euclidean cut and project schemes were discussed in some detail. For sufficiently nice windows, these sets are pure point diffractive, and the diffraction measure can be expressed explicitly in terms of the Fourier transform of the characteristic function of the window. It is possible to generalise results to weak model sets of maximal density, such as the set of visible (primitive) points of the square lattice. This subset of the lattice $\mathbb{Z}^2$ is not a Delone set, as it contains holes of arbitrary size (as a consequence of the Chinese remainder theorem), but can be interpreted as a model set with a window that has no interior and so consists just of its boundary. A weak model set of this type is still pure point diffractive if it has extremal density [3].

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### From potentials to minimizing structures


Laurent Bétermin

(joint work with Mircea Petrache, Peng Zhang)


A natural question arising in any crystallization problem in $\mathbb{R}^d$ (equipped with its euclidean norm $|.|$) with a central-force energy represented by an absolutely summable interaction potential $f : (0, +\infty) \to \mathbb{R}$ is the following:

$$\textit{What is the minimizer of } E_f[L] := \sum_{p \in L \setminus \{0\}} f(|p|^2) \textit{ among lattices } L\textit{?}$$

By comparing the energies of different crystal structures, we can exclude or keep possible minimizing lattices for the crystallization problem with potential $f$. We restrict our study to the class $\mathcal{L}_d$ of simple lattices $L = \bigoplus_{i=1}^{d} \mathbb{Z}u_i$ where $(u_i)_i$ is a basis of $\mathbb{R}^d$, and we denote by $\mathcal{L}_d^\circ(V)$ the space of simple lattices with a unit cell of volume $V$. Furthermore, $f$ is assumed to be the Laplace transform of a Radon measure $\mu_f$, i.e. $f(r) = \int_0^\infty e^{-rt} d\mu_f(t)$. We then ask the following fundamental questions:

- Q1: For which $f$ a lattice can be a minimizer of $E_f$ in $\mathcal{L}_d^\circ(V)$ for all $V$?
- Q2: If the minimizer is not the same for all the densities, what are the other candidates?
- Q3: What are the reasonable candidates for being a minimizer of $E_f$ in $\mathcal{L}_d$?

A key point to study these questions is to write $E_f$ in terms of theta functions:

$$E_f[L] = \int_0^\infty \left[\theta_L\left(\frac{t}{\pi}\right) - 1\right] d\mu_f(t), \quad \theta_L(\alpha) := \sum_{p\in L} e^{-\pi\alpha|p|^2}.$$

Thus, the minimizers of $L \mapsto \theta_L(\alpha)$ and the sign of $\mu_f$ can give some crucial information about the minimizers of $E_f$. Let us assume that $L \mapsto \theta_L(\alpha)$ has the same minimizer $L_0$ for all $\alpha > 0$ in $\mathcal{L}_d^\circ(1)$, which is the case for $d \in \{2, 8, 24\}$ and where $L_0$ is respectively the triangular lattice, $\mathbb{E}_8$ and the Leech lattice, as proved in [8, 6]. Then we have proved the following results in [4]:

(1) **Completely monotone functions.** If $\mu_f$ is nonnegative, then $L_0$ minimizes $E_f$ in $\mathcal{L}_d^\circ(V)$ for all $V > 0$.
(2) **Negativity of the measure $\mu_f$ near 0 and infinity.** If $\mu_f < 0$ on $(0, r_0)$ (resp. on $(r_0, \infty)$), then there exists $V_0$ such that for all $V > V_0$ (resp. for all $V < V_0$), $L_0$ is not a minimizer of $E_f$ in $\mathcal{L}_d^\circ(V)$.
(3) **Positivity of the measure $\mu_f$ near 0.** If $\mu_f > 0$ on $(0, r_0)$ or on $(r_0, \infty)$ and if $L$ minimizes $E_f$ on $\mathcal{L}_d^\circ(V)$ for all $V > 0$, then $L = L_0$.

The class of completely monotone functions answers question Q1, but it turns out that the problem of finding all the potentials $f$ answering this question is a difficult task. Indeed, in dimension $d = 2$ where the only lattice that can be a minimizer of $E_f$ at all the scales is the triangular one, we have found in [1] a positive, decreasing and convex function $f$ such that the triangular lattice is not a minimizer of $E_f$ in $\mathcal{L}_2^\circ(V)$ for some $V$ in an open interval. Furthermore, in [4], we have constructed a potential $f$ such that its measure $\mu_f$ is negative on an open interval and the minimizer of $E_f$ in $\mathcal{L}_2^\circ(V)$ is triangular for all $V > 0$. We also remark that the sign of the derivatives of $f_{\varepsilon_0}$ alternates until the fourth one only.

It is also possible to have some quantitative results for the optimality of the triangular lattice for $E_f$ in $\mathcal{L}_2^\circ(V)$. For example, in the Lennard–Jones case $f(r) = ar^{-p} - br^{-q}$, $p > q > 1$, in [5, 1], we have derived a new integral representation of $E_f$ and we have found an explicit bound $V_0$ such that the triangular lattice is a minimizer of $E_f$ in $\mathcal{L}_2^\circ(V)$ for all $V < V_0$. Furthermore, in [2], we

have numerically checked that the minimizer of $E_f$ in $\mathcal{L}_2^\circ(V)$ exhibits an interesting phase transition of the form 'triangular-rhombic-square-rectangular' as $V$ increases, the same behaviour being observed for the Morse potential in [3].

Finding the global minimizer of $E_f$ in $\mathcal{L}_d$ is also a difficult task. The integral representation showed in [1] implies the optimality of a triangular lattice for the Lennard–Jones potential with small parameters $p, q$, but the same result is expected for any values of the parameters, and a method to compare the possible global minima is explained in [4]. The Morse potential seems also to have a triangular lattice for global minimum, but in [4] we have constructed many examples of one-well potentials $f$ such that the minimizer of $E_f$ in $\mathcal{L}_2$ is not triangular.

Finally, an important result is the classification of all the lattices being critical points of $E_f$ in $\mathcal{L}_2^\circ(V)$ for all $V$ in some open interval. Using a result by Gruber [7] about the Epstein zeta function, we have shown in [3] that such lattices must have all their layers 'strongly eutactic'. These structures, answering question Q3, that are then the best candidates for being a global minimum of $E_f$, are the square and triangular lattices in dimension $d = 2$ and the BCC, FCC and simple cubic lattice $\mathbb{Z}^3$ in dimension $d = 3$.

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## The equilibrium measure for a non-local dislocation energy

Lucia Scardia

In this talk I presented the results in [7] and [1] on the characterisation of equilibrium measures for non-local and *anisotropic* weighted energies.

For $\alpha \in \mathbb{R}$ we consider the interaction energy

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

defined on probability measures $\mu$, where the interaction potential $W_\alpha$ is given by

$$W_\alpha(x) = -\log|x| + \alpha\frac{x_1^2}{|x|^2}, \qquad x = (x_1, x_2), \tag{2}$$

while the second term in the energy acts as a confinement.

The energy $I_\alpha$ is the continuum limit (via $\Gamma$-convergence) of the discrete interaction energy

$$I_{n,\alpha}(z_1,\dots,z_n) = \frac{1}{n^2}\sum_{i\neq j} W_\alpha(z_i - z_j) + \frac{1}{n}\sum_i |z_i|^2 \tag{3}$$

for $n \to \infty$. The non-local term in (1) describes the macroscopic effect of long-range interactions in the discrete energy (3). Note that $W_1$ is the interaction potential between positive edge dislocations with Burgers vector $\mathbf{e_1}$ (see [4]), and so the energy $I_{n,1}$ (and its continuum limit $I_1$) models the interaction of positive dislocations in the plane in the case of single slip.

We are interested in characterising the minimisers $\mu_\alpha$ of $I_\alpha$. We first focus on $\alpha = 1$. For $\alpha = 1$ the minimiser $\mu_1$ represents the equilibrium dislocation pattern at the mesoscale. Although such a minimiser has not been characterised analytically so far, neither at the micro nor at the mesoscale, it is conjectured to be a vertical wall (see, e.g., [2, 4]). This belief has triggered a considerable interest in dislocation walls in the engineering and mathematical literature, and interactions, upscaled behaviour and dynamics of walls have been thoroughly analysed. We also mention the remarkable result [5] where, starting from a nonlinear dislocation model, vertical walls, 'low-angle grain boundaries', are shown to have the optimal energy scaling in accordance with the celebrated Read-Shockley formula.

Formally, we can see how the interaction term in $I_{1,n}$ can be obtained starting from a dislocation model as the one considered in [5]. Indeed, consider the (linearised) energy

$$E_\varepsilon(\mu_n) = \frac{1}{2}\min_\beta \int_{\Omega\setminus B_\varepsilon(\mathrm{supp}\mu_n)} \mathcal{C}\beta : \beta dx,$$

where $\Omega$ is a bounded domain, $\mathcal{C}$ is the tensor of isotropic elasticity, $\varepsilon > 0$ is the length of the Burger's vector, $\mu_n = \frac{1}{n}\sum\delta_{z_i}$, and the minimum is taken over the strains $\beta$ such that $\mathrm{curl}\beta = \mathbf{e_1}\mu_n$. Roughly speaking, the energy contribution of $E_\varepsilon$ in the vicinity of the dislocations at $\{z_i\}$ is the so-called self-energy, which is constant (although a large constant) under the assumption that $|z_i - z_j| \gg \varepsilon$. The contribution away of the core regions, in the formal limit of $\Omega \to \mathbb{R}^2$, corresponds to

the energy $I_{n,1}$. So, minimising $I_{n,1}$ is very much in the same spirit as minimising $E_\varepsilon$, and it is natural to expect the minimiser of $I_{n,1}$ or $I_1$ to be a vertical structure, similarly as in [5] for $E_\varepsilon$.

This is what we prove in [7]: the minimiser of $I_1$ exists, is unique, and is given by a *one-dimensional, vertical* measure, namely the semi-circle law on the vertical axis

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

This proves the conjecture that positive edge dislocations form vertical structures to minimise their interaction energy. Note that the semi-circle law is well-known in the theory of Random Matrices, as it is the unique minimiser of the logarithmic one dimensional energy

$$I_{\log}(\mu) = -\iint_{\mathbb{R}\times\mathbb{R}} \log|x-y|\,d\mu(x)\,d\mu(y) + \int_{\mathbb{R}} |x|^2\,d\mu(x), \quad \mu \in \mathcal{P}(\mathbb{R}), \tag{4}$$

and represents the average distribution of the eigenvalues of a random matrix (with i.i.d. Gaussian entries) in the Hermitian case (see [6] and [9]). Curiously,

$$I_{\log}(\mu_1) = I_1(\mu_1),$$

namely the $2d$-dislocation energy $I_1$ coincides with the $1d$-logarithmic energy along the measure $\mu_1$ (in fact on every vertical measure, since the anisotropic term vanishes on those measures). Therefore if one could prove that the minimiser of $I_1$ is supported on the vertical axis, then the minimality of the semi-circle law would follow directly from [9].

This is however not the strategy we use in [7]. Our approach consists of two steps: We first prove the strict convexity of $I_1$ on the class of measures with compact support and finite interaction energy. Strict convexity implies uniqueness of the minimiser and the equivalence between minimality and the Euler-Lagrange conditions for $I_1$. As a second step, we show that the semi-circle law satisfies the Euler-Lagrange conditions and hence is the unique minimiser of $I_1$.

The proof of both steps is highly non-trivial. We could not rely on the machinery developed in the classical case of purely logarithmic potentials with external fields (see [8]), which is heavily based on $-\log|\cdot|$ being radially symmetric, and on it being the fundamental solution of the Laplace operator, since $W_1$ is neither. Similarly, although non-local energies are widely used and studied in the mathematical community, and the existence of their ground states and their qualitative properties have received great attention in recent years, the potential is typically required to be radially symmetric, or the singularity to be non-critical, so $W_1$ is not covered by their analysis.

Now, we consider the case of a general $\alpha \in \mathbb{R}$. Note that for $\alpha = 0$, corresponding to the Coulomb potential $W_0 = -\log|\cdot|$, the minimiser of $I_0$ in (1) is well-known and given by the circle law $\mu_0 := \frac{1}{\pi}\chi_{B_1(0)}$ (see, e.g., [3, 8], and the references therein). Although the radial component of the potential in (2) is exactly the Coulomb kernel $W_0$, the presence of the additional anisotropic term for $\alpha = 1$ has then a dramatic effect on the structure of the equilibrium measure.

Unlike $\mu_0$, the support of $\mu_1$ is one-dimensional and its density is not constant. It is then natural to consider the intermediate case of $\alpha \in (0,1)$, where we sort of interpolate between $W_0$ and $W_1$.

In this case we prove in [1] that the minimiser $\mu_\alpha$ of $I_\alpha$ is the (normalised) characteristic function of an ellipse of semi-axes $\sqrt{1 \pm \alpha}$. So $\alpha = 0$ indeed gives back the circle law $\mu_0$, and the case $\alpha = 1$ is singular, in the sense that one of the semi-axes is degenerate. This is indeed the case, as for $\alpha = 1$ we know that the minimiser is one-dimensional, and hence it can be considered as a 'singular' limit case.

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## Molecular dynamics simulations, with applications to quasicrystals

Franz Gähler

An overview of the molecular dynamics simulation technique and its application to the simulation of quasicrystals is given. More details can be found in the review [1]. Molecular dynamics is a low-level simulation technique, in which the equations of motion of an interacting system of particles are integrated numerically. One thereby performs a numerical experiment. The only modelling required is the choice of a suitable interaction model and, to some extent, the choice of an initial structure. For performance reasons, classical interaction potentials are preferred, whenever suitable potentials are available. Such potentials usually have to be constructed for a particular material.

Quite generally, complex intermetallics require potentials with Friedel oscillatations, but already very simple such potentials with just a second minimum, or even only a second maximum, can lead to complex quasicrystal phases. This was first observed by Dzugutov, who found dodecagonal random tiling quasicrystal phases upon slow cooling of a monoatomic liquid [2]. The very same structures, dodecagonal Frank-Kasper phases, actually occur also in many soft-matter quasicrystals. Later, Engel systematically investigated the phase diagram of simple oscillating

potentials, and found a region with decagonal random tiling quasicrystals in two dimensionals [3], and icosahedral quasicrystals in three dimensions [4].

For more realistic quasicrystal structures, also more realistic potentials are required. These are usually fitted to reproduce forces and energies of reference structures computed in ab-initio DFT simulations [5]. In this way, quantum mechanical information is made available also to classical simulations. As an illustrative example, simulations of Al diffusion in decagonal AlNiCo quasicrystals are presented. These have been performed with two kinds of potentials, derived analytically from density functional theory on the one hand, and fitted to ab-initio data on the other hand. Results for the two potential types are compared and discussed (see also [1]).

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## Dislocation lines in three-dimensional solids at low temperature, part I


Franz Merkl

(joint work with Roland Bauerschmidt, Diana Conache, Markus Heydenreich, Silke Rolles)


We propose a model for three-dimensional solids on a mesoscopic scale with a statistical mechanical description of dislocation lines in thermal equilibrium. The model has a linearized rotational symmetry, which is broken by boundary conditions. We show that this symmetry is spontaneously broken in the thermodynamic limit at small positive temperatures. This part I is continued by the talk of Diana Conache.

In a linear and continuum approximation, a deformed solid is modeled by a map $w : \mathbb{R}^3 \to \mathbb{R}^{3\times 3}$, describing locally the linear part of the deformation map.

**Total energy in the model.** The leading order total energy $H(w)$ of a deformed solid is modeled to consist of

$$H(w) = H_{\mathrm{el}}(w) + H_{\mathrm{disl}}(d_1 w), \tag{1}$$

with an "elastic" part

$$H_{\mathrm{el}}(w) = \int_{\mathbb{R}^3} F(w(x) + w(x)^t)\, dx, \quad F(U) = \frac{\lambda}{2}(\operatorname{tr} U)^2 + \mu |U|^2, \tag{2}$$

with Lamé coefficients $\lambda$ and $\mu$, and a local "dislocation"part $H_{\mathrm{disl}}(d_1 w)$, depending on the exterior derivative

$$b_{ijk} := (d_1 w)_{ijk} = \partial_i w_{jk} - \partial_j w_{ik} \tag{3}$$

of $w$, describing the Burgers vector density of dislocations in the solid.

**Coarse-grained model for dislocation lines.** Dislocation lines are only allowed in the set $\Lambda$ of undirected edges of a *mesoscopic* lattice in $\mathbb{R}^3$. Let $V_\Lambda$ denote its vertex set. As a lattice, the graph $(V_\Lambda, \Lambda)$ is of bounded degree. To model boundary conditions, we only allow dislocation lines on a finite subgraph $G = (V, E)$ of $(V_\Lambda, \Lambda)$, ultimately taking the thermodynamic limit $E \uparrow \Lambda$. The graph $(V_\Lambda, \Lambda)$ is *not* intended to describe the atomic structure of the solid, as it lives on a mesoscopic scale. Rather, it is just a tool to introduce a coarse-grained structure which eventually makes the model discrete.

**From dislocation lines to Burgers vector densities.** We model the Burgers vector densities with the help of vector-valued currents flowing along the edges of $\Lambda$, but smeared out with a smooth, compactly supported form function $\varphi : \mathbb{R}^3 \to \mathbb{R}_0^+$ with total mass $\|\varphi\|_1 = 1$ and $\varphi(0) > 0$. Let $\Gamma \subset \mathbb{R}^3$ be a lattice, interpreted as the *microscopic* lattice (scaled to length scale 1). It should not be confused with the *mesoscopic* lattice $V_\Lambda$. The Burgers vectors on the finite subgraph $G = (V, E)$ are encoded by a family $I = (I_e)_{e \in E} \in \Gamma^E$ of vector-valued currents flowing through the edges in counting direction. We set

$$\mathcal{I} = \mathcal{I}(E) = \{I \in \Gamma^E : \ \text{Kirchhoff's node rule holds for } I\}. \tag{4}$$

For $e = \{x, y\} \in \Lambda$, let $\lambda_e : \mathrm{Borel}(\mathbb{R}^3) \to \mathbb{R}_0^+$ denote the 1-dimensional Lebesgue measure on the line segment $[x, y]$. For every edge $e \in E$, let $n_e \in \mathbb{R}^3$ denote the unit vector pointing in its counting direction. Before smearing out, we model the vector-valued current associated to the current configuration $I$ to be described by the following matrix-valued measure $J(I) : \mathrm{Borel}(\mathbb{R}^3) \to \mathbb{R}^{3\times 3}$ on $\mathbb{R}^3$, supported on the union of all edges:

$$\mathrm{Borel}(\mathbb{R}^3) \ni B \mapsto J_{jk}(I)(B) = \sum_{e \in E} (n_e)_j (I_e)_k \lambda_e(B). \tag{5}$$

The Burgers vector density $b(I)$ associated to $I$ is then modeled by convolving $J(I)$ with the form function $\varphi$ and contracting it with the totally antisymmetric tensor $\epsilon_{ijk} = \det(e_i, e_j, e_k)$ with the standard unit vectors $e_i \in \mathbb{R}^3$:

$$b_{ijk}(I) = \sum_{l=1}^{3} \epsilon_{ijl} \varphi * \sum_{e \in E} (n_e)_l (I_e)_k \lambda_e. \tag{6}$$

**Dislocation part of the energy:** For the dislocation part of the total energy, we make the following assumptions:

- *Symmetry:* $H_{\mathrm{disl}}(b(I)) = H_{\mathrm{disl}}(b(-I))$ for all $I \in \mathcal{I}$.
- *Locality:* For $I = I_1 + I_2$ with $I_1, I_2 \in \mathcal{I}$ such that no edge in $\operatorname{supp} I_1$ has a common vertex with another edge in $\operatorname{supp} I_2$ we have $H_{\mathrm{disl}}(b(I)) = H_{\mathrm{disl}}(b(I_1)) + H_{\mathrm{disl}}(b(I_2))$. In particular, $H_{\mathrm{disl}}(0) = 0$.

- *Lower bound:* For some constant $c > 0$ and all $I \in \mathcal{I}$,

$$H_{\mathrm{disl}}(b(I)) \geq c \sum_{e \in E} |I_e|. \tag{7}$$

**Elastic part of the Hamiltonian of the model.** We define

$$H^*_{\mathrm{el}}(I) = \inf_{\substack{w \in C^\infty_c(\mathbb{R}^3, \mathbb{R}^{3\times 3}): \\ d_1 w = b(I)}} H_{\mathrm{el}}(w) \tag{8}$$

for all $I \in \mathcal{I}$. The condition that $w$ is compactly supported reflects the boundary condition: Close to infinity the solid must not be moved away from its reference location. The symmetry with respect to linearized global rotations is reflected by the fact $H_{\mathrm{el}}(w) = H_{\mathrm{el}}(w + w_{\mathrm{const}})$ for every constant antisymmetric matrix $w_{\mathrm{const}} \in \mathbb{R}^{3\times 3}$. Only the boundary condition, i.e. only the restriction that $w$ should have compact support, breaks this global symmetry.

**Partition sum and thermal measure:**

$$Z_{\beta,E} := \sum_{I \in \mathcal{I}(E)} e^{-\beta(H^*_{\mathrm{el}}(I) + H_{\mathrm{disl}}(b(I)))}, \tag{9}$$

$$P_{\beta,E} := \frac{1}{Z_{\beta,E}} \sum_{I \in \mathcal{I}(E)} e^{-\beta(H^*_{\mathrm{el}}(I) + H_{\mathrm{disl}}(b(I)))} \delta_I, \tag{10}$$

here $\delta_I$ denotes the Dirac measure in $I \in \mathcal{I}$.

**Comparison to the rotator model.** Purely elastic deformations in the present model correspond to "spin wave" contributions in the rotator model, while deformations induced by the Burgers vectors correspond to "vortex" contributions. In our model, the purely elastic deformations are orthogonal to the deformations induced by the Burgers vectors in a suitable inner product. Therefore, we do not model the purely elastic part stochastically. It would not be relevant for our purposes, because in a linearized model, it is expected to be independent of the Burgers vectors anyway.

**Statement of results.** The following lemma shows that any sequence of smooth configurations satisfying the boundary conditions with prescribed Burgers vectors has a limit $w^*$ in $L^2$ provided that the energy is approaching the infimum of all energies within the class.

**Lemma: Compactly supported approximations of the minimizer.** *For any $I \in \mathcal{I}$, there is a bounded smooth function $w^*(\cdot, I) \in L^2(\mathbb{R}^3, \mathbb{R}^{3\times 3})$ such that for any sequence $(w^n)_{n\in\mathbb{N}}$ in $C^\infty_c(\mathbb{R}^3, \mathbb{R}^{3\times 3})$ with $d_1 w^n = b(I)$ for all $n \in \mathbb{N}$ and $\lim_{n\to\infty} H_{\mathrm{el}}(w^n) = H^*_{\mathrm{el}}(I)$ we have $\lim_{n\to\infty} \|w^n - w^*(\cdot, I)\|_2 = 0$.*

The following theorem shows that the breaking of linearized rotational symmetry $w \rightsquigarrow w + w_{\mathrm{const}}$ induced by the boundary conditions persists in the thermodynamic limit $E \uparrow \Lambda$, provided that the inverse temperature $\beta$ is large enough.

**Theorem: Spontaneous breaking of linearized rotational symmetry.** *There is a constant $c_1 = c_1(\Gamma, \Lambda, c) > 0$ such that for all $\beta$ large enough and for all $t \in \mathbb{R}$,*

$$\inf_{E \Subset \Lambda} \inf_{x,y \in \mathbb{R}^3} \min_{i,j \in [3]} E_{P_{\beta,E}} \Big[ e^{it(w^*_{ij}(x,I) - w^*_{ij}(y,I))} \Big] \geq \exp\Big\{ - \frac{t^2}{2}\, e^{-c_1 \beta} \Big\}, \tag{11}$$

*and consequently*

$$\sup_{E \Subset \Lambda} \sup_{x,y \in \mathbb{R}^3} \max_{i,j \in [3]} \mathrm{Var}_{P_{\beta,E}} \big( w^*_{ij}(x,I) - w^*_{ij}(y,I) \big) \leq e^{-c_1 \beta}. \tag{12}$$

The presentation of Diana Conache provides the key ingredients for the proof of this theorem. Details are given in reference [1].

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## Dislocation lines in three-dimensional solids at low temperature, part II

Diana Conache

(joint work with Roland Bauerschmidt, Markus Heydenreich, Franz Merkl, Silke Rolles)

This talk is a continuation of the one by Franz Merkl and is based on [2]. The aim will be to prove the main theorem stated in his abstract and we therefore use the notation introduced there. Namely, we study the statistical mechanical properties of a random Burgers vector configuration, in the spirit of the Fröhlich–Spencer approach to the Villain model introduced in [1]. In particular, we show that the breaking of the linearized rotational symmetry persists in the thermodynamic limit.

In this sense, we consider the Sine-Gordon transformation of the Boltzmann factor of the elastic Hamiltonian $H_{\mathrm{el}}$, namely we introduce an auxiliary Gaussian field $\phi = (\phi_e)_{e \in E}$ in order to get rid of the non-locality of $H_{\mathrm{el}}$:

$$\mathbb{E}\big[\mathrm{e}^{\mathrm{i}\langle \phi, I \rangle}\big] = \mathrm{e}^{-\beta H^*_{\mathrm{el}}(I)}. \tag{1}$$

For any observable of the form $\mathcal{I} \ni I \mapsto \langle \sigma, I \rangle$ with $\sigma \in \mathbb{R}^E$ and $\beta > 0$, we define

$$\mathcal{Z}_{\beta,\phi} := \sum_{I \in \mathcal{I}} \mathrm{e}^{\mathrm{i}\langle \phi, I \rangle} \mathrm{e}^{-\beta H_{\mathrm{disl}}(I)}, \tag{2}$$

$$Z_\beta(\sigma) := \sum_{I \in \mathcal{I}} \mathrm{e}^{\mathrm{i}\langle \sigma, I \rangle} \mathrm{e}^{-\beta (H^*_{\mathrm{el}}(I) + H_{\mathrm{disl}}(I))} = \mathbb{E}\left[ \mathcal{Z}_{\beta, \sigma + \phi} \right]. \tag{3}$$

We prove via a cluster expansion a Gaussian lower bound for the Fourier transform of an observable with respect to the thermal measure, as follows. For $I \in \mathcal{I}$ we define its size to be $\operatorname{size} I := \|I\|_1 + \operatorname{diam} \operatorname{supp} I$ and note that there exists a

positive constant $c_4$ such that $H_{\mathrm{disl}}(I) \geq c_4 \mathrm{size}\, I$. An important observation at this point is that all constants that appear in our estimates are only dependent on the model, namely on the two lattices $\Lambda$ and $\Gamma$, on the constant $c$ appearing in the lower bound of $H_{\mathrm{disl}}$ and on the form function $\varphi$.

We denote by $\mathcal{J}$ the set of all $I \in \mathcal{I}$ with compact support and introduce the weights $K(J) := \mathrm{e}^{-\beta c_4 \mathrm{size}\, J}$, for $J \in \mathcal{J}$, and size function $a : \mathcal{J} \to \mathbb{R}_{>0}$, $a(J) := \beta c_5 \eta |\mathrm{supp}\, J|$, for $J \in \mathcal{J}$. We prove via a Peierls argument that the conditions for convergence of the cluster exansion are satisfied. We then show that the partial partition sums defined by

$$z(\beta, I) := \sum_{n=1}^{\infty} \sum_{(I_1,\ldots,I_n)\in\mathcal{J}^n} U(I_1,\ldots,I_n) 1_{\{I_1+\cdots+I_n=I\}} \prod_{j=1}^{n} \mathrm{e}^{-\beta H_{\mathrm{disl}}(I_j)} \in \mathbb{R}, \tag{4}$$

where $U$ are the Ursell functions, have exponential decay, despite some exponential corrections. Namely, the following lemma holds:

**Lemma: (Exponential decay of partial partition sums.)** *For all sufficiently large $\beta > 0$, the following holds with the positive constants $c_4$ and $c_7$:*

$$\sup_{E\Subset\Lambda} \sup_{o\in E} \sum_{\substack{I\in\mathcal{I}:\\ o\in supp\, I}} \mathrm{e}^{\beta c_4 size\, I} |z(\beta, I)| \leq \mathrm{e}^{-\beta c_7}. \tag{5}$$

Next, we apply a cluster expansion with $K(I, \phi) := \mathrm{e}^{\mathrm{i}\langle\phi, I\rangle} \mathrm{e}^{-\beta H_{\mathrm{disl}}(I)}$ to obtain a representation of $\mathcal{Z}_{\beta,\phi}$.

**Lemma: (Partition sums in the presence of $\phi$.)** *For all $\beta$ large enough the following identity holds for any $\phi \in \mathbb{R}^E$:*

$$0 < \mathcal{Z}_{\beta,\phi} = \exp\left(\sum_{I\in\mathcal{I}} z(\beta, I) \mathrm{e}^{\mathrm{i}\langle\phi, I\rangle}\right) = \exp\left(\sum_{I\in\mathcal{I}} z(\beta, I) \cos\langle\phi, I\rangle\right) < \infty. \tag{6}$$

This representation is now used to give a bound for the Fourier transform of the observable

**Lemma: (Gaussian lower bound for Fourier transforms.)** *For all $\beta$ large enough, the following holds for any observable $\sigma \in \mathbb{R}^E$:*

$$\mathbb{E}_{P_\beta}\left[\mathrm{e}^{\mathrm{i}\langle\sigma, I\rangle}\right] \geq \exp\left(-\frac{1}{2}\sum_{I\in\mathcal{I}} |z(\beta, I)| \langle\sigma, I\rangle^2\right). \tag{7}$$

**Choice of the observable:** For $x, y \in \mathbb{R}^3$, we choose $\sigma(x, y) = (\sigma_{ij}(x, y))_{i,j\in[3]} \in (\mathbb{R}^E)^{[3]\times[3]}$ satisfying the equation

$$\langle\sigma_{ij}(x, y), I\rangle = w^*_{ij}(x, I) - w^*_{ij}(y, I) \quad \text{for all } I \in \mathcal{I}.$$

By the previous lemma, in order to prove the main result one needs to bound $|z(\beta, I)| w^*_{ij}(x, I)^2$. This is done as follows.

**Lemma: (Bounding the observable.)** *There are a function* $W : \Lambda \times \mathbb{R}^3 \times \bigcup_{E \Subset \Lambda} (\mathcal{I}(E) \setminus \{0\}) \to \mathbb{R}_{\geq 0}$ *with*

$$c_{11} := \sup_{x \in \mathbb{R}^3} \sup_{E \Subset \Lambda} \sup_{I \in \mathcal{I}(E) \setminus \{0\}} \sum_{o \in \Lambda} W(o, x, I) < \infty \tag{8}$$

*and* $\beta_1 > 0$ *such that for all* $E \Subset \Lambda$, $I \in \mathcal{I}(E) \setminus \{0\}$, $o \in \operatorname{supp} I$, $x \in \mathbb{R}^3$, $\beta \geq \beta_1$ *and* $i, j \in [3]$ *we have*

$$w_{ij}^*(x, I)^2 \leq W(o, x, I) \mathrm{e}^{\beta c_4 \operatorname{size} I}. \tag{9}$$

The proof follows by a variant of the dipole expansion from magnetostatics.

The main result follows easily by a direct application of the Gaussian lower bound and the bound on the observable from the previous lemma.

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## Order versus disorder from a diffraction perspective

Michael Baake

The diffraction measure of a point set or pattern in Euclidean space is a natural tool to detect various forms of long-range positional order or disorder. This has been a powerful tool in crystallography for over 100 years, which has recently been developed also from a more mathematical point of view [9]; see [3, Chs. 8 and 9] for a systematic exposition. In recent times, diffraction has become important in the context of aperiodic systems as well; see [12, 7, 3, 10, 4] for general background.

Concretely, taking up from the initial overview given by U. Grimm, we assume that a translation-bounded Radon measure on $\mathbb{R}^d$ is given, such as the Dirac comb $\omega = \sum_{x \in \varLambda} \delta_x$ of a uniformly discrete point set $\varLambda \subset \mathbb{R}^d$. Then, its *autocorrelation* $\gamma_\omega$ is given by

$$\gamma_\omega \,=\, \omega \circledast \widetilde{\omega} \,:=\, \lim_{r \to \infty} \frac{\omega_r * \widetilde{\omega_r}}{\mathrm{vol}(B_r)} \,,$$

where $B_r$ denotes the ball of radius $r$ around 0, provided the limit exists (which can usually be ensured by mild assumptions or some ergodicity property). Then, $\gamma_\omega$ is a positive definite measure, which is thus Fourier transformable. Its Fourier transform, $\widehat{\gamma_\omega}$, is a positive measure, known as the *diffraction measure* of $\omega$.

By the Lebesgue decomposition theorem, one has the splitting

$$\widehat{\gamma_\omega} \,=\, \big(\widehat{\gamma_\omega}\big)_{\mathsf{pp}} + \big(\widehat{\gamma_\omega}\big)_{\mathsf{sc}} + \big(\widehat{\gamma_\omega}\big)_{\mathsf{ac}}$$

into the pure point (pp) part, which consists of at most countably many Dirac measures (or Bragg peaks), the absolutely continuous (ac) part, which is described by a locally integrable Radon–Nikodym density relative to Lebesgue measure (also known as diffuse background), and the singular continuous (sc) part, which is

concentrated to an uncountable Lebesgue null set. Usually, Bragg peaks signify a coherent long-range positional order, while the diffuse background is a strong indicator of disorder with entropic nature (though the Rudin–Shapiro sequence is a classic counterexample to this stereotype). The sc-part is somewhere in between, and often an indicator of long-range correlations of a different nature, for instance one with a more complex behaviour as a function of the system size.

In this survey talk, the basic structures were explained, with examples from perfect crystals and 'nice' cut and project sets, compare [11, 3], as used to model perfect quasicrystals (of energetically stabilised type). In a nutshell, all these results essentially rely on the Poisson summation formula for lattices, which can be written as

$$\widehat{\delta_{\varGamma}} \,=\, \mathrm{dens}(\varGamma)\, \delta_{\varGamma^*}$$

for a lattice $\varGamma$ in $\mathbb{R}^d$ and its dual, $\varGamma^*$. This extends to examples of number-theoretic origin [11, 5]. Various further examples with concrete expressions were discussed, including the classic Thue–Morse chain with singular diffraction of mixed type, where the sc-part of the diffraction measure is given by an infinite Riesz product,

$$\bigl(\widehat{\gamma}\bigr)_{\mathsf{sc}} \,=\, \prod_{\ell \geqslant 0} \cos\bigl(2^{\ell+1}\pi(.)\bigr),$$

with convergence in the vague topology; see [3, Sec. 10.1] for details. The associated inverse problem increases in complexity as the spectrum shows continuous components, which was illustrated by the Bernoullisation of the Rudin–Shapiro chain, taken from [3, Sec 11.2.2]. This also marked the crossover to the corresponding theory for general point processes in $\mathbb{R}^d$, as discussed in [2, 1, 6] and covered in more detail in H. Kösters' contribution to this workshop.

As one application, an argument was presented to corroborate the decay of long-range order in a one-dimensional model with Lennard–Jones type potential, presented by S. Jansen and B. Schmidt during the workshop. Here, the essence emerges from the observation that the sum

$$1 + \sum_{m=1}^{M} \exp\Bigl(2\pi\mathrm{i} \sum_{\ell=1}^{m} X_\ell\Bigr),$$

where the $X_j$ are i.i.d. random variables with values in $\mathbb{R}_+$, concentrates around 0 as $M$ grows, and suppresses other Bragg peaks, because its absolute square appears as an overall factor in the diffraction measure of the model.

Another application of diffraction methods is the detection of grain boundaries in (almost) single crystals. This leads to the classification problem of coincidence site lattices (CSLs) and modules; see [8] for a review and a comprehensive list of the existing literature. For 'nice' lattices (with large symmetry groups, say) in dimensions $d \leqslant 4$, the CSLs can be classified, and an efficient enumeration of the number of such lattices of a given index can be achieved via Dirichlet series generating functions and their expression in terms of Dedekind zeta functions of algebraic number fields and quaternion algebras.

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## Fourier spectra of quasipatterns and quasicrystals

Alastair M. Rucklidge
(joint work with Andrew J. Archer, Daniel J. Ratliff, Priya Subramanian)

Two-dimensional quasipatterns with 12-fold rotation symmetry are the soft analogues of the metallic quasicrystals that can be found in certain alloys. In the early 1990s [1, 2], quasipatterns were identified in the Faraday wave experiment, in which a thin layer of liquid is subjected to vertical vibrations strong enough that standing waves form when the flat surface becomes unstable. In models of soft matter, a similar transition corresponds to the formation of a crystal from a liquid. In the early 2000s [3], structures with 12-fold rotation symmetry were identified in a polymeric material. Here, large cone-shaped branched polymers self-assemble into spheres, which in turn assemble into quasicrystals that have 12-fold rotation symmetry in one plane while being periodic in the third dimension. The Faraday wave example is characterised as being more wave-like than particle-like, and here we use the word *quasipattern* to mean a structure with non-crystallographic symmetry (here, 12-fold rotation) that can be well approximated by a linear superposition of waves. In contrast, *quasicrystals* are better described as non-crystallographic arrangements of particles (or delta functions). The polymeric example, in which the density is not far from uniform, may be in between these two limits.

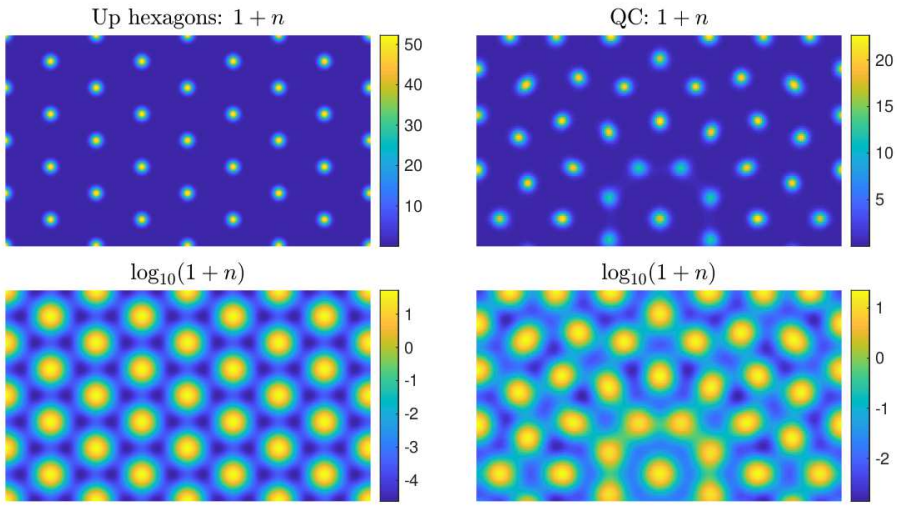


FIGURE 1. Triangular (also known as up hexagons, left) and approximate quasipattern (right) solutions of (1). The common parameters are $R = 5.0962$ and $\rho_0\beta\epsilon = 0.2455$. For the triangles, $\mu = 10.052$ in an $8 \times \frac{8}{\sqrt{3}}$ wavelengths domain; for the quasipatterns, $\mu = 4.0395$ in an $8 \times 8$ domain, partly shown.

Here, we focus on a description of soft matter (polymeric) crystallisation based on Density Functional Theory (DFT), which can span the wave-like to particle-like description of crystals, and in which entropy and energy are both taken into account. The density of centres of mass of soft particles is described by a field $\rho(\boldsymbol{x})$, and the Helmholtz free energy $\mathcal{F}$ for a collection of particles interacting through a pair potential $V(r)$ is

$$\mathcal{F} = kT\int \rho(\boldsymbol{x})\left(\log\rho(\boldsymbol{x}) - 1\right)\,\mathrm{d}\boldsymbol{x} + \frac{1}{2}\iint \rho(\boldsymbol{x})V(|\boldsymbol{x}-\boldsymbol{x}'|)\rho(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{x}',$$

where $T$ is the temperature and $k$ is Boltzmann's constant. The first term represents the entropy of non-interacting particles, and the second term is the energy of interaction. The free energy is minimised subject to the constraint of the total number of particles being constant. The chemical potential $\mu$ is the Lagrange multiplier for this constraint, so the equation that is solved is

$$\log(1+n(\boldsymbol{x})) + \rho_0\beta\int V(|\boldsymbol{x}-\boldsymbol{x}'|)n(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}' - \mu = 0, \tag{1}$$

where $\beta = 1/kT$ and the density is written in terms of a background density $\rho_0$ and a perturbation $n(\boldsymbol{x})$: $\rho = \rho_0(1+n)$.

Potentials $V(r)$ can be devised to make 12-fold quasipatterns the lowest (or nearly lowest) energy state [4, 5]. Here we focus on existence rather than stability,

and so we choose a simple potential $V(r) = \epsilon \exp((r/R)^4)$, where $\epsilon$ controls the strength of the interaction and $R$ its length scale. Triangles (figure 1, left) have the lowest free energy, but 12-fold approximate quasipatterns (figure 1, right) can also be found close to the transition point.

Small-amplitude approximate solutions to (1) can be found: if $\mu = \mathcal{O}(\epsilon)$, where $\epsilon \ll 1$, we scale $\mu \to \epsilon\mu$ and write

$$n = \epsilon n_1 + \epsilon^2 n_2 + \dots$$

This formal power series for quasipatterns does not converge for related problems [6], though asymptotic approximations can be found in a function space that requires the amplitudes of Fourier modes to decay at high order [7, 8]. Let the 12 basic wave-vectors of the quasipattern be $\boldsymbol{k}_1, \dots, \boldsymbol{k}_{12}$, where

$$\boldsymbol{k}_j = \left(\cos\left(\frac{2\pi}{12}(j-1)\right), \sin\left(\frac{2\pi}{12}(j-1)\right)\right),$$

and let $\boldsymbol{m} = (m_1, \dots, m_{12})$, with $m_j$ being non-negative integers, let $|\boldsymbol{m}| = \sum_j m_j$, and let $\boldsymbol{k}_{\boldsymbol{m}} = \sum_j m_j \boldsymbol{k}_j$. With these, define the truncated quasilattice $\Gamma_M$ to be the sum of all integer combinations of up to $M$ wave-vectors:

$$\Gamma_M = \{\boldsymbol{k}_{\boldsymbol{m}} \text{ such that } |\boldsymbol{m}| \le M\},$$

so $\Gamma_1$ is the set of the original 12 vectors, $\Gamma_2$ includes these and all pairwise sums, and so on. In the limit, the quasilattice of all integer combinations of the 12 wave-vectors forms a dense set $\Gamma$ [6].

Braaskma *et al.* [8] proved that quasipattern solutions of a partial differential equation related to (1) can be found in a Hilbert space $\mathcal{H}_s$ defined by

$$\mathcal{H}_s = \left\{ n(\boldsymbol{x}) = \sum_{\boldsymbol{k}\in\Gamma} n_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}} : ||n||_s^2 = \sum_{\boldsymbol{k}\in\Gamma} \left(1 + N_{\boldsymbol{k}}^2\right)^s |n_{\boldsymbol{k}}|^2 < \infty \right\},$$

where $s > 4$, and the order $N_{\boldsymbol{k}}$ of a wave-vector is the smallest $M = |\boldsymbol{m}|$ such that $\boldsymbol{k} \in \Gamma_M$. In this space, amplitudes of Fourier modes $\exp(i\boldsymbol{k}_{\boldsymbol{m}} \cdot \boldsymbol{x})$ decay both as $|\boldsymbol{k}_{\boldsymbol{m}}| \to \infty$ and as $|\boldsymbol{m}| \to \infty$.

The triangle and quasipattern shown in figure 1 are members of families of solutions of (1) parameterised by the parameter $\mu$. As $\mu$ increases, the quasipattern becomes less wave-like and more particle-like, in the sense that the density (top row of figure 1) varies over increasingly many orders of magnitude and the maxima become larger and sharper as $\mu$ increases. Nonetheless, for both triangles and the quasipattern, the *logarithm* of the density (bottom row of figure 1) remains smooth. The reason that $\log(1+n)$ is smooth is that the integral in (1) damps high-wavenumber Fourier modes: even as the density becomes sharper, the logarithm of the density remains well behaved. This is reflected in the Fourier spectra of the two fields: amplitudes of the Fourier modes of the logarithm of the density drop of sharply, while the Fourier spectrum of the density becomes flatter as $\mu$ increases.

Perhaps this dichotomy will allow a connection to be made to aperiodic structures derived from tilings, which have Fourier spectra that do not decay at high

wavenumber [9]. This connection may clarify the connection between these wave-like quasipatterns and quasicrystals characterised by aperiodic arrangements of atoms, tilings or cut-and-project sets.

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## Long-range order in atomistic equilibrium distributions with dislocations


Florian Theil

(joint work with Alessandro Giuliani)


The Ariza–Ortiz energy [1] is a discrete model for elastic crystals with dislocations. To define the model properly we need the concept of cellular lattice complexes.

### 1. Notation

We assume that $\mathcal{L}$ is a three-dimensional lattice. The domains of the elastic configurations with dislocations are $p$-dimensional cells, denoted by $E_p$.

- Oriented vertices $E_0$ are a finite subset of $\mathcal{L}$.
- Oriented edges $E_1$ are vertex pairs,
- Oriented faces $E_2$ are polygons where the sides are a subset of the $E_1$,
- Oriented volumes $E_3$ are a tessellation of $\mathbb{R}^3$ such that the boundary of each volume is a collection of faces.

A key property of the cells is that the boundary of each cell $e \in E_p$ is a subset of $E_{p-1}$. It is important to remember that the boundary of an oriented cell consists of a collection of oriented cells, for example the boundary of an edge are two oppositely oriented vertices.

Maps from $E_p$ to $\mathbb{R}^3$ which are equivariant under the change of orientation are called $p$-forms:

$$\Omega_p = \{u : E_p \to \mathbb{R}^3 \text{ s.t. } u(-e) = -u(e) \text{ for all } e \in E_p\},$$

where $-e_p$ denotes the cell $e_p$ with opposite orientation. The motivation for introducing $p$-forms is that that we can define the exterior derivative operators $\mathrm{d}_p : \Omega_p \to \Omega_{p+1}$ by the formula

$$\mathrm{d}_p u(f) = \sum_{e \in \partial f} u(e).$$

We assume from now on that $\mathcal{L}$ is the 3-dimensional face centered cubic lattice:

$$\mathcal{L} = \left\{ \sum_{j=1}^{3} l_j b_j \ : \ l \in \mathbb{Z}^3 \right\} \text{ with basis vectors } b_1 = \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \ b_2 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \ b_3 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix},$$

and $E_1$ are the nearest neighbor pairs. The Ariza–Ortiz energy is a functional on $\Omega_0 \times \Omega_1$:

$$H_{\mathrm{AO}}(u, \sigma) = \frac{1}{2} \sum_{e \in E_1} \left[ \mathrm{d}e \cdot (\mathrm{d}u(e) - \sigma(e)) \right]^2,$$

with the convention that d$e$ is an abbreviation for $\mathrm{d}\,\mathrm{Id}(e)$ where $\mathrm{Id} \in \Omega_0$ is the identity map. The 1-form $\sigma$ is called slip field and assumes only values in $\mathcal{L}$. The 0-form $u$ is called displacement. The case of the face centered cubic lattice is motivated by a particularly simple notation because it suffices to consider only nearest neighbor interactions. Of course it is possible to consider less restrictive settings as well.

## 2. Symmetries

We observe that $H_{\mathrm{AO}}$ is invariant under a large group of transformations.

Classical models with continuous spins such as the $X - Y$-model or the Villain model have two symmetries: Continuous translations and discrete translations.

The Ariza–Ortiz energy is invariant under the classical symmetries and an additional symmetry which yields new and interesting configurations with low energy.

**Proposition 2.1.** *The Ariza–Ortiz energy $H_{\mathrm{AO}}$ admits the following invariance:*

$$H(u, \sigma) = H(u + v + s + t, \sigma + \mathrm{d}v)$$

*for all $u, v, s, t \in \Omega_0$ and $\sigma \in \Omega_1$ if $t$ is constant and there exists a skew-symmetric $3 \times 3$ matrix $S$ such that $s(x) = S\,x$ for all $x \in E_0$.*

**Remark 2.2.** *The interpretation of the symmetries is that*

- *$t$ generates continuous translations,*
- *$s$ generates linearized rotations,*
- *$v$ generates discrete translations (lattice slips).*

### 3. Main result

We consider the Boltzmann–Gibbs measure

$$P(u,\sigma) = \frac{1}{Z(\beta)} \exp(-\beta\, H(u,\sigma)),$$

where $Z(\beta)$ is the partition function, $u \in \Omega_0$ and $\sigma \in \Omega_1/\sim$ with the convention that

(1) $\sigma$ is lattice valued, i.e. $\sigma(e) \in \mathcal{L}$ for each bond $e$.
(2) Two slip fields $\sigma$ and $\sigma'$ are equivalent if $\sigma - \sigma'$ is exact (i.e. $\sigma - \sigma' = \mathrm{d}v$ for some $v \in \Omega_0$).

Our main result is that the Boltzmann-Gibbs measure breaks the translational symmetry of the energy if the temperature is low.

**Theorem 3.1** (In preparation 2019)**.** *Let $b \in \mathcal{L}^*$ be an element of the reciprocal lattice. Then*

$$\lim_{|x-x'|\to\infty} \lim_{|E_0|\to\infty} \mathbb{E}_\beta(\cos((u(x) - u(x')) \cdot b)) = 1 + O(\beta^{-1}), \qquad \beta \ll 1$$

This result has been previously established by Fröhlich and Spencer in [2] for models without rotational invariance like the $X - Y$ model. Franz Merkl et al studied a mesoscopic version of this model which is invariant under linearized rotations, [3]. They establish the weaker notion of orientational order.

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## Percolation of two-dimensional hard disks

Alexander Magazinov

How closely can we pack unit disks in the Euclidean plane? A result, generally attributed to Thue [6], asserts that the density of any packing (informally, the number of centers per unit area) is at most $\frac{1}{2\sqrt{3}}$ (see also [3]). The packing, where the centers of the disks are the points of a triangular lattice with edges of triangles equal to 2, realizes the maximal density. But one can ask the following question — are there properties of the triangular lattice that are retained by packings of slightly sub-optimal density (say, $\frac{1}{2\sqrt{3}} - \delta$)?

Let us connect two centers of a packing by an edge if the distance between them is at most $2 + \varepsilon$. Is it true that the resulting graph has an infinite connected component? Bowen, Lyons, Radin and Winkler [2] explicitly conjectured that an infinite connected component can be found almost surely in any model obtained

as a weak-$*$ limit ($N \to \infty$) of a random $N\mathbb{Z}^2$-periodic packings with density $d_N$, provided that $\liminf_{N\to\infty} d_N > \frac{1}{2\sqrt{3}} - \delta(\varepsilon)$.

Aristoff [1] addressed a similar question to that of [2]: does percolation at distance $2+\varepsilon$ occur almost surely for Gibbs states of the hard-disk model if the intensity parameter $\lambda$ satisfies $\lambda > \lambda(\varepsilon)$? Aristoff managed to provide a positive answer for $\varepsilon > 1$. Passing from intensity to density is indeed relevant; the former has control over the latter (see [5, Subsection 2.2 and Appendix A]).

In this talk we focus on generalizing of Aristoff's result by eliminating the restriction $\varepsilon > 1$. This result strongly supports the conjecture by Bowen, Lyons, Radin and Winkler, although the definition of a model just by density, as in [2], may, a priori, be less restrictive than the definition via the Grand canonical ensemble.

Define

$$\Omega := \{\xi \subset \mathbb{R}^2 : \|x - y\| > 2 \text{ for all } x, y \in \xi,\ x \neq y\}.$$

Let $D \subset \mathbb{R}^2$ be a bounded open set and let $\zeta \in \Omega$. Assume that $\lambda$ is a positive real number. Consider the Poisson point process $\eta$ in $D$ with intensity $\lambda$. With this notation, the *Poisson hard-disk model* on $D$ with intensity $\lambda$ and boundary conditions $\zeta$ is, by definition, the random point set

$$\eta^{[\lambda]}(D, \zeta) := \big(\eta \cup (\zeta \setminus D)\big)\,\big|_{\eta\cup(\zeta\setminus D)\in\Omega}.$$

(Note that the conditioning implies $\eta^{[\lambda]}(D, \zeta) \in \Omega$ a.s.)

The random set $\eta^{[\lambda]}(D, \zeta)$ will be treated as the set of centers for a random packing of unit disks.

Let a packing of unit disks be given by the set $\xi \in \Omega$ of its centers. We denote by $G_\varepsilon(\xi)$ the above mentioned graph, where the edges connect each pair of centers at distance at most $2 + \varepsilon$.

Now, using the notation $Q_N := [-N, N]^2 \subset \mathbb{R}^2$, the main result of the talk can be stated as follows.

**Theorem.** *For any $\varepsilon > 0$ there exists a positive number $\lambda_0$ such that the following holds. For every $\lambda > \lambda_0$, $M > 10$ and $L > 3M$, and for arbitrary boundary conditions $\zeta \in \Omega$ one has*

$$\Pr\Big(G_\varepsilon\left(\eta^{[\lambda]}(Q_L, \zeta)\right) \text{ contains a connected component } \Gamma \text{ such that } V(\Gamma) \cap Q_M \neq \emptyset \text{ and } V(\Gamma) \cap Q_{L-M} \neq \emptyset\Big) \geq 1 - e^{-cM},$$

*where $c$ is a positive constant depending only on $\varepsilon$.*

In other words, for a Poisson hard disk model of sufficiently high intensity in a large square box $Q$ there is a high probability to find a connected component of the graph $G_\varepsilon$ that closely approaches both the center and the boundary of $Q$.

This talk is based on the paper [4].

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## Surface energy and boundary layers for a chain of atoms at low temperature: analytic aspects


Bernd Schmidt

(joint work with Sabine Jansen, Wolfgang König, and Florian Theil)


We report on recent results obtained in [2] on the low-temperature behavior for a one-dimensional chain of atoms that interact via a Lennard–Jones type potential. In particular we (1) provide a detailed analysis of the boundary layers and surface energy at temperature $T = 0$, (2) show that at $T > 0$ the Gibbs measures $\mu_\beta$ and $\nu_\beta$ for infinite chains and semi-infinite chains satisfy path large deviations principles and find that the surface correction to the Gibbs free energy converges to the zero temperature surface energy, and (3) derive bounds on the decay of correlations. Further developments, in particular, a detailed description of the typical atomic configurations at low temperature and low density which fill space by alternating approximately crystalline domains ("clusters") with empty domains ("cracks") that can be obtained with the results discussed below are the subject of another abstract within this report given by Sabine Jansen, see [3].

**1. Set-up** Consider a system of $N$ particles with interparticle spacings $z_1, \dots, z_N > 0$ whose Gibbs energy at zero temperature and (small) pressure $p$ is given by

$$\mathcal{E}_N(z_1, \dots, z_{N-1}) = \sum_{\substack{1 \le i < j \le N \\ |i-j| \le m}} v(z_i + \cdots + z_{j-1}) + p \sum_{j=1}^{N-1} z_j,$$

$m \in \mathbb{N} \cup \{\infty\}$ fixed. The pair interaction potential $v$ is assumed to satisfy a set of generic conditions, which in particular allows for the Lennard–Jones potential $v(r) = r^{-12} - r^{-6}$. It is characterized by $r_{\mathrm{hc}} \in [0, \infty)$ (a hard core) and special values $z_{\max} > z_{\min} > r_{\mathrm{hc}}$ such that $v$ attains its unique (negative) minimum at $z_{\max}$, $v(z_{\min}) > 0$ is large and $v$ is strictly convex in $[z_{\min}, z_{\max}]$ (see [2] for details).

**2. Results at zero temperature.** Our first result can be seen as an extension of a result by Gardner and Radin [1] to a generic setting.

**Theorem A** (Bulk properties)

(a) *For every $N \geq 2$, $\mathcal{E}_N$ has a unique minimizer $(z_1^{(N)}, \dots, z_{N-1}^{(N)})$. The mimizer has all its spacings $z_j^{(N)}$ in $[z_{\min}, z_{\max}]$.*

(b) *As $j, N \to \infty$ along $N - j \to \infty$, we have $z_j^{(N)} \to a$ where $a \in (z_{\min}, z_{\max}]$ is the unique minimizer of $\mathbb{R}_+ \ni r \mapsto pr + \sum_{k=1}^m v(kr)$.*

(c) *The limit $e_0 = \lim_{N\to\infty}(\min \mathcal{E}_N/N) < 0$ exists and is given by*

$$e_0 = pa + \sum_{k=1}^m v(ka) = \min_{r>0}\Big(pr + \sum_{k=1}^m v(kr)\Big).$$

Our next goal is to provide a finer analysis which not only captures bulk energy effects (of order $N$) but also the surface corrections (of order 1). For this we set for sequences $(z_j)_{j\in\mathbb{N}}$ with none or at most finitely many elements different from $a$

$$\mathcal{E}_{\rm surf}\big((z_j)_{j\in\mathbb{N}}\big) = \sum_{j=1}^\infty \Big(-e_0 + pz_j + \sum_{k=1}^m v(z_j + \cdots + z_{j+k-1})\Big).$$

$\mathcal{E}_{\rm surf}$ is the Gibbs energy of a semi-infinite chain, with additive constant chosen in such a way that at spacings $z_j \equiv a$ the Gibbs energy is zero. Let $\mathcal{D} = \{(z_j)_{j\in\mathbb{N}} \in (r_{\rm hc}, \infty)^{\mathbb{N}} \mid \sum_{j=1}^\infty (z_j - a)^2 < \infty\}$ be the space of square summable strains.

**Theorem B** (Surface energy) *Equip $\mathcal{D}$ with the $\ell^2$-metric. Then*

(a) *$\mathcal{E}_{\rm surf}$ extends to a continuous functional on $\mathcal{D}$.*

(b) *On $\mathcal{D} \cap [z_{\min}, z_{\max}]^{\mathbb{N}}$ it is strictly convex.*

(c) *$\mathcal{E}_{\rm surf}$ has a unique minimizer. The minimizer lies in $\mathcal{D} \cap [z_{\min}, z_{\max}]^{\mathbb{N}}$.*

(d) *The limit $e_{\rm surf} = \lim_{N\to\infty}(\min \mathcal{E}_N - Ne_0)$ exists and is given by*

$$e_{\rm surf} = 2 \min_{\mathcal{D}} \mathcal{E}_{\rm surf} - pa - \sum_{k=1}^m kv(ka).$$

**3. Results at (small) positive temperature.** Here we assume $r_{\rm hc} > 0$ and $p > 0$ (small). Let $\mathbb{Q}_N^{(\beta)}$ be the probability measure on $\mathbb{R}_+^{N-1}$ defined by

$$\mathbb{Q}_N^{(\beta)}(A) = \frac{1}{Q_N(\beta)} \int_A \mathrm{e}^{-\beta \mathcal{E}_N(z_1,\dots,z_{N-1})} \mathrm{d}z_1 \cdots \mathrm{d}z_{N-1}$$

with $Q_N(\beta) = \int_{\mathbb{R}_+^{N-1}} \mathrm{e}^{-\beta \mathcal{E}_N(z_1,\dots,z_{N-1})} \mathrm{d}z_1 \cdots \mathrm{d}z_{N-1}$. Standard arguments show that there are uniquely defined surface and bulk Gibbs measures $\nu_\beta$ on $\mathbb{R}_+^{\mathbb{N}}$ and $\mu_\beta$ on $\mathbb{R}_+^{\mathbb{Z}}$, respectively, such that for every bounded continuous test function $f$ which only depends on $z_1, \dots, z_k$ for a $k \in \mathbb{N}$,

$$\lim_{N\to\infty} \langle f, \mathbb{Q}_N^{(\beta)} \rangle = \langle f, \nu_\beta \rangle \quad \text{and} \quad \lim_{\substack{N\to\infty \\ (i_N, N-i_N\to\infty)}} \langle f \circ \tau^{i_N}, \mathbb{Q}_N^{(\beta)} \rangle = \langle f, \mu_\beta \rangle,$$

where $\tau$ denotes the left shift on $\mathbb{Z}$. Let $\mathbb{R}_+^{\mathbb{N}}$ and $\mathbb{R}_+^{\mathbb{Z}}$ be equipped with the product topology and extend $\mathcal{E}_{\mathrm{surf}}$ and $\mathcal{E}_{\mathrm{bulk}}$ to all of $\mathbb{R}^{\mathbb{N}}$, resp., $\mathbb{R}^{\mathbb{N}}$ with value $+\infty$ where not defined previously. With the help of these functionals we can quantify the asymptotic behavior at small temperature as follows.

**Theorem C** (Large deviations) *As $\beta \to \infty$, $(\nu_\beta)_{\beta>0}$ and $(\mu_\beta)_{\beta>0}$ satisfy large deviations principles with speed $\beta$ and respective rate functions $\mathcal{E}_{\mathrm{surf}} - \min \mathcal{E}_{\mathrm{surf}}$ and $\mathcal{E}_{\mathrm{bulk}}$. The rate functions are* good*, i.e., lower semi-continuous with compact level sets.*

For the asymptotic behavior of the Gibbs free energy we get:

**Theorem D** (Zero temperature limit of the Gibbs free energy) *The Gibbs free energy $g(\beta)$ per particle in the bulk and the surface correction $g_{\mathrm{surf}}(\beta)$ given by*

$$g(\beta) = -\lim_{N\to\infty} \frac{1}{\beta N} \log Q_N(\beta), \qquad g_{\mathrm{surf}}(\beta) = \lim_{N\to\infty} \Big( -\frac{1}{\beta} \log Q_N(\beta) - N g(\beta) \Big),$$

*are well-defined. They satisfy*

$$\lim_{\beta\to\infty} g(\beta) = e_0, \qquad \lim_{\beta\to\infty} g_{\mathrm{surf}}(\beta) = e_{\mathrm{surf}}.$$

At last we mention an estimate on the decay of correlations which is exponential for finite range interactions and algebraic for unbounded interaction ranges.

**Theorem E** (Decay of correlations) *There exist $c, C > 0$ such that for all $\beta, p > 0$, $k \in \mathbb{N}$, and bounded $f, g : \mathbb{R}_+^k \to \mathbb{R}$,*

$$\begin{aligned} &\big| \mu_\beta(fg \circ \tau^n) - \mu_\beta(f)\mu_\beta(g) \big| \\ &\le \min_{\substack{q\in\mathbb{N}: \\ 1\le q\le n/k}} \Big( (1 - \mathrm{e}^{-c\beta})^q + \mathrm{e}^{c\beta} (\mathrm{e}^{C\beta (q/n)^{s-2}} - 1) \Big) \|f\|_\infty \|g\|_\infty. \end{aligned}$$

*When $m$ is finite and $k = m - 1$, we have the stronger bound*

$$\big| \mu_\beta(fg \circ \tau^n) - \mu_\beta(f)\mu_\beta(g) \big| \le (1 - \mathrm{e}^{-c\beta})^{n/k} \|f\|_\infty \|g\|_\infty.$$

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## Surface energy and boundary layers for a chain of atoms at low temperature: probabilistic aspects

Sabine Jansen
(joint work with Wolfgang König, Bernd Schmidt, and Florian Theil)

The talk is a continuation of a talk by Bernd Schmidt, we use the same notation. We complement the zero-temperature results and the rough a priori estimate on the decay of correlations by the following: (1) improved estimates on the decay of correlations that are uniform in the temperature, and (2) results on the Gaussian approximation to the bulk Gibbs measure.

Concretely, we prove the following.

**Theorem E** Let $m \in \mathbb{N} \cup \{\infty\}$. There exists $c > 0$ such that for all $\beta, p > 0$, smooth $f, g : \mathbb{R}_+ \to \mathbb{R}$, and $i \neq j$,

$$\Big|\tilde\mu_\beta(f_i g_j) - \tilde\mu_\beta(f_i)\tilde\mu_\beta(g_j)\Big| \le \frac{c}{\beta|i-j|^s}\Big(\tilde\mu_\beta(f_i'^2)\ \tilde\mu_\beta(g_j'^2)\Big)^{1/2}.$$

**Theorem F** Assume $2 \le m < \infty$, $p \in (0, p^*)$, and $r_{\mathrm{hc}} > 0$. There exists $\gamma > 0$ such that for all sufficiently large $\beta$, suitable $C(\beta)$, all $n \in \mathbb{N}$, and all $f, g : \mathbb{R}_+^d \to \mathbb{R}$, we have

$$\big|\mu_\beta(f_0 g_n) - \mu_\beta(f_0)\mu_\beta(g_n)\big| \le C(\beta)\mathrm{e}^{-\gamma n}||f_0||_\infty\, ||g_n||_\infty.$$

If $m = 2$, we can pick $C(\beta) = 1$.

For the Gaussian approximation, let $\mathcal{H}_{ij} = \partial_i\partial_j\mathcal{E}_{\mathrm{bulk}}((z_i)_{i\in\mathbb{Z}})$. The Hessian $(\mathcal{H}_{ij})_{i,j\in\mathbb{Z}}$ is diagonally dominant and defines a bounded, positive-definite operator in $\ell^2(\mathbb{Z})$. Let $\mu^{\mathrm{Gauss}}$ is the distribution of a Gaussian process $(N_j)_{j\in\mathbb{Z}}$ with mean zero and covariance $\mathbb{E}[N_iN_j] = (\mathcal{H}^{-1})_{ij}$. We identify the measure $\mu_\beta$ on $\mathbb{R}_+^{\mathbb{Z}}$ with the measure $\mathbf{1}_{\mathbb{R}_+^{\mathbb{Z}}}\mu_\beta$ on $\mathbb{R}^{\mathbb{Z}}$. We exclude the trivial case $m = 1$.

**Theorem G** Assume $2 \le m < \infty$, $p \in (0, p^*)$, and $r_{\mathrm{hc}} > 0$. Then for every $n \in \mathbb{N}$, the $n$-dimensional marginals of $\mu_\beta$ and $\mu^{\mathrm{Gauss}}$ have probability density functions $\rho_n^{(\beta)}$ and $\rho_n^{\mathrm{Gauss}}$, and

$$\lim_{\beta\to\infty}\int_{\mathbb{R}^n}\Big|\beta^{-n/2}\rho_n^{(\beta)}\big(a+\beta^{-1/2}s_1,\dots,a+\beta^{-1/2}s_n\big) - \rho_n^{\mathrm{Gauss}}(s_1,\dots,s_n)\Big|\mathrm{d}s_1\dots\mathrm{d}s_n = 0.$$

We also provide a result on the Gaussian approximation to the Gibbs free energy.

**Theorem H** Assume $2 \le m < \infty$, $p \in (0, p^*)$, and $r_{\mathrm{hc}} > 0$. The Gibbs free energy satisfies, as $\beta \to \infty$,

$$g(\beta) = e_0 - \frac{1}{\beta}\log\sqrt{\frac{2\pi}{\beta(\det C)^{1/d}}} + o(\beta^{-1})$$

where $d = m - 1$ and $C$ is a $d \times d$ positive-definite matrix.
The matrix $C$ is a function of the Hessian of the energy.

Theorem F is instrumental in examining the distribution of micro-cracks at vanishing pressure $p = p(\beta) \to 0$ / average spacing $\ell > a_0$, with $a_0$ the minimizer of the Cauchy–Born density $r \mapsto \sum_{k=1}^{\infty} v(kr)$ at zero pressure: In a forthcoming article [2] we treat the elongated chain of atoms with an effective model consisting of a lattice gas of defects. The "sites" of the effective lattice gas correspond to nearest-neighbor bonds $\{i, i+1\}$ of the atomic model, and a defect occurs if the spacing $z_i = x_{i+1} - x_i$ is larger than some cut-off parameter $R > a$. The parameter is chosen in such a way that the entropic push for large spacings overcomes the attractive interaction between particles. The estimates on the decay of correlations allow us to show, under some additional assumptions, that the effective interaction between defects decays exponentially when defects are separated by many non-broken bonds.

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### On the diffraction spectra of some random point sets

Holger Kösters

One approach to identifying long-range order is via diffraction. Since real-world crystals and quasicrystals are never perfect, it is natural to ask for the effects of randomness. We survey selected examples of random structures for which the autocorrelation measure $\gamma$ and the diffraction measure $\widehat{\gamma}$ may be calculated explicitly. For background information and further examples, we refer to [1, 2, 5].

*Random modifications of deterministic point sets.* Here we start from a "nice" deterministic point set $\Lambda \subset \mathbb{R}^d$ of density 1 (e.g. a lattice or a model set) such that $\gamma_\Lambda$ and $\widehat{\gamma}_\Lambda$ exist and make random modifications at each point of $\Lambda$. In the *random weight model* [1], we take $\Phi = \sum_{x \in \Lambda} \xi_x \delta_x$, where $(\xi_x)_{x \in \Lambda}$ is a family of independent copies of a real random variable $\xi$ with $\mathbb{E}|\xi|^2 < \infty$. Then, almost surely,

$$\gamma_\Phi = |\mathbb{E}\xi|^2 \, \gamma_\Lambda + (\mathbb{E}|\xi|^2 - |\mathbb{E}\xi|^2) \, \delta_0 \,, \quad \widehat{\gamma}_\Phi = |\mathbb{E}\xi|^2 \, \widehat{\gamma}_\Lambda + (\mathbb{E}|\xi|^2 - |\mathbb{E}\xi|^2) \, \text{𝕜}^d \,.$$

In the *random displacement model* [9, 1], we take $\Phi = \sum_{x \in \Lambda} \delta_{x + Y_x}$, where $(Y_x)_{x \in \Lambda}$ is a family of independent copies of an $\mathbb{R}^d$-valued random vector $Y$ with law $\nu$. Then, almost surely,

$$\gamma_\Phi = (\nu * \widetilde{\nu}) * \gamma_\Lambda + (\delta_0 - \nu * \widetilde{\nu}) \,, \quad \widehat{\gamma}_\Phi = |\widehat{\nu}|^2 \, \widehat{\gamma}_\Lambda + (1 - |\widehat{\nu}|^2) \, \text{𝕜}^d \,.$$

Similar results hold for the *random cluster model* [1], where each point of $\Lambda$ is replaced with a copy of a finite random cluster. In all cases, $\widehat{\gamma}_\Phi$ consists of two parts, a first part which is related to $\widehat{\gamma}_\Lambda$ and a second part which is absolutely continuous.

In particular, if $\widehat{\gamma}_\Lambda$ is pure point, then the first part of $\widehat{\gamma}_\Phi$ is also pure point, i.e. the random modification has a modulating but not a smoothing effect.

More general weighting schemes where the weights are distributed according to some finite-range Gibbs measure have also been investigated [3, 10, 6, 7]. Moreover, in $d = 1$, one may also consider renewal processes where the increments between the points are i.i.d. random variables [1].

*Completely random point sets.* Here we do not have a reference point set in the background anymore, but we start from a stationary and ergodic point process $\Phi$ with density 1 and reduced second-order correlation function $1+g$, with $g \in L^1(\mathbb{A}^d)$ [1, 5]. Then, almost surely,

$$\gamma_\Phi = \delta_0 + (1+g)\,\mathbb{A}^d\,, \quad \widehat{\gamma}_\Phi = \delta_0 + (1+\widehat{g})\,\mathbb{A}^d\,.$$

Thus, apart from the Bragg peak at the origin, $\widehat{\gamma}_\Phi$ is absolutely continuous. Examples include

(i) the homogeneous Poisson process, for which $g = 0$ and $\widehat{g} = 0$,

(ii) determinantal point processes [5], for which $g = -|\widehat{\varphi}|^2$ and $\widehat{g} = -(\varphi * \widetilde{\varphi})$, for some probability density $\varphi$ on $\mathbb{R}^d$ taking values in $[0, 1]$.

(iii) permanental point processes [5], for which $g = +|\widehat{\varphi}|^2$ and $\widehat{g} = +(\varphi * \widetilde{\varphi})$, for some probability density $\varphi$ on $\mathbb{R}^d$.

A famous example of type (ii) is the sine process with $d = 1$, $g(x) = -(\frac{\sin \pi x}{\pi x})^2$ and $\widehat{g}(k) = -(1 - |k|)^+$. It arises as the limit (after appropriate rescaling) of the eigenvalue ensembles of Gaussian Hermitian random matrices. More generally, one might consider the corresponding limits for the Gaussian beta ensembles [8], which interpolate between the homogeneous Poisson process (for $\beta \to 0$) and the integer lattice (for $\beta \to \infty$). It would be interesting to describe the transition from complete disorder to perfect order at the level of the diffraction spectrum, at least qualitatively. The diffraction is known explicitly for $\beta \in \{1, 2, 4\}$, see e.g. [4], but not for general $\beta > 0$.

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## The Widom–Rowlinson model: metastability, mesoscopic and microscopic fluctuations for the critical droplet

Elena Pulvirenti

(joint work with Frank den Hollander, Sabine Jansen and Roman Kotecký)

Metastability is a widely observed phenomenon where a system, subject to *random dynamics*, moves between regions of its state space on different *time scales*. In the context of statistical physics, metastability is the dynamical manifestation of a first-order phase transition, e.g. condensation. In this case, the crossover from one phase to the other is triggered by the formation of a *critical droplet* of the new phase (liquid) inside the old phase (gas). While in the metastable state, the system makes many unsuccessful attempts to form a critical droplet, because this requires the system to climb an energetic barrier, and returns many times to the bottom of the valley it resides in. As a consequence, metastability is a *non-equilibrium* phenomenon and the crossover time is random (for an overview see the monograph by Bovier and den Hollander [1]).

We study metastability for a model of continuum interacting particle systems displaying condensation. The microscopic model that we consider is a non - equilibrium version of the *static* Widom–Rowlinson model introduced in [7], which describes a classical fluid in thermodynamic equilibrium and is one of the few models in the continuum for which the occurrence of condensation has been rigorously proven (first by Ruelle [6], then by Chayes, Chayes and Kotecký [2]). The phase transition occurs as the chemical potential, controlling the density of the particles, changes from a subcritical value to a supercritical value. It is therefore very natural to expect that it displays a metastable behaviour, once we choose a random dynamics.

This model possesses a dual description. In the first one, it is a binary gas with hard-core repulsion between particles of different types. In the second one, particles are viewed as points carrying $d$-dimensional disks and the energy of a particle configuration is the volume of the union of the disks minus the sum of the volumes of the disks. Consequently, the interaction between the particles is attractive.

We consider a *dynamic* version of the WR model on a two dimensional torus, where the system is subject to a Metropolis random dynamics associated with the Hamiltonian of the model. This means that the configuration is viewed as a continuous-time Markov process where particles are randomly created and annihilated according to an infinite reservoir with a given chemical potential.

Our main goal is to study the metastable behaviour of the dynamic WR model in the regime of *low temperature* when the chemical potential is *supercritical*. In

particular, we start with the empty torus (which represents the vapour phase) and are interested in how the dynamics tunnels to the configuration in which the torus is full, i.e., the torus is fully covered by disks (which represents the liquid state). In order to achieve the transition from empty to full, the system needs to create a sufficiently large droplet of overlapping disks, which plays the role of the critical droplet that triggers the crossover. In the limit as the temperature tends to zero, we

- characterize the size and the shape of the critical droplet, which is created in the condensation process under the above dynamics
- compute the average crossover time which the system takes to pass from the empty to the full configuration and identify its asymptotics.

In the average crossover time we compute not only the leading order term (which corresponds to the classical Arrhenius law) but also the correction term, which is large and represents a substantial deviation from this law. While the first one represents the *volume free energy* of the critical droplet, the second one is instead a *surface free energy* contribution. The above results rely on a detailed study of the fluctuations of the surface of the critical droplet in the static WR model. In order to analyze the *mesoscopic fluctuations* for the critical droplet, we find asymptotics for the partition function on the configurations where the union of the disks is close to the critical disk both in volume and in Hausdorff distance. In order to control the mesoscopic fluctuations, we need also to prove the existence of the free energy associated with the *microscopic fluctuations* of the surface. This relies on the study of a model for a $1 + 1$-dimensional interface, which arises as an effective interface model for the WR model. This model is a variant of the discrete one-dimensional Gaussian free field, where the underlying deterministic lattice is replaced by a random point configuration on the line and where an additional multy-body hard-core interaction coming from a geometric constraint is added. This project is in collaboration with F. den Hollander, S. Jansen and R. Kotecký.

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## Gradient fields for non-linear elasticity

Stefan Adams
(joint work with Simon Buchholz, Roman Kotecký, and Stefan Müller)

We study gradient fields as effective models for non-linear elasticity. The talk is based on recent work with S. Müller and R. Kotecký joined by S. Buchholz this year, see [1, 2, 3]. We consider models of discrete elasticity and analyse local convexity properties of the free energy. We consider vector-valued fields $\varphi\colon \Lambda \to \mathbb{R}^d$ on some torus $\Lambda$ in the integer lattice and interactions beyond nearest neighbour interactions. An additional difficulty in discrete non-linear elasticity is that the invariance under rotations leads a degeneracy of the quadratic form in the measure usually considered. We will overcome this difficulty by adding a suitable discrete null Lagrangian, see [3]. Gradient systems are defined as Gibbs distributions for Hamiltonian functions depending solely on the gradients of the given field $\varphi$, where $\varphi_x$ is the displacement of atom with label '$x$'. The logarithm of the normalisation of these Gibbs distributions, called partition function in statistical mechanics, is the free energy. Our aim is to show that the free energy is uniformly convex as a function of the applied boundary condition. The strong dependence on the boundary condition, which in our case is given by $F\colon \mathbb{F}^d \to \mathbb{R}^d$, is different from typical models in statistical mechanics. For the setting, let $A$ be a finite subset of $\mathbb{Z}^d$ and let $U\colon (\mathbb{R}^d)^A \to \mathbb{R}$ be an interaction potential. The *Hamiltonian* with boundary $F$ is then

$$H_\Lambda(\varphi) = \sum_{x\in\Lambda} U\big(\big(\varphi + F\big)_{\tau_x(A)}\big)\,, \tag{1}$$

where $\tau_x(A)$ denotes the set $A$ translated by $x \in \Lambda$, $\tau_x(A) = A + x$. For simplicity (and without loss of generality), we suppose that the support set $A$ of the potential $U$ contains the unit cell of $\mathbb{Z}^d$, $\{0,1\}^d \subset A$. For a linear map $F\colon \mathbb{R}^d \to \mathbb{R}^d$ we consider the extension to $(\mathbb{R}^d)^A$ given by $(F\psi)(x) = F(\psi(x))$. Gradient models are well understood when the interaction potential is quadratic. Then the Gibbs distributions are Gaussian measures and are a model for linear elasticity due to the quadratic nature of the interaction. In [2], using renormalisation group techniques in conjunction with [1], it was shown that models for real-valued fields $\varphi\colon \Lambda \to \mathbb{R}$ with non-convex potentials can be analysed, showing in particular that the free energy is strictly convex as a function of the applied boundary condition, extending well-known results in [5] to a class of non-convex potentials. Recently, this study has been extended to non-linear discrete elasticity using vector-valued fields under a certain class of non-convex potentials $U$. We assume that the potential $U$ satisfies the following conditions.

(H1) *Invariance under rotations and shifts:* We have

$$U(\psi) = U(\mathbf{R}(t_a\psi))$$

for any $\psi \in (\mathbb{R}^d)^A$ and any $\mathbf{R} \in SO(d)$, $a \in \mathbb{R}^d$, with $\mathbf{R}(t_a\psi)(x) = \mathbf{R}(\psi(x) + a)$.

(H2) *Ground state:* $U(\psi) \geq 0$ and $U(\psi) = 0$ if and only if $\psi$ is a rigid body rotation, i.e., there exists $\mathbf{R} \in \mathrm{SO}(d)$ and $a \in \mathbb{R}^d$ such that $\psi(x) = \mathbf{R}x + a$ for any $x \in A$.

(H3) *Smoothness and convexity:* Let $\mathsf{1} \in (\mathbb{R}^d)^A$ denote the identity configuration $\mathsf{1}(x) = x$. Assume that $U$ is a $C^2$ function and $D^2U(\mathsf{1})$ is positive definite on the subspace orthogonal to shifts and infinitesimal rotations given by skew-symmetric linear maps.

(H4) *Growth at infinity:*

$$\liminf_{|\psi|\to\infty} \frac{U(\psi)}{|\psi|^d} > 0.$$

(H5) *Additional smoothness and sub-gaussian bound:* $U \in C^{r_0+r_1}$ with $r_0 \geq 3$ and $r_1 \geq 0$ and

$$\lim_{|\psi|\to\infty} |\psi|^{-2} \ln\Big( \sum_{2\leq|\alpha|\leq r_0+r_1} \frac{1}{\alpha!} |\partial_\psi^\alpha U(\psi)| \Big) = 0\,.$$

The first four conditions are the same as in [4]. The last condition is a minor additional regularity assumption for the potential. It was stated as a separate item to make clear that it is only required in the renormalisation group analysis.

In [4] these assumptions are used to prove that the *Cauchy–Born rules* holds at zero temperature.

Here we use this result as a starting point for a study of the Gibbs distribution for the Hamiltonian $H_\Lambda$ at low temperatures using the renormalisation group approach. The ground state in the setting of discrete elasticity corresponds to the affine deformation given by the identity. Therefore we consider deformations $F \in \mathbb{R}^{d\times d}$ for which $F - \mathsf{1}$ is small. For a linear function $F$, its restriction to $A$ and to $\tau_x(A)$ differ by the constant vector $F(x) \in \mathbb{R}^d$ and thus $U(F|_A) = U(F|_{\tau_x(A)})$.

We define the free energy as

$$W_{N,\beta}(F) := -\frac{\ln Z_{N,\beta}(F,0)}{\beta L^{Nd}}.$$

Note that $W_{N,\beta}$ inherits the rotational invariance of $U$.

**Theorem:**

Suppose the potential $U$ satisfies the assumptions $(H1)$ to $(H5)$ with $r_0 = 3$ and $r_1 \geq 0$. There exists a subsequence $(N_\ell)$ such that $W_{N_\ell,\beta}$ converges in $C^{r_1-1}$ to the free energy $W_\beta(F)$. For $r_1 \geq 3$ the second derivative $D^2W_\beta(\mathsf{1})$ is strictly positive on the subspace orthogonal to the skew-symmetric matrices.

**Remark:**

The second part of the theorem asserts that $W_{N,\beta}$ is uniformly convex near $\mathsf{1}$ modulo rotational invariance. Equivalently this can be stated as follows. Since $W_{N,\beta}$ is rotational invariant there exists a smooth function $\hat{W}_{N,\beta}$, defined in a small neighbourhood of $\mathsf{1}$ such that $W_{N,\beta}(F) = \hat{W}_{N,\beta}(F^TF)$. Then $\hat{W}$ is uniformly convex in a neighbourhood of $\mathsf{1}$, uniformly in $N$.

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