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Spin field topological linear defects in quasicrystals with magnetic order

Paolo Maria Mariano

DICeA, Università di Firenze, via Santa Marta 3, I-50139 Firenze, Italy

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ABSTRACT

It is proven that magnetizable quasicrystals undergoing large deformations admit elastic ground states characterized by a net of linear topological defects for the magnetic spin field.

Quasicrystals are aluminium-based alloys characterized by a quasi-periodic distribution of atoms in space. Their structure is made of prevailing atomic clusters having incompatible symmetry with the periodic tiling of the ambient space, and sparse additional atomic structures. The latter clusters (sometimes called worms) are generated by local rearrangements of atoms and produce the characteristic quasi-periodicity (see, e.g., [11,18]). In principle it is not known where worms are placed: they can be nucleated and annihilated in any place as a consequence of external actions. There is an interplay between macroscopic deformation and local formation or annihilation of worms: macroscopic deformations alter the energetic content of a generic crystalline cell and may favour or obstruct local rearrangements in the atomic clusters. There is also difference between the effects of infinitesimal and finite deformation. In the latter case, a fully non-linear theory is necessary (see results in [12,16,13]). Moreover, quasicrystals may admit magnetic order (see [10,17]).

For such classes of quasicrystals I describe here conditions allowing the existence of elastic ground states which admit a net of linear defects in the magnetic spin field. Relevant experiments should be then necessary to corroborate the theoretical result.

Conditions of magnetic saturation are assumed to hold. The deformation setting is fully non-linear. Uniform thermal bath is presumed.

$\mathcal{B}$ is the regular[1] region of the three-dimensional ambient space occupied by the body under scrutiny and taken as a reference place for the sake of convenience. New places are reached by *deformations* $x \mapsto u(x) \in \mathbb{R}^3$, x in $\mathcal{B}$. They are differentiable one-to-one maps which are also orientation preserving (i.e. $\det Du(x) > 0$, where Du is the spatial derivative of u) and satisfy a global invertibility condition specified later. The macroscopic configuration reached after the deformation is $u(\mathcal{B})$ and has the same topological properties of $\mathcal{B}$ itself.

Besides the degrees of freedom in the ambient space, the ones exploited in the macroscopic deformation, inner degrees of freedom are accounted for to represent local atomic rearrangements (see, e.g., [9]) due to jumps between neighboring positions with a similar local environment [3], or collective atomic modes generated for example by the flipping of crisscrossing worms needed to maintain matching rules [7]. They are commonly called *phason degrees of freedom*. A differentiable vector field $x \mapsto \nu_p(x) \in \tilde{\mathbb{R}}^3$, x in $\mathcal{B}$, collects them — the index p indicates phason. $\tilde{\mathbb{R}}^3$ is an isomorphic copy of $\mathbb{R}^3$, distinguished from it.[2]

A differentiable field $x \mapsto \nu_s(x) \in S^2$, x in $\mathcal{B}$, of *Heisenberg spins* ν_s — the index s means spin — describes locally the magnetization in saturation conditions.

These three fields and their spatial derivatives enter the energy. If the picture accounts only for first-neighborhoud interactions, the energy to be considered has density of the form $\tilde{e}(x, u, Du, D\nu_p, \nu_s, D\nu_s)$. No external bulk actions acting directly on the possible atomic rearrangements appear. Moreover, experiments exclude also the dependence of the internal energy on ν_p (see, e.g., [18,7]). Here a less general energy is considered. It reads

E-mail address: paolo.mariano@unifi.it.

[1] Regularity is intended here in the sense that $\mathcal{B}$ is considered as an open, connected set in the three-dimensional ambient space, with surface-like boundary oriented by the normal at each point, to within a finite number of corners and edges.

[2] Such a representation of the morphology of quasicrystals falls within the model-building framework of the mechanics of complex bodies (see [13] for details; see also [14,15]).

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$$\int_{\mathcal{B}} e(x, u, Du, D\nu_p, \nu_s)\, dx + \frac{1}{2} c \int_{\mathcal{B}} |D\nu_s|^2\, dx,$$

with c a constitutive constant with appropriate physical dimensions. The gradient magnetization energy density $|D\nu_s|^2$ of Dirichlet type is suggested by Ginzburg–Landau theory (see [1,8,2]). The energy density

$$e(x, u, Du, D\nu_p, \nu_s) + \frac{1}{2} c |D\nu_s|^2$$

is the difference between the internal energy $\hat{e}(x, Du, D\nu_p, \nu_s) + \frac{1}{2} c |D\nu_s|^2$ and the potential of external bulk actions $w(u, \nu_s)$.

Boundary conditions are here of Dirichlet type. The possibility to prescribe the three fields introduced above over at least part of the boundary of $\mathcal{B}$ is then presumed. The prescription of the deformation is natural. A bit arduous is the practical assignment of phason degrees of freedom and spins. In any case, it is possible to imagine that at the boundary, or in a thin layer comprising it, the phason field is zero and that also part of the boundary is insulated with respect to the magnetic action.

The question here is existence and essential physical properties of ground states for the energy. The existence of ground states for quasicrystals undergoing large deformations has been proven in [15] as a special case of a general existence theorem of ground states of generic complex bodies. Here, with respect to standard quasicrystals, the setting is enriched by the presence of the spin field. However, although the situation tackled here can be embedded in the general theory developed in [15], the specificity of the situation puts in evidence peculiar physical features. The analysis starts from the choice of the function spaces in which one looks for minimizers of the energy. Such a choice has constitutive nature. The strategy is, in fact, to select maps which may be reasonable descriptors of some physical behaviour under analysis, then to prove possibly their ability to be minimizers of the energy selected, under appropriate assumptions on the structure of the energy. Another crucial point is that the functional choice made can suggest modifications of the energy structure in a way discussed later.

1. Elastic setting is considered. Deformations can be thus perfectly recovered, and the body can deform at will, without any threshold and, in principle, without end. Deformations are then considered to be compatible when they do not imply nucleation of fractures and/or holes which pertain to the elastic-brittle behaviour. These considerations drive the choice of the functional setting for u. For instance, if the Sobolev space $W^{1,p}(\mathcal{B}, \mathbb{R}^3)$ — a space hosting maps with first distributional derivative having integrable p-power, i.e. the first derivative is in L^p — is considered as the set of deformations, for $p < 3$ it should be possible to find maps with graphs admitting boundaries with projections into the interior of $\mathcal{B}$. Such boundaries represent then 'holes' and/or 'fractures' not admitted in the elastic setting accepted here. In fact, it is necessary to impose a constraint forbidding these boundaries. To do this, the first step is to remind that the presence of boundaries in the graph of a map can be checked through some special linear functionals called *currents*. Their definition requires a few preliminary notions. First, remind that 3-*vectors* over $\mathbb{R}^3 \times \mathbb{R}^3$, where the graph of the deformation is placed, are rank-3 skew-symmetric tensors. Their space is indicated by $\Lambda_3(\mathbb{R}^3 \times \mathbb{R}^3)$ and has natural dual $\Lambda^3(\mathbb{R}^3 \times \mathbb{R}^3)$. Maps of the type $\omega : \mathbb{R}^3 \to \Lambda^3(\mathbb{R}^3 \times \mathbb{R}^3)$ are called 3-*forms*, their space is indicated by $\mathcal{D}^3(\mathbb{R}^3 \times \mathbb{R}^3)$. 3-forms with compact support in $\mathcal{B} \times \mathbb{R}^3$ are maps of the type $\omega : \mathcal{B} \to \Lambda^3(\mathbb{R}^3 \times \mathbb{R}^3)$. Given a deformation $x \mapsto u(x) \in \mathbb{R}^3$, $x \in \mathcal{B}$, a 3-vector $M(Du)$ is naturally associated with the gradient of deformation Du. Its components at x are 1 and the entries of $Du(x)$, $\operatorname{adj} Du(x)$, $\det Du(x)$. In other words, all elements characterizing the deformation of lines, areas, and volume in $\mathcal{B}$ are included in $M(Du)$. The 3-*current integration* G_u (*current* for short) over the rectifiable part of the graph of u is then defined as a linear functional on smooth 3-forms $\omega \in \mathcal{D}^3(\mathbb{R}^3 \times \mathbb{R}^3)$ with compact support in $\mathcal{B} \times \mathbb{R}^3$:

$$G_u := \int_{\mathcal{B}} \langle \omega\big(x, u(x)\big), M\big(Du(x)\big) \rangle\, dx.$$

The number $\mathbf{M}(G_u) := \int_{\mathcal{B}} |M(Du(x))|\, dx$ indicates the so-called *mass* of the current, with $|M(Du(x))|$ the modulus of $M(Du(x))$. A functional named *boundary current* can be associated with G_u: it is indicated by ∂G_u and defined by duality, namely $\partial G_u(\omega) := G_u(d\omega)$, $\forall \omega \in \mathcal{D}_c^2(\mathcal{B} \times \mathbb{R}^3)$, with $\mathcal{D}_c^2(\mathcal{B} \times \mathbb{R}^3)$ the space of 2-forms over $\mathbb{R}^3 \times \mathbb{R}^3$ with compact support in $\mathcal{B} \times \mathbb{R}^3$. The notion of boundary current has stringent physical meaning: when the graph of u is free of boundaries inside the interior of $\mathcal{B}$, $\partial G_u(\omega) = 0$ for any $\omega \in \mathcal{D}_c^2(\mathcal{B} \times \mathbb{R}^3)$ (see [5] for the theory of currents in n-dimensional space).

All these notions allow one to define the appropriate functional class that can represent adequately physically significant elastic (meaning fully recoverable) deformation. The class is the one of *weak diffeomorphisms*. A map u in $W^{1,1}(\mathcal{B}, \mathbb{R}^3)$ is said to be a weak diffeomorphism (in short $u \in dif^{1,1}(\mathcal{B}, \mathbb{R}^3)$), when [5] (i) $\det Du(x) > 0$ for almost every $x \in \mathcal{B}$, (ii) $|M(Du)| \in L^1(\mathcal{B})$, (iii) $\partial G_u(\omega) = 0$ for any $\omega \in \mathcal{D}^2(\mathcal{B} \times \mathbb{R}^3)$, (iv) the inequality

$$\int_{\mathcal{B}} f\big(x, u(x)\big) \det Du(x)\, dx \leqslant \int_{\mathbb{R}^3} \sup_{x \in \mathcal{B}} f(x, z)\, dz$$

holds for any $f \in C_c^\infty(\mathcal{B} \times \mathbb{R}^3)$.

Condition (i) prescribes that the transplacement be an orientation preserving map. Item (ii) is a regularity condition allowing the measure of averages of the gradient of deformation, the volume change, the overall deformation of surfaces inside the body. Item (iii) is a constraint excluding the formation of fractures and holes due to cavitation, as it is expected in pure elasticity. The inequality (iv) is a global invertibility condition allowing self-contact between parts of the boundary of $\mathcal{B}$, and excluding self-penetration of the matter along the deformation. A closure theorem for the space of weak diffeomorphisms is available (see [5]).

A role is played later by a regularized class $dif^{p,1}(\mathcal{B}, \mathbb{R}^3)$ of weak diffeomorphism constituted by maps $u \in dif^{1,1}(\mathcal{B}, \mathbb{R}^3)$ such that $|M(Du)| \in L^p(\mathcal{B})$.

2. The conditions determined by the requirement that the transplacement be orientation preserving and the boundary of the body can have self-contact but not self-penetration along a generic deformation do not play role for the phason field ν_p. Physics does not suggest further special restrictions. For this reason it is possible (and also natural) to select the field ν_p in the Sobolev space $W^{1,s}(\mathcal{B}, \tilde{\mathbb{R}}^3)$ for some $s > 1$. The choice of s has also constitutive character.

3. Rather subtle is the functional choice for the spin field. Here the aim is to check whether it is possible to have ground states for the energy — the one having the rather general form prescribed hitherto — with topological linear defects. A reasonable way of investigation is then to select a space of fields having in their graphs such defects and then to check whether an existence theorem of minimizers can be proven in such a space. The functional choice can be then made just in terms of currents thanks to results in [5,4,6], which are briefly recalled here. Given a differentiable spin field ν_s, its associated Dirichlet energy is just the integral

$$\frac{1}{2} \int_{\mathcal{B}} |D\nu_s|^2\, dx.$$