Stability of Objective Structures: General Criteria and Applications

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Abstract

We develop a general stability analysis for objective structures, which constitute a far reaching generalization of crystal lattice systems. We show that these particle systems, although in general neither periodic nor space filling, allow for the identification of stability constants in terms of representations of the underlying symmetry group and interaction potentials. From our representation results a general computational algorithm to test objective structures for their stability is derived. By way of example we show that our method can be applied to verify the stability of carbon nanotubes with chirality.

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1 Introduction

A fundamental problem in material science is to investigate elastic structures for their stability properties. In classical continuum mechanics stability criteria can be derived from positivity properties of the Hessian of the stored energy function such as the classical Legendre-Hadamard condition. For atomistic systems the continuum approach, however, can imply stability only in a regime in which the Cauchy-Born rule is known to be valid and small scale oscillations are excluded a priori. In such a regime individual atoms follow the macroscopic deformation so that the configurational energy can effectively be described by a macroscopic continuum stored energy function.

In general, however, stability conditions in the continuum cannot detect small wavelength instabilities when modes at the interatomic length-scale are excited. While systems of only few atoms may be investigated by computational methods, in high dimensional systems with many or even an infinite number of particles a direct and fully discrete numerical approach is not feasible. It is thus a fundamental challenge to identify classes of structures that, on the one hand, are general enough to cover many interesting and physically relevant examples and, on the other hand, are still amenable to a quantitative stability analysis.

Due to their ubiquity in nature, crystalline atomic systems have been extensively investigated over the last decades by physicists and material scientists, cp. [6, 33, 43]. More recently, there has been a vital interest also within the applied analysis community to rigorously substantiate the connection of atomistic systems and effective continuum models. A brief review of some key results is provided below.

The main objective of the current contribution is to go beyond the periodic setting of crystals, and to extend a stability analysis to the class of objective structures. These structures, introduced by James in [31], constitute a far reaching generalization of lattice systems. They are relevant in a remarkable number of models ranging from biology (to describe, e.g., parts of viruses) to nanoscience (to model carbon nanotubes), see, e.g., [21, 17, 14, 23]. Their defining feature is that, up to rigid motions of the surrounding space, any two particles are embedded in an identical environment of other particles. (In a lattice, this would be the case even up to translations.) This entails that objective structures are described by orbits of a single reference point under the action of a general discrete group of Euclidean isometries, cf. [31, 32], and allows to resort to ideas in harmonic analysis. However, the symmetry of objective structures in general is considerably more complex than that of a periodic crystal and the adaption of methods and results for lattices has only been achieved in a few cases so far such as, notably, an algorithm for the Kohn-Sham equations for clusters [4] and the X-ray analysis of helical structures in [25].

Our endeavor is to provide an in-depth study of stability properties of general objective structures. As detailed below, we will derive explicit formulae for stability constants which are not only interesting from a theoretical point of view but directly lead to an efficient computational algorithm for these quantities. The strength of our method is demonstrated by showing stability of a carbon nanotube with non-trivial chirality. Yet, the non-periodicity and possible lower dimensionality of objective structures poses severe analytical changes as compared to crystals.

For a crystal, in the seminal contribution [26] Friesecke and Theil have shown the validity of the Cauchy-Born rule for small strains in a two-dimensional mass spring model. Their results were then extended to arbitrary dimensions and more general atomistic interactions in [13]. We refer to the survey article [20] for a general review on the Cauchy-Born rule. These results are the first step of various variational discrete-to-continuum
Gamma-convergence results for energy functionals on lattices in which the limiting model is identified explicitly in terms of the effective Cauchy-Born stored energy function, see \cite{37} and \cite{8} for linear and nonlinear elastic bulk systems, respectively, and \cite{36, 10} for thin films.

An alternative approach to establish the Cauchy-Born rule for crystals has been set forth by E and Ming in \cite{18} where they show that under suitable atomistic stability assumptions solutions of the equations of continuum elasticity theory on a flat torus and subject to smooth body forces are approximated by associated atomistic equilibrium configurations. These results have been generalized to the whole space and only mild regularity assumptions in \cite{34} and to boundary value problems in \cite{9}. Even the dynamic setting has been considered in \cite{18, 34, 7}.

At the core of all the aforementioned contributions lies a stability condition for lattice systems. This seems to have been analyzed in detail for the first time by Hudson and Ortner in \cite{29}. Motivated by their results, an explicitly computable stability constant for lattice system has been derived in \cite{9} which permits a direct comparison with the corresponding continuum Legendre-Hadamard continuum stability constant in a long wave-length regime. The main technical tool which allows for an efficient analysis of discrete and continuum stability constants and their interrelation is the Fourier transform. Due to the periodicity of the underlying lattice, the atomistic stability can be determined on a diverging series of finite boxes with periodic boundary conditions, i.e., larger and larger tori, invading the whole space to define a stability constant for the infinite particle system eventually in the limit.

At this point it becomes apparent why the extension to general objective structures is challenging. First, these structures need not be periodic. While their group theoretic description allows for the definition of a Fourier transform, it is a priori not clear in which sense a large wave-length limit with diverging tori can be performed. Second, these structures may be lower dimensional, both macroscopically and microscopically. This leads to the possibility of buckling modes that might impair stability. A related problem is that novel Korn-type inequalities are necessary in order to control atomistic strain measures in terms of configurational energy expressions.

In our recent contribution \cite{38} we have provided an efficient and extensive description of the dual space of a general discrete group of Euclidean isometries in terms of a finite union of ‘wave vector domains’ which can be related to a specific ‘translation type’ subgroup of finite index. This subgroup in turn allows to define a notion of periodicity and to construct seminorms that measure the local difference of discrete gradients to the set of rigid motions. These seminorms and, in particular, Korn type inequalities for objective structures in terms of these seminorms are studied in detail in our companion paper \cite{39}.

The main goal of the present contribution is, departing from \cite{38, 39} to obtain a general stability criterion for objective structures which identifies an appropriate stability constant and which leads to a directly implementable numerical algorithm. We achieve this in Theorem 5.10 which gives an abstract representation result in Fourier space, and Theorem 5.12 which provides an explicit formula in terms of the above mentioned wave vector domains. It turns out interesting to consider two stability constants \(\lambda_0\) and \(\lambda_{0,0}\) which measure the stability against displacements from the set of rigid motions in two different seminorms \(\|\cdot\|_R\) and \(\|\cdot\|_{R,0}\). While in the important special cases of finite structures and of space filling structures these seminorms are equivalent, this is not the case for lower dimensional infinite systems. There the distinction between these seminorms allows for a fine analysis of systems at the onset of instabilities, that may be caused by buckling modes.
As our stability constants are lower bounds on the Hessian operator of the configura
tional energy, it is worth noticing that we also have results on matching upper bounds:
Theorem 4.4 provides strong bounds for structures with equilibrized onsite potentials and
Corollary 4.15 summarizes a full and rather demanding analysis for general structures.
The algorithm resulting from Theorem 5.12 is spelled out as Algorithm 6.1. The power
of our approach is demonstrated by applying our scheme to the physically most relevant
example of a carbon nanotube [30, 15]. These structures have attracted an immense
attention in the literature due to their extraordinary mechanical and electronic properties
[11, 42, 12, 11]. A carbon nanotube can be visualized by rolling up a portion of a regular
hexagonal lattice along a lattice vector, so that a long hollow cylinder emerges on the
surface of which the atoms are bonded in a seamless way. Except for special choices of
the winding direction the nanotube will possess a non-trivial chirality.

In spite of the tremendous boom in the physical and material science literature, rigorous
analytical results are comparatively scarce and primarily focused on continuum models
such as [11, 3, 22]. Notable exceptions are [19], where under the assumption of stability
a discrete Saint-Venant principle is established for a general class of nanotubes, and the
recent contribution [24]. In [24], which appears to provide the farthest reaching results on
carbon nanotubes to date, the Cauchy-Born rule is established rigorously for an atomistic
model for stretched tubes under the assumption that the tubes be achiral. In fact, for
tubes without chirality the authors show that the stability of the cell problem can be
upscaled to the whole structure.

Our harmonic analysis based scheme in fact also applies to general carbon nanotubes
with non-trivial chirality. By way of example we explicitly apply our algorithm to a so-
called (5, 1) nanotube and a relaxed version thereof. We investigate the stability both for
stretched and natural reference configurations, see Example 6.3. While in the stretched
regime both stability constants \( \lambda_a \) and \( \lambda_{a,0,0} \) are indeed positive, we see that at the onset
of buckling \( \lambda_{a,0,0} \) vanishes while the weaker constant \( \lambda_a \) still remains positive.

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2 Objective structures

We begin by collecting some basic results on the group theoretic description of objective
structures and the quantitative analysis of their deformations in terms of suitable seminorms, cf. [38, 39].

2.1 Discrete subgroups of the Euclidean group

We collect some basic material on discrete subgroups of the Euclidean group acting on \( \mathbb{R}^d \)
from [38]. For references and proofs we refer to [38].

The Euclidean group \( E(d) \) in dimension \( d \in \mathbb{N} \) is the set of all Euclidean distance
preserving transformations of \( \mathbb{R}^d \) into itself, their elements are called Euclidean isometries.
It may be described as \( E(d) = O(d) \times \mathbb{R}^d \), the outer semidirect product of \( \mathbb{R}^d \) and
the orthogonal group \( O(d) \) in dimension \( d \) with group operation given by

\[
(A_1, b_1)(A_2, b_2) = (A_1 A_2, b_1 + A_1 b_2)
\]
for \((A_1, b_1), (A_1, b_2) \in E(d)\). We set
\[
L: E(d) \to O(d), \quad (A, b) \mapsto A \quad \text{and} \quad \tau: E(d) \to \mathbb{R}^d, \quad (A, b) \mapsto b
\]
and for \((A, b) \in E(d)\) we call \(L((A, b))\) the linear component and \(\tau((A, b))\) the translation component of \((A, b)\) so that
\[
g = (I_d, \tau(g))(L(g), 0)
\]
for each \(g \in E(d)\). An Euclidean isometry \((A, b)\) is called a translation if \(A = I_d\). The set \(\text{Trans}(d) := \{I_d\} \times \mathbb{R}^d\) of translations forms an abelian subgroup of \(E(d)\). \(E(d)\) acts on \(\mathbb{R}^d\) via
\[
(A, b) \cdot x := Ax + b \quad \text{for all } (A, b) \in E(d) \text{ and } x \in \mathbb{R}^d.
\]
For a group \(G < E(d)\) the orbit of a point \(x \in \mathbb{R}^d\) under the action of the group is
\[
G \cdot x := \{g \cdot x \mid g \in G\}.
\]
In the following we will consider discrete subgroups of the Euclidean group, which are those \(G < E(d)\) for which every orbit \(G \cdot x, x \in \mathbb{R}^d\), is discrete.

Particular examples of discrete subgroups of \(E(d)\) are the so-called space groups. These are those discrete groups \(G < E(d)\) that contain \(d\) translations whose translation components are linearly independent. Their subgroup of translations is generated by \(d\) such linearly independent translations and forms a normal subgroup of \(G\) which is isomorphic to \(\mathbb{Z}^d\).

In general, discrete subgroups of \(E(d)\) can be characterized as follows. Recall that two subgroups \(G_1, G_2 < E(d)\) are conjugate in \(E(d)\) if there exists some \(g \in E(d)\) such that \(g^{-1}G_1g = G_2\). (This corresponds to a rigid coordinate transformation in \(\mathbb{R}^d\).)

**Theorem 2.1.** Let \(G < E(d)\) be discrete, \(d \in \mathbb{N}\). There exist \(d_1, d_2 \in \mathbb{N}_0\) such that \(d = d_1 + d_2\), a \(d_2\)-dimensional space group \(S\) and a discrete group \(G' < O(d_1) \oplus S\) such that \(G\) is conjugate under \(E(d)\) to \(G'\) and \(\pi(G') = S\), where \(\pi\) is the natural surjective homomorphism \(O(d_1) \oplus E(d_2) \to E(d_2), A \oplus g \mapsto g\).

Here \(\oplus\) is the group homomorphism
\[
\oplus: O(d_1) \times E(d_2) \to E(d_1 + d_2)
\]
\[
(A_1, (A_2, b_2)) \mapsto A_1 \oplus (A_2, b_2) := \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ b_2 \end{pmatrix}
\]
and \(O(d_1) \oplus S\) is understood to be \(O(d)\) if \(d_1 = d\) and to be \(S\) if \(d_1 = 0\). The theorem allows us to assume that \(G\) is of the form \(G'\) which we will do henceforth with no loss of generality.

Such a group \(G\) can be efficiently described in terms of the space group \(S\), the kernel \(\mathcal{F}\) of \(\pi|_G\) and a section \(T \subset G\) of the translation group \(T_S\) of \(S\), i.e., a set \(T \subset G\) such that the map \(T \to T_S, g \mapsto \pi(g)\) is bijective. The group \(T \mathcal{F} = \pi|_G^{-1}(T_S)\) is a normal subgroup of \(G\) of finite index. We remark that the quantities \(d, d_1, d_2, \mathcal{F}, S\) and \(T_S\) are uniquely defined by \(G\). However, in general there is no canonical choice for \(T\), it might not be a group and the elements of \(T\) might not commute. Yet, a main result of [RS] states that there is an \(m_0 \in \mathbb{N}\) such that \(T^N = \{t^N \mid t \in T\}\) is a normal subgroup of \(G\) if and only if \(N\) is a multiple of \(m_0\):
\[
T^N \triangleleft G \iff N \in M_0 := m_0\mathbb{N}.
\]
For each \( N \in M_0 \), \( \mathcal{T}^N \) is isomorphic to \( \mathbb{Z}^{d_2} \) and of finite index in \( \mathcal{G} \). We then denote the quotient group \( \mathcal{G}/\mathcal{T}^N \) by \( \mathcal{G}_N \).

The set \( \mathcal{T} \) allows to introduce a notion of periodicity for functions defined on \( \mathcal{G} \). For a set \( S \) and \( N \in M_0 \) we say that a function \( u : \mathcal{G} \to S \) is \( \mathcal{T}^N \)-periodic if

\[
  u(g) = u(gt) \quad \text{for all} \ g \in \mathcal{G} \text{ and } t \in \mathcal{T}^N.
\]

It is called periodic if there exists some \( N \in M_0 \) such that \( u \) is \( \mathcal{T}^N \)-periodic. We also set

\[
  \mathcal{L}_{\text{per}}^\infty(\mathcal{G}, \mathbb{C}^{m \times n}) := \{ u : \mathcal{G} \to \mathbb{C}^{m \times n} \mid u \text{ is periodic} \}.
\]

(Throughout \( \mathbb{C}^{m \times n} \) is equipped with the usual Frobenius inner product and induced norm \( \| \cdot \| \).) We notice that the above definition of periodicity is independent of the choice of \( \mathcal{T} \) and that \( \mathcal{L}_{\text{per}}^\infty(\mathcal{G}, \mathbb{C}^{m \times n}) \) is a vector space. In fact, one has

\[
  \mathcal{L}_{\text{per}}^\infty(\mathcal{G}, \mathbb{C}^{m \times n}) = \left\{ \mathcal{G} \to \mathbb{C}^{m \times n}, g \mapsto u(g\mathcal{T}^N) \mid N \in M_0, u : \mathcal{G}_N \to \mathbb{C}^{m \times n} \right\}.
\]

For each \( N \in M_0 \) we now fix a representation set \( \mathcal{C}_N \) of \( \mathcal{G}/\mathcal{T}^N \) and we equip \( \mathcal{L}_{\text{per}}^\infty(\mathcal{G}, \mathbb{C}^{m \times n}) \) with the inner product \( \langle \cdot , \cdot \rangle \) given by

\[
  \langle u, v \rangle := \frac{1}{|\mathcal{C}_N|} \sum_{g \in \mathcal{C}_N} \langle u(g), v(g) \rangle \quad \text{if } u \text{ and } v \text{ are } \mathcal{T}^N\text{-periodic}
\]

for all \( u, v \in \mathcal{L}_{\text{per}}^\infty(\mathcal{G}, \mathbb{C}^{m \times n}) \). The induced norm is denoted by \( \| \cdot \|_2 \).

We denote by \( \widehat{\mathcal{G}} \) the dual space of \( \mathcal{G} \), which consists of all equivalence classes of irreducible (unitary) representations of the group \( \mathcal{G} \). (Recall that a (unitary) representation \( \rho \) of dimension \( d_\rho \) of \( \mathcal{G} \) is a homomorphism from \( \mathcal{G} \) to the unitary matrices in \( \mathbb{C}^{d_\rho \times d_\rho} \), that two representations \( \rho, \rho' \) are said to be equivalent if \( d_\rho = d_{\rho'} \) and \( T^* \rho(g)T = \rho'(g) \) for all \( g \in \mathcal{G} \) and some unitary \( d_\rho \times d_\rho \) matrix \( T \) and that \( \rho \) is said to be irreducible if the only subspaces of \( \mathbb{C}^{d_\rho} \) invariant under \( \{ \rho(g) \mid g \in \mathcal{G} \} \) are \{0\} and \( \mathbb{C}^{d_\rho} \).) We further remark that the dimensions \( d_\rho \) of irreducible representations \( \rho \) of \( \mathcal{G} \) are uniformly bounded. One-dimensional representations will be denoted by the symbol \( \chi \) and called characters. Their equivalence class is a singleton. If \( \mathcal{G} \) is abelian, then every irreducible representation of \( \mathcal{G} \) is of dimension one. In particular, \( \mathcal{T}^{m_0} \) consists of all homomorphisms from \( \mathcal{G} \) to the complex unit circle.

Observe that a representation \( \rho \) of \( \mathcal{G} \) is \( \mathcal{T}^N \)-periodic, \( N \in M_0 \), if and only if \( \rho|_{\mathcal{T}^N} = I_{d_\rho} \). We fix a representation set \( \mathcal{E} \) of \( \{ \rho \in \widehat{\mathcal{G}} \mid \rho \text{ is periodic} \} \) and define the Fourier transform as follows.

**Definition 2.2.** If \( u \in \mathcal{L}_{\text{per}}^\infty(\mathcal{G}, \mathbb{C}^{m \times n}) \) and \( \rho \) is a periodic representation of \( \mathcal{G} \), we set

\[
  \hat{u}(\rho) := \frac{1}{|\mathcal{C}_N|} \sum_{g \in \mathcal{C}_N} u(g) \otimes \rho(g) \in \mathbb{C}^{(md_\rho) \times (nd_\rho)},
\]

where \( N \in M_0 \) is such that \( u \) and \( \rho \) are \( \mathcal{T}^N \)-periodic and \( \otimes \) denotes the Kronecker product, see \([59]\).

**Proposition 2.3** (The Plancherel formula). *The Fourier transformation*

\[
  \hat{\cdot} : \mathcal{L}_{\text{per}}^\infty(\mathcal{G}, \mathbb{C}^{m \times n}) \to \bigoplus_{\rho \in \mathcal{E}} \mathbb{C}^{(md_\rho) \times (nd_\rho)}, \quad u \mapsto (\hat{u}(\rho))_{\rho \in \mathcal{E}}
\]
is well-defined and bijective. Moreover, the Plancherel formula
\[ \langle u, v \rangle = \sum_{\rho \in \mathcal{E}} d_{\rho} \langle \hat{u}(\rho), \hat{v}(\rho) \rangle \quad \text{for all } u, v \in L^\infty_{\text{per}}(\mathcal{G}, \mathbb{C}^{m \times n}) \]
holds true.

We remark that for all \( u : \mathcal{G} \rightarrow \mathbb{C}^{m \times n} \) and \( N \in M_0 \) such that \( u \) is \( T^N \)-periodic, one gets
\[ \{ \rho \in \mathcal{E} \mid \hat{u}(\rho) \neq 0 \} \subset \{ \rho \in \mathcal{E} \mid \rho \text{ is } T^N \text{-periodic} \}. \]

The following lemma provides the Fourier transform of a translated function.

**Lemma 2.4.** Let \( f \in L^\infty_{\text{per}}(\mathcal{G}, \mathbb{C}^{m \times n}) \), \( g \in \mathcal{G} \) and \( \tau_g f \) denote the translated function \( f(\cdot, g) \). Then we have \( \tau_g f \in L^\infty_{\text{per}}(\mathcal{G}, \mathbb{C}^{m \times n}) \) and
\[ \widehat{\tau_g f}(\rho) = \hat{f}(\rho)(I_n \otimes \rho(g^{-1})) \]
for all periodic representations \( \rho \) of \( \mathcal{G} \).

**Definition 2.5.** For all \( u \in L^1(\mathcal{G}, \mathbb{C}^{m \times n}) \) and all representations \( \rho \) of \( \mathcal{G} \) we define
\[ \hat{u}(\rho) := \sum_{g \in \mathcal{G}} u(g) \otimes \rho(g). \]

Note that if \( \mathcal{G} \) is finite and \( u \in L^1(\mathcal{G}, \mathbb{C}^{m \times n}) = L^\infty_{\text{per}}(\mathcal{G}, \mathbb{C}^{m \times n}) \), then the Definitions 2.2 and 2.5 for \( \hat{u} \) differ by the multiplicative constant \( |\mathcal{G}| \), but it will always be clear from the context which of the two is meant. If \( \mathcal{G} \) is infinite, there is no ambiguity as then \( L^1(\mathcal{G}, \mathbb{C}^{m \times n}) \cap L^\infty_{\text{per}}(\mathcal{G}, \mathbb{C}^{m \times n}) = \{0\} \).

**Definition 2.6.** For all \( u \in L^1(\mathcal{G}, \mathbb{C}^{l \times m}) \) and \( v \in L^\infty_{\text{per}}(\mathcal{G}, \mathbb{C}^{m \times n}) \) we define the convolution \( u * v \in L^\infty_{\text{per}}(\mathcal{G}, \mathbb{C}^{l \times n}) \) by
\[ u * v(g) := \sum_{h \in \mathcal{G}} u(h)v(h^{-1}g) \quad \text{for all } g \in \mathcal{G}. \]

**Lemma 2.7.** Let \( u \in L^1(\mathcal{G}, \mathbb{C}^{l \times m}) \), \( v \in L^\infty_{\text{per}}(\mathcal{G}, \mathbb{C}^{m \times n}) \) and \( \rho \) be a periodic representation of \( \mathcal{G} \). Then
(i) the convolution \( u * v \) is \( T^N \)-periodic if \( v \) is \( T^N \)-periodic and
(ii) we have \( \hat{u} \ast \hat{v}(\rho) = \hat{u}(\rho) \hat{v}(\rho) \).

**Wave vector characterization of the dual space**

A main result of [38] which is vital to our stability analysis is an efficient description of the dual space \( \hat{\mathcal{G}} \). It is obtained by lifting the characters on \( \mathcal{T}_S \) via \( \pi^{-1} \) to \( \mathcal{T}F = \pi^{-1}(\mathcal{T}_S) \) and then considering those representations on \( \mathcal{G} \) that are induced by representations of \( \mathcal{T}F \).

**Definition 2.8.** For all \( k \in \mathbb{R}^{d_2} \) we define the one-dimensional representation \( \chi_k \in \hat{\mathcal{T}F} \) by
\[ \chi_k(g) := \exp(2\pi i(k, \tau(\pi(g)))) \quad \text{for all } g \in \mathcal{T}F, \]
where \( \pi : \mathcal{T}F \rightarrow \mathcal{T}_S \) is the natural surjective homomorphism.
Let \( L_S < \mathbb{R}^{d_2} \) be the lattice of translational components of \( T_S \) and \( L_S^* \) its dual lattice:

\[
L_S := \tau(T_S), \quad L_S^* := \{x \in \mathbb{R}^{d_2} \mid \langle x, y \rangle \in \mathbb{Z} \text{ for all } y \in L_S\}.
\] (1)

Characters that are trivial on \( T^n \) are characterized as follows.

**Lemma 2.9.** For each \( n \in \mathbb{N} \) one has

\[
L_{S}^*/n = \{k \in \mathbb{R}^{d_2} \mid \chi_k|_{T^n} = 1\}.
\]

As \( T\mathcal{F} \) is a normal subgroup of \( G \), \( G \) acts on the set of irreducible representations of \( T\mathcal{F} \) via \( g \cdot \rho(h) = \rho(g^{-1}hg) \) for all \( h \in T\mathcal{F} \) for any \( g \in G \) and irreducible representation \( \rho \) of \( T\mathcal{F} \). This induces an action of \( G \) on \( \hat{T\mathcal{F}} \). The characters of \( T\mathcal{F} \) act on \( \hat{T\mathcal{F}} \) by multiplication.

**Definition 2.10.** We define the relation \( \sim \) on \( \hat{T\mathcal{F}} \) by

\[
(\rho \sim \rho') \iff (\exists g \in G \exists k \in \mathbb{R}^{d_2} : g \cdot \rho = \chi_k \rho').
\]

Indeed, \( \sim \) is an equivalence relation on \( \hat{T\mathcal{F}} \). The following provides an algorithm for the determination of a representation set of \( \hat{T\mathcal{F}}/\sim \).

**Lemma 2.11.**

(i) Every representation set of \( \{\rho \in \hat{T\mathcal{F}} \mid \rho|_{T^{m_0}_0} = I_{d_ρ}\}/\sim \) is a representation set of \( \hat{T\mathcal{F}}/\sim \).

(ii) The map

\[
(\hat{T\mathcal{F}})_{m_0} \to \{\rho \in \hat{T\mathcal{F}} \mid \rho|_{T^{m_0}_0} = I_{d_ρ}\}, \quad \rho \mapsto \rho \circ \pi
\]

where \( \pi: T\mathcal{F} \to (\hat{T\mathcal{F}})_{m_0} \) is the natural surjective homomorphism, is bijective. In particular, the set \( \{\rho \in \hat{T\mathcal{F}} \mid \rho|_{T^{m_0}_0} = I_{d_ρ}\} \) is finite.

(iii) Let \( K \) be a representation set of \( (L_{S}^*/m_0)\)/\( L_{S}^* \) and \( \mathcal{P} \) be a representation set of \( G/(T\mathcal{F}) \). Then, for all \( \rho, \rho' \in \{\hat{\rho} \in \hat{T\mathcal{F}} \mid \hat{\rho}|_{T^{m_0}_0} = I_{d_ρ}\} \) it holds

\[
(\rho \sim \rho') \iff (\exists g \in \mathcal{P} \exists k \in K : g \cdot \rho = \chi_k \rho').
\]

In particular, the set \( \hat{T\mathcal{F}}/\sim \) is finite. We now associate a special space group acting on \( \mathbb{R}^{d_2} \) to any \( \rho \in \hat{T\mathcal{F}} \).

**Definition 2.12.** For all \( \rho \in \hat{T\mathcal{F}} \) we define the set

\[
G_\rho := \{(L(\pi(g)), k) \mid g \in G, k \in \mathbb{R}^{d_2} : g \cdot \rho = \chi_k \rho\} \subset E(d_2),
\]

where \( \pi: G \to S \) is the natural surjective homomorphism. We also set \( G_{\rho'} := G_\rho \) if \( \rho' \in \rho \).

**Proposition 2.13.** For each \( \rho \in \hat{T\mathcal{F}} \) the set \( G_\rho \) is a \( d_2 \)-dimensional space group. It holds

\[
L_{S}^* \leq \{k \in \mathbb{R}^{d_2} \mid (I_{d_2}, k) \in G_\rho\} \leq L_{S}^*/m_0.
\]

Moreover, if \( \rho|_{T_N} = I_{d_ρ} \) with \( N \in M_0 \), then the set \( L_{S}^*/N \) is invariant under \( G_\rho \).

We can now state the main results from [38] on the structure of the set of (equivalence classes of) representations of \( G \) that are induced by (equivalence classes of) irreducible representations of \( T\mathcal{F} \). We make the following definition, cp., e.g., [40, Section 8.2].
Definition 2.14. Let $\mathcal{H}$ be a subgroup of $\mathcal{G}$ of finite index $n = |\mathcal{G} : \mathcal{H}|$. Choose a complete set of representatives $\{k_1, \ldots, k_n\}$ of the left cosets of $\mathcal{H}$ in $\mathcal{G}$. If $\rho : \mathcal{H} \to \text{U}(d_{\rho})$ is a representation of $\mathcal{H}$, we set

$$
\hat{\rho}(g) := \begin{cases} 
\rho(g) & \text{if } g \in \mathcal{H}, \\
0_{d_{\rho}, d_{\rho}} & \text{else}
\end{cases}
$$

for all $g \in \mathcal{G}$. The induced representation $\text{Ind}_{\mathcal{H}}^\mathcal{G} \rho : \mathcal{G} \to \text{U}(nd_{\rho})$ is defined by

$$
\text{Ind}_{\mathcal{H}}^\mathcal{G} \rho(g) = \left[ \hat{\rho}(k_1^{-1} g k_1) \cdots \hat{\rho}(k_n^{-1} g k_n) \right] \text{ for all } g \in \mathcal{G}.
$$

The induced representation of an equivalence class of representations is the equivalence class of the induced representation of a representative. Moreover, let $\text{Ind}_{\mathcal{H}}^\mathcal{G}(\mathcal{H})$ denote the set of all induced representations of $\mathcal{H}$. We also write $\text{Ind}$ instead of $\text{Ind}_{\mathcal{H}}^\mathcal{G}$ if $\mathcal{H}$ and $\mathcal{G}$ are clear by context.

Note that the set $R$ in the following theorems is finite.

Theorem 2.15. Let $R$ be a representation set of $\overline{T F}/\sim$. Then, the map

$$
\bigsqcup_{\rho \in R} \mathbb{R}^{d_2}/\mathcal{G}_{\rho} \to \text{Ind}_{\mathcal{H}}^\mathcal{G}(\overline{T F}), \\
(\mathcal{G}_{\rho} \cdot k, \rho) \mapsto \text{Ind}_{\mathcal{H}}^\mathcal{G}(\chi_{k \rho}),
$$

where $\bigsqcup$ is the disjoint union, is bijective.

Here the quotient space $\mathbb{R}^{d_2}/\mathcal{G}_{\rho}$ denotes the set of orbits of $\mathbb{R}^{d_2}$ under the action of $\mathcal{G}_{\rho}$. There is also a version of this result for periodic representations.

Theorem 2.16. Let $R$ be a representation set of $\{\rho \in \overline{T F} | \rho|_{T^M_0} = I_{d_{\rho}}\}/\sim$. Then the maps

(i) $\bigsqcup_{\rho \in R} \{k/N | k \in L_{\mathcal{S}}^+, N \in M_0\}/\mathcal{G}_{\rho} \to \text{Ind}(\{\rho \in \overline{T F} | \exists N \in M_0 : \rho|_{T^N} = I_{d_{\rho}}\})$

$$(\mathcal{G}_{\rho} \cdot (k/N), \rho) \mapsto \text{Ind}(\chi_{k/N \rho})$$

(ii) $\bigsqcup_{\rho \in R} (L_{\mathcal{S}}^+/N)/\mathcal{G}_{\rho} \to \text{Ind}(\{\rho \in \overline{T F} | \rho|_{T^N} = I_{d_{\rho}}\})$

$$(\mathcal{G}_{\rho} \cdot k, \rho) \mapsto \text{Ind}(\chi_{k \rho})$$

where $\bigsqcup$ is the disjoint union, $\text{Ind} = \text{Ind}_{\mathcal{H}}^\mathcal{G}$ and $N \in M_0$ in (ii) is arbitrary, are bijective.

Here the quotient spaces are well-defined in view of Proposition 2.13. As a consequence of these theorems one has the following result on the full dual space $\hat{\mathcal{G}}$.

Corollary 2.17. Let $R$ be as in Theorem 2.15. For every $\sigma \in \hat{\mathcal{G}}$ there exists a $\rho \in R$ and a $k \in \mathbb{R}^{d_2}$ such that $\sigma$ is a subrepresentation of $\text{Ind}_{\mathcal{H}}^\mathcal{G}(\chi_{k \rho})$. If moreover $R$ is as in Theorem 2.16 and $\rho|_{T^N} = I_{d_{\rho}}$ for an $N \in M_0$, then $k$ can be chosen in $L_{\mathcal{S}}^+/N$.

Remark 2.18. Although we will not need it in the sequel, we mention that even a complete characterization of $\hat{\mathcal{G}}$ up to (suitably defined) negligible sets can be achieved along the lines of the above theorems, see [38, Theorem 4.19].
2.2 Orbits of discrete subgroups of the Euclidean group

Following James [31] we define an objective (atomic) structure as a discrete point set \( S \) in \( \mathbb{R}^d \) such that for any two elements \( x_1, x_2 \in S \) there is an isometry \( g \in E(d) \) with \( g \cdot S = S \) and \( g \cdot x_1 = x_2 \). An equivalent characterization is that \( S \) be an orbit of a point under the action of a discrete subgroup of \( E(d) \), see, e.g., [32, Proposition 3.14]. With only minor loss of generality (cp. [39] Remark 2.6(ii)) we assume that the point \( x_0 \in \mathbb{R}^d \) is such that the map \( G \to \mathbb{R}^d, g \mapsto g \cdot x_0 \) is injective.

The following elementary lemmas, proved in [39], show that by changing coordinates we may without loss of generality assume that objective structures \( G \cdot x_0 \) lie in \( \{0_{d-d_{aff}}\} \times \mathbb{R}^{d_{aff}} \), where \( d_{aff} \) is their affine dimension, and that \( G \) acts trivially on \( \mathbb{R}^{d-d_{aff}} \times \{0_{d_{aff}}\} \). We denote by \( \text{aff}(A) \) the affine hull of a set \( A \subset \mathbb{R}^d \) and by \( \text{dim}(A) := \text{dim}(\text{aff}(A)) \) its affine dimension.

**Lemma 2.19.** Let \( G < E(d) \) be discrete and \( x_0 \in \mathbb{R}^d \) such that the map \( G \to \mathbb{R}^d, g \mapsto g \cdot x_0 \) is injective. Let \( d_{aff} = \text{dim}(G \cdot x_0) \). Then there exists some \( a \in E(d) \) such that for the discrete group \( G' = aGa^{-1} \) and \( x'_0 = a \cdot x_0 \) it holds

\[
\text{aff}(G' \cdot x'_0) = \{0_{d-d_{aff}}\} \times \mathbb{R}^{d_{aff}}.
\]

The map \( G' \to \mathbb{R}^d, g \mapsto g \cdot x'_0 \) is injective and we have \( G' \cdot x'_0 = a \cdot (G \cdot x_0) \).

**Lemma 2.20.** Let \( G < E(d) \) be discrete and \( x_0 \in \mathbb{R}^d \) such that \( \text{aff}(G \cdot x_0) = \{0_{d-d_{aff}}\} \times \mathbb{R}^{d_{aff}} \), where \( d_{aff} = \text{dim}(G \cdot x_0) \). Then we have \( G < \text{O}(d-d_{aff}) \oplus E(d_{aff}) \).

**Lemma 2.21.** If in addition to the assumptions of Lemma 2.20 the map \( G \to \mathbb{R}^d, g \mapsto g \cdot x_0 \) is injective, then \( G' = \{I_{d-d_{aff}} \oplus g : g \in E(d_{aff}), \exists A \in \text{O}(d-d_{aff}) : A \oplus g \in G\} < E(d) \) is isomorphic to \( G \), \( G \cdot x_0 = G' \cdot x_0 \) and the map \( G' \to \mathbb{R}^d, g \mapsto g \cdot x_0 \) is injective.

2.3 Deformations and local rigidity seminorms

We consider deformations \( y : G \cdot x_0 \to \mathbb{R}^d \) of the structure \( G \cdot x_0 \). As \( G \to G \cdot x_0 \), \( g \mapsto g \cdot x_0 \) is bijective, they can be written in terms of a ‘group deformation’ \( y_G : G \to \mathbb{R}^d \) via \( y_G(g) = y(g \cdot x_0) \). It will be convenient to consider the pulled back quantities \( g^{-1} \cdot y_G(g) \) and to associate a ‘group displacement mapping’ \( u : G \to \mathbb{R}^d \) by defining \( u(g) = g^{-1} \cdot y_G(g) - x_0 \), so that

\[
y_G(g) = g \cdot (x_0 + u(g)) \quad \text{for all } g \in G. \tag{2}
\]

In particular, \( y_G \) is the translation \( y_G(g) = g \cdot x_0 + a \) for all \( g \in G \) and an \( a \in \mathbb{R}^d \) if and only if \( L(g)u(g) = a \) for all \( g \in G \) and \( y_G \) is the rotation \( y_G(g) = R(g \cdot x_0) \) for all \( g \in G \) and an \( R \in \text{SO}(d) \) if and only if \( L(g)u(g) = (R - I_d)(g \cdot x_0) \) for all \( g \in G \).

For brevity we introduce the notation

\[
U_{\text{per},C} := L^\infty_{\text{per}}(G, \mathbb{C}^{d \times 1}) = \{u : G \to \mathbb{C}^d \mid u \text{ is periodic}\},
\]

\[
U_{\text{per}} := \{u : G \to \mathbb{R}^d \mid u \text{ is periodic}\} \subset U_{\text{per},C}.
\]

We will measure the deviation of a displacement from the set of rigid motions or a specific subset thereof locally for a given interaction range \( R \) in terms of certain seminorms on \( U_{\text{per}} \). In particular, \( || \cdot ||_R \) will measure the local distances from the set of all infinitesimal rigid motions. While the linear component of a general rigid motion is a generic skew symmetric matrix \( S \in \text{Skew}(d) \), stronger seminorms are obtained by restricting to specific
linear components. The seminorm $\| \cdot \|_{R,0}$ will measure the local distances to those rigid motions that fix $\{0_d\} \times \mathbb{R}^{d_2}$ intrinsically, corresponding to $S \in \text{Skew}(d)$ whose lower right $d_2 \times d_2$ block vanishes, while $\| \cdot \|_{R,0,0}$ will measure the local distances to those rigid motions that fix $\{0_d\} \times \mathbb{R}^{d_2}$ in $\mathbb{R}^d$, corresponding to $S = S_1 \oplus 0_{d_2,d_2}$ with $S_1 \in \text{Skew}(d_1)$. In particular, we will have $\| \cdot \|_R \leq \| \cdot \|_{R,0} \leq \| \cdot \|_{R,0,0}$.

**Definition 2.22.** For all $R \subset G$ we define the vector spaces

\[
U_{\text{trans}}(R) := \left\{ u : R \rightarrow \mathbb{R}^d \mid \exists a \in \mathbb{R}^d \forall g \in R : L(g)u(g) = a \right\},
\]

\[
U_{\text{rot}}(R) := \left\{ u : R \rightarrow \mathbb{R}^d \mid \exists S \in \text{Skew}(d) \forall g \in R : L(g)u(g) = S(g \cdot x_0 - x_0) \right\},
\]

\[
U_{\text{rot},0}(R) := \left\{ u : R \rightarrow \mathbb{R}^d \mid \exists S \in \text{Skew}(d) \forall g \in R : L(g)u(g) = S(g \cdot x_0 - x_0) \right\},
\]

\[
U_{\text{rot},0,0}(R) := \left\{ u : R \rightarrow \mathbb{R}^d \mid \exists S \in \text{Skew}(d) \forall g \in R : L(g)u(g) = S(g \cdot x_0 - x_0) \right\},
\]

where for $S = \begin{pmatrix} S_1 & S_2 \\ -S_2^T & S_3 \end{pmatrix} \in \text{Skew}(d)$ with $S_1 \in \text{Skew}(d_1), S_2 \in \mathbb{R}^{d_1 \times d_2}, S_3 \in \text{Skew}(d_2)$ we have written $S \in \text{Skew}(d)$ if $S_3 = 0$ and $S \in \text{Skew}(0,0,d)$ if $S_3 = 0$ and $S_2 = 0$. We also set

\[
U_{\text{iso}}(R) := U_{\text{trans}}(R) + U_{\text{rot}}(R),
\]

\[
U_{\text{iso},0}(R) := U_{\text{trans}}(R) + U_{\text{rot},0}(R),
\]

\[
U_{\text{iso},0,0}(R) := U_{\text{trans}}(R) + U_{\text{rot},0,0}(R).
\]

Clearly, $U_{\text{rot},0,0}(R) \subset U_{\text{rot},0}(R) \subset U_{\text{rot}}(R)$ and $U_{\text{iso},0,0}(R) \subset U_{\text{iso},0}(R) \subset U_{\text{iso}}(R)$. The following elementary proposition fixes coordinates on these sets.

**Proposition 2.23.** Suppose that $R \subset G$, $i_d \in R$ and $\text{aff}(R \cdot x_0) = \text{aff}(G \cdot x_0)$. Then the maps

\[
\varphi_1 : \mathbb{R}^d \rightarrow U_{\text{trans}}(R)
\]

\[
a \mapsto (R \rightarrow \mathbb{R}^d, g \mapsto L(g)^T a),
\]

\[
\varphi_2 : \mathbb{R}^{d_3 \times d_2} \times \text{Skew}(d_2) \rightarrow U_{\text{rot}}(R)
\]

\[
(A_1, A_2) \mapsto (R \rightarrow \mathbb{R}^d, g \mapsto L(g)^T \begin{pmatrix} 0 & A_1 \\ -A_1^T & A_2 \end{pmatrix} (g \cdot x_0 - x_0)),
\]

\[
\varphi_3 : \mathbb{R}^{d_3 \times d_2} \times \mathbb{R}^{d_3 \times d_2} \times \text{Skew}(d_4) \times \mathbb{R}^{d_2 \times d_2} \times U_{\text{rot},0}(R)
\]

\[
(A_1, A_2, A_3, A_4) \mapsto (R \rightarrow \mathbb{R}^d, g \mapsto L(g)^T \begin{pmatrix} 0 & A_1 \\ -A_1^T & A_2 \\ -A_3^T & A_4 \end{pmatrix} (g \cdot x_0 - x_0)),
\]

and

\[
\varphi_4 : \mathbb{R}^{d_3} \times \text{Skew}(d_4) \rightarrow U_{\text{rot},0,0}(R)
\]

\[
(A_1, A_2) \mapsto (R \rightarrow \mathbb{R}^d, g \mapsto L(g)^T \left( \begin{pmatrix} 0 & A_1 \\ -A_1^T & A_2 \end{pmatrix} \oplus 0_{d_2,d_2} \right) (g \cdot x_0 - x_0))
\]

are isomorphisms, where $d_3 = d - d_2$ and $d_4 = d_2 - d_2$. Moreover we have

\[
U_{\text{iso}}(R) = U_{\text{trans}}(R) \oplus U_{\text{rot}}(R),
\]

\[
U_{\text{iso},0}(R) = U_{\text{trans}}(R) \oplus U_{\text{rot},0}(R)
\]

and

\[
U_{\text{iso},0,0}(R) = U_{\text{trans}}(R) \oplus U_{\text{rot},0,0}(R).
\]
Remark 2.24. In Proposition 3.19 we show that indeed $U_{iso}(R)$ is the set of infinitesimally rigid displacements of $R$ which is the tangent space at the identity mapping to the space of finite rigid deformations.

Definition 2.25. Let $R \subset G$ be a finite set. We denote by

$$\| \cdot \|: \{ u: R \to R^d \} \to [0, \infty), \quad u \mapsto \left( \sum_{g \in R} \| u(g) \|^2 \right)^{\frac{1}{2}}$$

the Euclidean norm on $(R^d)^R$. We define three seminorms $\| \cdot \| \leq \| \cdot \|_{R,0} \leq \| \cdot \|_{R,0,0}$ on $U_{per}$ by setting

$$\| u \|_R = \left( \frac{1}{|CN|} \sum_{g \in CN} \| \pi_{U_{iso}}(R)(u(g \cdot))\|^2 \right)^{\frac{1}{2}},$$

$$\| u \|_{R,0} = \left( \frac{1}{|CN|} \sum_{g \in CN} \| \pi_{U_{iso,0}}(R)(u(g \cdot))\|^2 \right)^{\frac{1}{2}},$$

$$\| u \|_{R,0,0} = \left( \frac{1}{|CN|} \sum_{g \in CN} \| \pi_{U_{iso,0,0}}(R)(u(g \cdot))\|^2 \right)^{\frac{1}{2}},$$

whenever $u$ is $T^N$-periodic. Here $\pi_{U_{iso}}(R), \pi_{U_{iso,0}}(R), \pi_{U_{iso,0,0}}(R)$ are the orthogonal projections on $\{ u: R \to R^d \}$ with respect to the norm $\| \cdot \|$ with kernels $U_{iso}(R), U_{iso,0}(R)$ and $U_{iso,0,0}(R)$, respectively.

Due to the discrete nature of the underlying objective structure these seminorms can equivalently be described as seminorms on (discrete) gradients.

Definition 2.26. For all $u \in U_{per}$ and finite sets $R \subset G$ we define the discrete derivative

$$\nabla_R u: G \to \{ v: R \to R^d \}
\quad g \mapsto (\nabla_R u(g)): R \to R^d, h \mapsto u(gh) - L(h)^T u(g)).$$

Definition 2.27. For each finite set $R \subset G$ we define the seminorms $\| \cdot \|_{R,\nabla} \leq \| \cdot \|_{R,\nabla,0} \leq \| \cdot \|_{R,\nabla,0,0} \leq \| \nabla_R \cdot \|_2$ on $U_{per}$ by setting

$$\| u \|_{R,\nabla} = \left( \frac{1}{|CN|} \sum_{g \in CN} \| \pi_{U_{rot}}(R)(\nabla_R u(g))\|^2 \right)^{\frac{1}{2}},$$

$$\| u \|_{R,\nabla,0} = \left( \frac{1}{|CN|} \sum_{g \in CN} \| \pi_{U_{rot,0}}(R)(\nabla_R u(g))\|^2 \right)^{\frac{1}{2}},$$

$$\| u \|_{R,\nabla,0,0} = \left( \frac{1}{|CN|} \sum_{g \in CN} \| \pi_{U_{rot,0,0}}(R)(\nabla_R u(g))\|^2 \right)^{\frac{1}{2}},$$

$$\| \nabla_R u \|_2 = \left( \frac{1}{|CN|} \sum_{g \in CN} \| \nabla_R u(g)\|^2 \right)^{\frac{1}{2}},$$

whenever $u$ is $T^N$-periodic. Here $\pi_{U_{rot}}(R), \pi_{U_{rot,0}}(R), \pi_{U_{rot,0,0}}(R)$ are the orthogonal projections on $\{ u: R \to R^d \}$ with respect to the norm $\| \cdot \|$ with kernels $U_{rot}(R), U_{rot,0}(R)$ and $U_{rot,0,0}(R)$, respectively.

Remark 2.28. (i) If $u \in U_{per}$ is $T^N$-periodic for some $N \in M_0$ and $R \subset G$ is finite, then also the discrete derivative $\nabla_R u$ is $T^N$-periodic.
The definitions of $\| \cdot \|_{\mathcal{R},0}$, $\| \cdot \|_{\mathcal{R},0,0}$, $\| \cdot \|_{\mathcal{R},\nabla,0}$, $\| \cdot \|_{\mathcal{R},\nabla,0,0}$ and $\| \nabla \mathcal{R} \cdot \|_2$ are independent of the choice of $\mathcal{C}_N$.

The main result of [39] is summarized in the following Theorem 2.30 on the equivalence of seminorms whenever the range $\mathcal{R}$ is rich enough. For this we first introduce the following notation.

**Definition 2.29.** We say $\mathcal{R} \subset \mathcal{G}$ has Property 1 if $\mathcal{R}$ is finite, $id \in \mathcal{R}$ and

$$\text{aff}(\mathcal{R} \cdot x_0) = \text{aff}(\mathcal{G} \cdot x_0).$$

We say $\mathcal{R} \subset \mathcal{G}$ has Property 2 if $\mathcal{R}$ is finite and there exist two sets $\mathcal{R}', \mathcal{R}'' \subset \mathcal{G}$ such that $id \in \mathcal{R}'$, $\mathcal{R}'$ generates $\mathcal{G}$, $\mathcal{R}''$ has Property 1 and $\mathcal{R}'\mathcal{R}'' \subset \mathcal{R}$.

**Theorem 2.30.** Suppose that $\mathcal{R}_1, \mathcal{R}_2 \subset \mathcal{G}$ have Property 2. Then the seminorms $\| \cdot \|_{\mathcal{R}_1}$, $\| \cdot \|_{\mathcal{R}_2}$, $\| \cdot \|_{\mathcal{R}_1,0}$, $\| \cdot \|_{\mathcal{R}_2,0}$, $\| \cdot \|_{\mathcal{R}_1,\nabla}$, $\| \cdot \|_{\mathcal{R}_2,\nabla}$, $\| \cdot \|_{\mathcal{R}_1,\nabla,0}$ and $\| \cdot \|_{\mathcal{R}_2,\nabla,0}$ are equivalent and their kernel is $U_{\text{iso},0,0} \cap U_{\text{per}}$.

**Remark 2.31.** (i) The highly non-trivial part of this theorem is that for an $\mathcal{R} \subset \mathcal{G}$ with Property 2 the two seminorms $\| \cdot \|_{\mathcal{R}}$ and $\| \cdot \|_{\mathcal{R},0}$ are equivalent. This is a discrete Korn inequality for objective structures.

(ii) Examples show that in general $\| \cdot \|_{\mathcal{R}}$ and $\| \cdot \|_{\mathcal{R},0,0}$ are not equivalent.

For the stronger seminorms we have:

**Theorem 2.32.** (i) Suppose that $\mathcal{R}_1, \mathcal{R}_2 \subset \mathcal{G}$ have Property 2. Then the seminorms $\| \cdot \|_{\mathcal{R}_1,0}$, $\| \cdot \|_{\mathcal{R}_1,0,0}$, $\| \cdot \|_{\mathcal{R}_2,0}$, $\| \cdot \|_{\mathcal{R}_2,0,0}$, $\| \cdot \|_{\mathcal{R}_1,\nabla,0}$, $\| \cdot \|_{\mathcal{R}_2,\nabla,0}$ are equivalent and their kernel is $U_{\text{iso},0,0} \cap U_{\text{per}}$.

(ii) Let $\mathcal{R}_1, \mathcal{R}_2 \subset \mathcal{G}$ be finite generating sets of $\mathcal{G}$. Then the seminorms $\| \nabla \mathcal{R}_1 \cdot \|_2$ and $\| \nabla \mathcal{R}_2 \cdot \|_2$ on $U_{\text{per}}$ are equivalent and their kernel is $U_{\text{trans}} \cap U_{\text{per}}$.

For space groups this leads to a full Korn inequality:

**Theorem 2.33.** Suppose that $\mathcal{G}$ is a space group and $\mathcal{R} \subset \mathcal{G}$ has Property 2. Then the seminorms $\| \cdot \|_{\mathcal{R}}$, $\| \cdot \|_{\mathcal{R},0}$ and $\| \nabla \mathcal{R} \cdot \|_2$ are equivalent and their kernel is $U_{\text{trans}}$.

### 3 Energy, criticality and stability

#### 3.1 Configurational energy and stability constants

We assume that the configurational energy of a deformed objective structure is given as a sum of site potentials that describe the interaction of any single atom with all other atoms. Although we will consider bounded perturbations of the identity eventually, it will be convenient to define the interaction potential on all of $(\mathbb{R}^d)^{\mathcal{G}\setminus\{id\}}$, cf. Remark 3.2(iv) below.

**Definition 3.1.** Let

$$V: (\mathbb{R}^d)^{\mathcal{G}\setminus\{id\}} \to \mathbb{R}$$

be the interaction potential. We assume that $V$ has the following properties:

(H1) (Invariance under $O(d)$) For all $R \in O(d)$ and $y: \mathcal{G} \setminus \{id\} \to \mathbb{R}^d$ we have

$$V(Ry) = V(y).$$
(H2) (Smoothness) For all \( y : \mathcal{G} \setminus \{id\} \to \mathbb{R}^d \) the function
\[
L^\infty(\mathcal{G} \setminus \{id\}, \mathbb{R}^d) \to \mathbb{R}
\]
\[
z \mapsto V(y + z)
\]
is two times continuously Fréchet differentiable, where \( L^\infty(\mathcal{G} \setminus \{id\}, \mathbb{R}^d) \) is the vector space of all bounded functions from \( \mathcal{G} \setminus \{id\} \) to \( \mathbb{R}^d \) equipped with the uniform norm \( \| \cdot \|_\infty \).

For all \( y : \mathcal{G} \setminus \{id\} \to \mathbb{R}^d \) and \( g, h \in \mathcal{G} \setminus \{id\} \) we define the partial Jacobian row vector \( \partial_y V(y) \in \mathbb{R}^d \) by
\[
(\partial_y V(y))_i := V'(y)(\delta_y e_i)
\]
and the partial Hessian matrix \( \partial_y \partial_h V(y) \in \mathbb{R}^{d \times d} \) by
\[
(\partial_y \partial_h V(y))_{ij} := V''(y)(\delta_y e_i, \delta_h e_j)
\]
where \( \delta_y : \mathcal{G} \setminus \{id\} \to \{0, 1\}, l \mapsto \delta_{k,l} \) for all \( k \in \mathcal{G} \).

(H3) (Summability) For all \( y : \mathcal{G} \setminus \{id\} \to \mathbb{R}^d \) we have
\[
\sum_{g \in \mathcal{G} \setminus \{id\}} \| \partial_y V(y) \| < \infty \quad \text{and} \quad \sum_{g, h \in \mathcal{G} \setminus \{id\}} \| \partial_y \partial_h V(y) \| < \infty.
\]

We say a set \( \mathcal{R}_V \subset \mathcal{G} \setminus \{id\} \) is an interaction range of \( V \) if for all \( y : \mathcal{G} \setminus \{id\} \to \mathbb{R}^d \) we have \( V(y) = V(\chi_{\mathcal{R}_V} y) \), where \( \chi_{\mathcal{R}_V} \) is the indicator function. We denote \( y_0 = (g \cdot x_0 - x_0)_{g \in \mathcal{G} \setminus \{id\}} \in (\mathbb{R}^d)^{\mathcal{G} \setminus \{id\}} \). If \( V \) has finite interaction range, then we extend the domain of \( V'(y_0) \) and \( V''(y_0) \) to \( \{ z : \mathcal{G} \setminus \{id\} \to \mathbb{R}^d \} \) and \( \{ z : \mathcal{G} \setminus \{id\} \to \mathbb{R}^d \}^2 \), respectively, by
\[
V'(y_0)z_1 := V'(y_0)(\chi_{\mathcal{R}_V} z_1)
\]
and
\[
V''(y_0)(z_1, z_2) := V''(y_0)(\chi_{\mathcal{R}_V} z_1, \chi_{\mathcal{R}_V} z_2)
\]
for all \( z_1, z_2 \in \{ z : \mathcal{G} \setminus \{id\} \to \mathbb{R}^d \} \setminus \mathcal{R}_V \) and \( L^\infty(\mathcal{G} \setminus \{id\}, \mathbb{R}^d) \), where \( \mathcal{R}_V \) is a finite interaction range of \( V \).

Remark 3.2. (i) For all \( y : \mathcal{G} \setminus \{id\} \to \mathbb{R}^d \) and \( z, z_1, z_2 \in L^\infty(\mathcal{G} \setminus \{id\}, \mathbb{R}^d) \) we have
\[
V'(y)z = \sum_{g \in \mathcal{G} \setminus \{id\}} \partial_y V(y)z(g)
\]
and
\[
V''(y)(z_1, z_2) = \sum_{g, h \in \mathcal{G} \setminus \{id\}} z_1(g)^T \partial_y \partial_h V(y)z_2(h).
\]

(ii) In Section 3.3 and Section 4 we assume that \( V \) has finite interaction range.

(iii) If \( V \) has finite interaction range, then [H2] implies [H3].

(iv) For simplicity we assume that the domain of \( V \) is the whole space \((\mathbb{R}^d)^{\mathcal{G} \setminus \{id\}}\). It would be sufficient if \( V \) is defined only on \( O(d)y_0 + U \), where \( U \) is a small neighbourhood of \( 0 \in (\mathbb{R}^d)^{\mathcal{G} \setminus \{id\}} \) with respect to the uniform norm.
Example 3.3. An example of an interaction potential consisting of pair potentials is
\[ V : (\mathbb{R}^d)^G \setminus \{id\} \to \mathbb{R}, \quad y \mapsto \sum_{g \in G \setminus \{id\}} v(||y(g)||), \]
where
\[ v : (0, \infty) \to \mathbb{R}, \quad r \mapsto r^{-12} - r^{-6} \]
is the Lennard-Jones potential.

Recall from (2) that, for a given displacement \( u : G \to \mathbb{R}^d \) the physical particles are at the points \((y_G(g))_{g \in G} = (g \cdot (x_0 + u(g))_{g \in G}\) and in particular \( u = 0 \) for the identity mapping. It will be convenient to write the energy as a functional acting on \( w = \chi_G x_0 + u \) so that \( y_G(g) = g \cdot w(g) \) for \( g \in G \) and \( w = \chi_G x_0 \) corresponds to the identity deformation.

Definition 3.4. Let
\[ E : U_{\text{per}} \to \mathbb{R} \]
\[ w \mapsto \frac{1}{|C_N|} \sum_{g \in C_N} V\left(\left(gh \cdot w(gh) - g \cdot w(g)\right)_{h \in G \setminus \{id\}}\right) \]
if \( w \) is \( T^N \)-periodic and \( N \in M_0 \)
be the configurational energy.

Remark 3.5. The function \( E \) is well-defined and independent of the choice of the representation set \( C_N \) for all \( N \in M_0 \).

Lemma 3.6. The function \( E \) is two times continuously Fréchet differentiable with respect to the uniform norm \( \| \cdot \|_\infty \). We have
\[ E(\chi_G x_0) = V(y_0), \]
\[ E'(\chi_G x_0)u = \frac{1}{|C_N|} \sum_{g \in C_N} V'(y_0)(L(h)u(gh) - u(g))_{h \in G \setminus \{id\}}, \]
and
\[ E''(\chi_G x_0)(u, v) = \frac{1}{|C_N|} \sum_{g \in C_N} V''(y_0)\left(\left((L(h)u(gh) - u(g))_{h \in G \setminus \{id\}}, (L(h)v(gh) - v(g))_{h \in G \setminus \{id\}}\right)\right) \]
for all \( u, v \in U_{\text{per}} \) and \( N \in M_0 \) such that \( u \) and \( v \) are \( T^N \)-periodic.

Proof. By \([H1]\) we have
\[ E(u) = \frac{1}{|C_N|} \sum_{g \in C_N} V\left(\left(h \cdot u(gh) - u(g)\right)_{h \in G \setminus \{id\}}\right) \tag{3} \]
for all \( u \in U_{\text{per}} \) and \( N \in M_0 \) such that \( u \) is \( T^N \)-periodic. By \([H2]\) the function \( V \) is two times Fréchet differentiable. We define the vector space
\[ W = \left\{ w : G \to L^\infty(G \setminus \{id\}, \mathbb{R}^d) \mid w \text{ is periodic} \right\} \]
and equip \( U_{\text{per}} \) and \( W \) each with the uniform norm \( \| \cdot \|_\infty \). The linear map
\[ \varphi_1 : U_{\text{per}} \to W \]
\[ u \mapsto \left( G \to L^\infty(G \setminus \{id\}, \mathbb{R}^d), g \mapsto (L(h)u(gh) - u(g))_{h \in G \setminus \{id\}} \right) \]

is bounded and thus two times continuously Fréchet differentiable. The first and second derivative of the function
\[
\varphi_2: W \to \mathbb{R}
\]
\[
w \mapsto \frac{1}{|C_N|} \sum_{g \in C_N} V((\tau(h))_{h \in G \setminus \{id\}} + w(g)) \quad \text{if } w \text{ is } T^N\text{-periodic}
\]
is given by
\[
\varphi_2'(w)w_1 = \frac{1}{|C_N|} \sum_{g \in C_N} V'((\tau(h))_{h \in G \setminus \{id\}} + w(g))w_1(g)
\]
and
\[
\varphi_2''(w)(w_1, w_2) = \frac{1}{|C_N|} \sum_{g \in C_N} V''((\tau(h))_{h \in G \setminus \{id\}} + w(g))(w_1(g), w_2(g))
\]
for all \(w, w_1, w_2 \in W\) and \(N \in M_0\) such that \(w, w_1\) and \(w_2\) are \(T^N\)-periodic. Thus \(\varphi_2\) is two times continuously Fréchet differentiable. Since \(E = \varphi_2 \circ \varphi_1\), also the function \(E\) is two times continuously Fréchet differentiable.

Equation (3) also implies the representations of \(E(\chi_G x_0), E'(\chi_G x_0)\) and \(E''(\chi_G x_0)\).

\[\Box\]

Remark 3.7. (i) If the map in [H2] is \(n\) times (continuously) Fréchet differentiable for some natural number \(n\), then also \(E\) is \(n\) times (continuously) Fréchet differentiable with respect to the uniform norm \(\| \cdot \|_\infty\). The proof is analogous.

(ii) The function \(E\) need not be continuous with respect to the norm \(\| \cdot \|_2\). In particular \(E\) is not two times Fréchet differentiable with respect to \(\| \nabla_R \cdot \|_2\) although in other models a similar proposition is true, see, e.g., [34, Theorem 1].

We fix a finite set \(R \subset G\) with Property 2. Furthermore we assume that \(G\) is not the trivial group such that \(\lambda_a < \infty\) and \(\lambda_{a,0,0} < \infty\) in the following.

Definition 3.8. We say that \(w \in U_{\text{per}}\) is a critical point of \(E\) if \(E'(w) = 0\). We say that \((G, x_0, V)\) is stable (in the atomistic model) with respect to \(\| \cdot \|_R\) (resp. \(\| \cdot \|_{R,0,0}\)) \(\lambda_a < \infty\) and \(\lambda_{a,0,0} < \infty\) in the following.

We define the constants
\[
\lambda_a := \sup \{ c \in \mathbb{R} \mid \forall u \in U_{\text{per}} : c\|u\|_R^2 \leq E''(\chi_G x_0)(u, u) \} \in \mathbb{R} \cup \{-\infty\}
\]
and
\[
\lambda_{a,0,0} := \sup \{ c \in \mathbb{R} \mid \forall u \in U_{\text{per}} : c\|u\|_{R,0,0}^2 \leq E''(\chi_G x_0)(u, u) \} \in \mathbb{R} \cup \{-\infty\}.
\]

Remark 3.9. (i) The bilinear form \(E''(\chi_G x_0)\) is coercive with respect to the seminorm \(\| \cdot \|_R\) (resp. \(\| \cdot \|_{R,0,0}\)) if and only if \(\lambda_a > 0\) (resp. \(\lambda_{a,0,0} > 0\)).

(ii) If \((G, x_0, V)\) is stable with respect to \(\| \cdot \|_{R,0,0}\), then \((G, x_0, V)\) is also stable with respect to \(\| \cdot \|_R\), since \(\| \cdot \|_R \leq \| \cdot \|_{R,0,0}\).

(iii) The above definition of the stability and the constant \(\lambda_a\) generalizes the definition in [29] where these terms are defined for lattices. For lattices we have \(\lambda_a = \lambda_{a,0,0}\) since then \(\| \cdot \|_R = \| \cdot \|_{R,0,0}\).
(iv) By Theorem 2.30 the stability of $\mathcal{G}, x_0, V$ is independent of the choice of $\mathcal{R}$.

(v) The constants $\lambda_a$ and $\lambda_{a,0,0}$ need not be finite, see Example 4.16 and Example 4.17. In Section 4 we present sufficient conditions for both $\lambda_a \in \mathbb{R}$ and $\lambda_{a,0,0} \in \mathbb{R}$.

The following proposition states a characterization of $\lambda_a$ and $\lambda_{a,0,0}$ by means of the dual problem.

**Proposition 3.10.** We have

$$
\lambda_a = \inf\{E''(\chi_G x_0)(u, u) \mid u \in U_{\text{per}}, \|u\|_R = 1\}
$$

and

$$
\lambda_{a,0,0} = \inf\{E''(\chi_G x_0)(u, u) \mid u \in U_{\text{per}}, \|u\|_{R,0,0} = 1\}.
$$

**Proof.** We denote $\text{RHS} = \inf\{E''(\chi_G x_0)(u, u) \mid u \in U_{\text{per}}, \|u\|_R = 1\}$. It is clear that $\lambda_a \leq \text{RHS}$. Let $c \in \mathbb{R}$ be such that $c > \lambda_a$. There exists some $u \in U_{\text{per}}$ such that $c\|u\|_R^2 > E''(\chi_G x_0)(u, u)$. By Theorem 2.30, Proposition 2.23 and since the group $\mathcal{G}$ is not trivial, we have $\ker(\| \cdot \|_R) \neq U_{\text{per}}$. Thus and since $\| \cdot \|_R \leq \sqrt{\|R\|} \| \cdot \|_\infty$, we may assume that $\|u\|_R = 1$. Thus we have RHS $\leq c$. Since $c$ was arbitrary, we have $\lambda_a \geq \text{RHS}$.

The proof of the characterization of $\lambda_{a,0,0}$ is analogous.

\[ \square \]

### 3.2 Characterization of a critical point

**Definition 3.11.** We define the row vector

$$
e_V := \sum_{g \in \mathcal{G}\backslash\{id\}} \partial_g V(y_0)(L(g) - I_d) \in \mathbb{R}^d
$$

and the function $f_V \in L^1(\mathcal{G}, \mathbb{R}^{d \times d})$ by

$$
f_V(g) := \sum_{h_1, h_2 \in \mathcal{G}\backslash\{id\}} \left( \delta_{g,h_2^{-1}h_1} L(h_2)^T \partial_{h_2} \partial_{h_1} V(y_0) L(h_1) - \delta_{g,h_2^{-1}h_1} L(h_2)^T \partial_{h_2} \partial_{h_1} V(y_0) \right)

- \delta_{g,h_1} \partial_{h_1} \partial_{h_1} V(y_0) L(h_1) + \delta_{g,0} \partial_{h_2} \partial_{h_1} V(y_0)
$$

for all $g \in \mathcal{G}$.

**Remark 3.12.** (i) By (H3) the function $f_V$ is well-defined and we have

$$
\sum_{g \in \mathcal{G}} f_V(g) = \sum_{h_1, h_2 \in \mathcal{G}\backslash\{id\}} (L(h_2) - I_d)^T \partial_{h_2} \partial_{h_1} V(y_0) (L(h_1) - I_d).
$$

(ii) If $\mathcal{R}_V$ is an interaction range of $V$, then we have

$$
\text{supp } f_V \subset \mathcal{R}_V^{-1} \mathcal{R}_V \cup \mathcal{R}_V^{-1} \cup \mathcal{R}_V.
$$

In particular, if $V$ has finite interaction range, then the support of $f_V$ is finite.

**Definition 3.13.** For all $N \in M_0$ and $g, h \in \mathcal{G}_N$ we define the partial Jacobian row vector $\partial_g E(\chi_G x_0) \in \mathbb{R}^d$ by

$$
(\partial_g E(\chi_G x_0))_i := E'(\chi_G x_0)(\delta_g e_i)
$$

and the partial Hessian matrix $\partial_g \partial_h E(\chi_G x_0) \in \mathbb{R}^{d \times d}$ by

$$
(\partial_g \partial_h E(\chi_G x_0))_{ij} := E''(\chi_G x_0)(\delta_g e_i, \delta_h e_j)
$$

for all $i, j \in \{1, \ldots, d\}$, where $\delta_k : \mathcal{G} \to \{0,1\}$, $l \mapsto \delta_{k,l} \text{ for all } k \in \mathcal{G}_N$. 

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The following lemma characterizes the first and second derivative of $E$.

**Lemma 3.14.** Let $N \in M_0$. We have

$$\partial g E(\chi_G x_0) = \frac{1}{|C_N|} e_V$$

for all $g \in G_N$

and

$$\partial g_2 \partial g_1 E(\chi_G x_0) = \frac{1}{|C_N|} \sum_{g \in g_2^{-1} g_1} f_V(g)$$

for all $g_1, g_2 \in G_N$.

In particular we have

$$\partial g E(\chi_G x_0) = \partial \text{id} E(\chi_G x_0)$$

for all $g \in G_N$

and

$$\partial g_2 \partial g_1 E(\chi_G x_0) = \partial \text{id} \partial g_2^{-1} g_1 E(\chi_G x_0)$$

for all $g_1, g_2 \in G_N$.

**Proof.** Let $N \in M_0$, $g_1, g_2 \in G$ and for all $g \in G_N$ let $\delta_g$ be as in Definition 3.13. Since $T^N$ is a normal subgroup of $G$, we have

$$\sum_{g \in C_N} \delta_{g_1 T^N} (gh) = \sum_{g \in C_N} \sum_{t \in T^N} \delta_{g_1 t^{-1} g_1 t} = 1$$

for all $h \in G$. (4)

Using Lemma 3.6, Remark 3.2(i) and (4), we have

$$\partial_{g_1 T^N} E(\chi_G x_0) = (E'(\chi_G x_0)(\delta_{g_1 T^N} e_i))_{i \in \{1, \ldots, d\}}$$

$$= \frac{1}{|C_N|} \sum_{g \in C_N} \sum_{h \in G \setminus \{id\}} \partial h V(y_0)((\delta_{g_1 T^N} (gh) L(h) - \delta_{g_1 T^N} (g) I_d)$$

$$= \frac{1}{|C_N|} \sum_{h \in G \setminus \{id\}} \partial h V(y_0)(L(h) - I_d)$$

$$= \frac{1}{|C_N|} e_V.$$ (5)

The right hand side of (5) is independent of $g_1 T^N$ and in particular, we have

$$\partial_{g_1 T^N} E(\chi_G x_0) = \partial T^N E(\chi_G x_0).$$

Since $T^N$ is a normal subgroup of $G$, for all $h_1, h_2 \in G$ we have

$$\sum_{g \in C_N} \delta_{g_2 T^N} (gh_2) \delta_{g_1 T^N} (gh_1) = \sum_{g \in C_N} \sum_{t,s \in T^N} \delta_{g_2 h_2^{-1} g_1 h_1^{-1} t g s}$$

$$= \sum_{t \in T^N} \delta_{g_2 h_2^{-1} g_1 h_1^{-1} t}$$

$$= \sum_{t \in T^N} \delta_{h_2^{-1} h_1 g_2^{-1} g_1 t}.$$ (6)
Using Lemma 3.6 and Remark 3.2(i) and (ii), we have

\[
\frac{\partial_{g_2 T_N} \partial_{g_1 T_N}}{E(\chi G x_0)} = (E'(\chi G x_0)(\delta_{g_2 T_N} e_i, \delta_{g_1 T_N} e_j))_{i,j \in \{1,\ldots,d\}} \]

\[
\frac{1}{|CN|} \sum_{g \in C_N} \sum_{h_1, h_2 \in G \{id\}} (\delta_{g_2 T_N} (gh_2) L(h_2) - \delta_{g_2 T_N} (g) I_d) \partial h_2 \partial h_1 V(y_0)
\]

\[
(\delta_{g_1 T_N} (g_1) L(h_1) - \delta_{g_1 T_N} (g) I_d)
\]

\[
= \frac{1}{|CN|} \sum_{t \in T_N} \sum_{h_1, h_2 \in G \{id\}} (\delta_{h_1^{-1} h_2^{-1} g_1} L(h_2) \partial h_1 V(y_0) - \delta_{h_1, h_2^{-1} g_1} \partial h_2 \partial h_1 V(y_0) L(h_1) + \delta_{v, g_1} \partial h_2 \partial h_1 V(y_0))
\]

\[
= \frac{1}{|CN|} \sum_{t \in T_N} f_V(g_2^{-1} g_1 t).
\]

The right hand side of (7) is only dependent on \(g_2^{-1} g_1 T_N\) and in particular, we have

\[
\frac{\partial_{g_2 T_N} \partial_{g_1 T_N}}{E(\chi G x_0)} = \partial_{v} \partial_{g_2^{-1} g_1 T_N} E(\chi G x_0).
\]

**Remark 3.15.**

(i) The configurational energy is left-translation-invariant, i.e. for all \(w \in U_{per}\) and \(g \in G\) it holds \(E(w) = E(w)\). This implies that also \(E'(\chi G x_0)\) and \(E''(\chi G x_0)\) are left-translation-invariant, i.e. \(E'(\chi G x_0) u = E'(\chi G x_0) u(g \cdot).\) and \(E''(\chi G x_0) u, v = E'(\chi G x_0) (u(g \cdot) , v(g \cdot))\) for all \(u \in U_{per}\) and \(g \in G\). This directly shows that \(\partial_{g_1} E(\chi G x_0) = \partial_{v} \partial_{g_1} E(\chi G x_0) = \partial_{g_1} \partial_{v} E(\chi G x_0) = \partial_{v} \partial_{g_1} E(\chi G x_0) = \partial_{v} \partial_{g_1} E(\chi G x_0)\) for all \(N \in M_0\) and \(g_1, g_2 \in G N\).

(ii) By the above lemma we have

\[
e_V = (E'(\chi G x_0)(\chi G e_i))_{i \in \{1,\ldots,d\}}.
\]

Now we suppose that \(V\) has finite interaction range \(R_V \subset G \{id\}.\) By Remark 3.12(ii) we have

\[
supp f_V \subset R_V^{-1} R_V \cup R_V \cup R_V^{-1} =: R_{f_V}
\]

and by the above lemma we have

\[
f_V(g) = \begin{cases} |CN| \partial_{id} \partial_{g T_N} E(\chi G x_0) & \text{for all } g \in R_{f_V} \\ 0, & \text{else} \end{cases}
\]

for all \(N \in M_0\) large enough, precisely for all \(N \in M_0\) such that

\[
T_N \cap R_{f_V}^{-1} R_{f_V} \subset \{id\}.
\]

**Corollary 3.16.** It holds \(E'(\chi G x_0) = 0\) if and only if \(e_V = 0\)

**Proof.** This is clear by Lemma 3.14.

**Corollary 3.17.** Suppose that \(G < \text{Trans}(d)\). Then we have \(E'(\chi G x_0) = 0\).

**Proof.** This is clear by Corollary 3.16.

**Corollary 3.18.** The triple \((G, x_0, V)\) is stable with respect to \(\| \cdot \|_R\) (resp. \(\| \cdot \|_{R_0,0}\)) if and only if \(e_V = 0\) and \(\lambda_n > 0\) (resp. \(\lambda_{n,0,0} > 0\)).

**Proof.** This is clear by Corollary 3.16 and Remark 3.1.
3.3 A sufficient condition for a local minimum

We now prove that, in case $d_1 \in \{0, 1, d\}$, stable critical points are local minima of the energy functional. In the following $\mathcal{R} \subset \mathcal{G}$ is a finite set with Property 2. We first notice that the space $U_{iso}(\mathcal{R})$ of infinitesimally rigid displacements of $\mathcal{R}$ is indeed the tangent space at the identity mapping to the space of nonlinearly rigid deformations.

**Proposition 3.19.** There exists an open neighborhood $U \subset E(d)$ of $id$ such that the set

$$\{ u: \mathcal{R} \to \mathbb{R}^d \mid \exists a \in U \forall g \in \mathcal{R}: g \cdot (x_0 + u(g)) = a \cdot (g \cdot x_0) \}$$

is a manifold and $U_{iso}(\mathcal{R})$ is its tangent space at the point 0.

**Proof.** Let $B = \{ S \in \text{Skew}(d) \mid \| S \| < c \}$ with $c > 0$ so small that the matrix exponential $\exp: B \to \exp(B)$ is a diffeomorphism onto a neighborhood $\exp(B)$ of $I_d$ in $SO(d)$. Let $log$ be its inverse map. Let $U \subset \text{Skew}((d - d_{aff}) + d_{aff})$ be a neighborhood of 0 such that the map

$$f: U \to \text{Skew}(d)
\begin{pmatrix}
S_1 & A \\
-A^T & S_2
\end{pmatrix} \mapsto \log\left(\exp\left(\begin{pmatrix} 0 & A \\ -A^T & \text{Id} \end{pmatrix}\right)\exp\left(\begin{pmatrix} S_1 & 0 \\ 0 & 0 \end{pmatrix}\right)\right)$$

is well-defined. By the inverse function theorem there exists an open neighborhood $V \subset U$ of 0 such that $W := f(V)$ is an open neighborhood of 0 and the map $f|_V: V \to W$ is a diffeomorphism. Without loss of generality we may assume that

$$V = \left\{ \begin{pmatrix} S_1 & A \\
-A^T & S_2 \end{pmatrix} \bigg| S_1 \in V_1, (A, S_2) \in V_2 \right\},$$

where $V_1 \subset \text{Skew}(d-d_{aff})$ is an open neighborhood of 0 and $V_2 \subset \mathbb{R}^{(d-d_{aff}) \times d_{aff}} \times \text{Skew}(d_{aff})$ is an open neighborhood of 0. The set $X := \{(\exp(T), b) \mid T \in \mathbb{R}, b \in \mathbb{R}^d \} \subset E(d)$ is an open neighborhood of $id$. We have

$$M := \{ u: \mathcal{R} \to \mathbb{R}^d \mid \exists a \in X \forall g \in \mathcal{R}: g \cdot (x_0 + u(g)) = a \cdot (g \cdot x_0) \}$$

$$= \left\{ (L(g)^T(b + (\exp(T) - I_d)(g \cdot x_0)))_{g \in \mathcal{R}} \bigg| b \in \mathbb{R}^d, T \in W \right\}$$

$$= \left\{ (L(g)^T(b + \left(\exp\left(\begin{pmatrix} 0 & A \\ -A^T & \text{Id} \end{pmatrix}\right) - I_d\right)(g \cdot x_0 - x_0))_{g \in \mathcal{R}} \bigg| b \in \mathbb{R}^d, (A, S) \in V_2 \right\}$$

since $g \cdot x_0 - x_0 \in \{0_{d-d_{aff}}\} \times \mathbb{R}^{d_{aff}}$ for all $g \in \mathcal{R}$. Thus the map

$$h: \mathbb{R}^d \times V_2 \to M
(b, A, S) \mapsto \left(L(g)^T(b + \left(\exp\left(\begin{pmatrix} 0 & A \\ -A^T & S \end{pmatrix}\right) - I_d\right)(g \cdot x_0 - x_0))\right)_{g \in \mathcal{R}}$$

is surjective. Since $\mathcal{R} \subset \mathcal{G}$ has Property 1, there exists some $C = (c_g)_{g \in \mathcal{R}} \in \mathbb{R}^{d_{aff} \times |\mathcal{R}|}$ of rank $d_{aff}$ such that $(g \cdot x_0 - x_0)_{g \in \mathcal{R}} = (0_0)$. We have

$$h'(0): \mathbb{R}^d \times V_2 \to (\mathbb{R}^d)^\mathcal{R}
(b, A, S) \mapsto \left(L(g)^T(b + \left(\begin{pmatrix} A\cdot b \\ S\cdot c_g \end{pmatrix}\right))\right)_{g \in \mathcal{R}}.$$
Remark 3.20. A chart of the manifold of the above theorem is given in the proof.

The following theorem gives a sufficient condition for $\chi_G x_0$ to be a minimum point of $E$ in case $G$ is finite, a space group, or $d_1 = 1$.

Theorem 3.21. Suppose that $d_1 \in \{0, 1, d\}$, $V$ has finite interaction range, $e_V = 0$ and $\lambda_{a,0,0} > 0$. Then $E$ has a local minimum point at $\chi_G x_0$ with respect to $\|\cdot\|_\infty$, i.e. there exists a neighborhood $U \subset U_{per}$ of 0 with respect to $\|\cdot\|_\infty$ such that

$$E(\chi_G x_0 + u) \geq E(\chi_G x_0) \quad \text{for all } u \in U.$$ 

Proof. First we assume that $d_1 \in \{0, 1\}$. Let $R_V \subset G \setminus \{id\}$ be a finite interaction range of $V$. Since $e_V = 0$, by Corollary 3.16 we have $E'(\chi_G x_0) = 0$. By Theorem 2.32(1) there exists a constant $c_1$ such that $\|\cdot\|_R,0,0 \geq c_1 \|\cdot\|_{R \cup R_V, \nabla,0,0}$. Let $c_2 = c_1^2 \lambda_{a,0,0}/2 > 0$. We have

$$E''(\chi_G x_0)(u,u) \geq \lambda_{a,0,0} \|u\|_{R,0,0}^2$$

$$\geq \lambda_{a,0,0} \|u\|_{R,0,0}^2 + c_2 \|u\|_{R \cup R_V, \nabla,0,0}^2$$

$$\geq \lambda_{a,0,0} \|u\|_{R,0,0}^2 + c_2 \|u\|_{R_V, \nabla,0,0}^2$$

$$= \lambda_{a,0,0} \|u\|_{R,0,0}^2 + c_2 \|\nabla_{R_V} u\|_2^2$$

(8)

for all $u \in U_{per}$. In the last step we used that $\|\cdot\|_{R_V, \nabla,0,0} = \|\nabla_{R_V} \cdot\|_2$ since $d_1 \in \{0, 1\}$ and thus $U_{\text{rot,0,0}}(R_V) = \{0\}$. Since $R_V$ is a finite interaction range of $V$, by Taylor’s theorem there exists some $\varepsilon > 0$ such that for all $u: G \setminus \{id\} \to \mathbb{R}^d$ with $\|u\|_\infty < \varepsilon$ we have

$$V(y_0 + u) \geq V(y_0) + V'(y_0)u + V''(y_0)(u,u) - c_2 \|u\|_{R_V}^2.$$  

(9)

For all $u \in U_{per}$ with $\|u\|_\infty < \varepsilon/2$ we have

$$E(\chi_G x_0 + u) = \frac{1}{|C_N|} \sum_{g \in C_N} V((h \cdot (x_0 + u(gh)) - (x_0 + u(g)))_{h \in G \setminus \{id\}})$$

$$\geq \frac{1}{|C_N|} \sum_{g \in C_N} \left( V(y_0) + V'(y_0)(L(h)u(gh) - u(g))_{h \in G \setminus \{id\}} + V''(y_0)((L(h)u(gh) - u(g))_{h \in G \setminus \{id\}} - c_2 \|\nabla_{R_V} u(g)\|_2^2)\right)$$

$$= E(\chi_G x_0) + E'(\chi_G x_0)u + E''(\chi_G x_0)(u,u) - c_2 \|\nabla_{R_V} u\|_2^2$$

$$\geq E(\chi_G x_0) + \frac{\lambda_{a,0,0}}{2} \|u\|_{R,0,0}^2,$$

where $N \in M_0$ such that $u$ is $T^N$-periodic and we used [H1] in the first, [9] in the second, Lemma 3.6 in the third and [8] in the last step.

Now we assume that $d_1 = d$, i.e. $G$ is finite. Thus we have $U_{\text{iso}}(R) = U_{\text{iso},0,0}(R)$. By Proposition 3.19 there exists a neighborhood $U \subset E(d)$ of $id$ such that the set

$$M := \{u \in U_{per} \mid \exists a \in U \forall g \in G : g \cdot (x_0 + u(g)) = a \cdot (g \cdot x_0)\}$$

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is a manifold and $U_{iso,0,0}$ is its tangent space at 0. For all $u \in M$ and $v \in U_{per}$ we have
\[
E(\chi_Gx_0 + u + v) = E(\chi_Gx_0 + (Lg)^T(b + (A - I_d)(g \cdot x_0)))
\]
\[
= \frac{1}{|G|} \sum_{g \in G} \left( (gh) \cdot (x_0 + L(g)^T(b + (A - I_d)(g \cdot x_0)) + v(gh)) - g \cdot (x_0 + L(g)^T(b + (A - I_d)(g \cdot x_0)) + v(g)) \right)
\]
\[
= \frac{1}{|G|} \sum_{g \in G} \left( (A((gh) \cdot (x_0 + w(gh))) - g \cdot (x_0 + w(g))) \right)
\]
\[
= \frac{1}{|G|} \sum_{g \in G} \left( ((gh) \cdot (x_0 + w(gh))) - g \cdot (x_0 + w(g)) \right)
\]
\[
= E(\chi_Gx_0 + w),
\]
where $a = (A, b) \in U$ such that $g \cdot (x_0 + u(g)) = a \cdot (g \cdot x_0)$ for all $g \in G$, the function $w: G \to \mathbb{R}^d$ is defined by $g \mapsto L(g)^TA^TL(g)v(g)$, and we used (H1) in the second to last step. In particular we have
\[
E(\chi_Gx_0 + u) = E(\chi_Gx_0) \quad \text{for all } u \in M. \tag{11}
\]
Since $v_V = 0$, by (10) and Corollary 3.16 for all $u \in M$ and $v \in U_{per}$ we have
\[
E'(\chi_Gx_0 + u)v = \lim_{t \to 0} \frac{E(\chi_Gx_0 + u + tv) - E(\chi_Gx_0 + u)}{t}
\]
\[
= \lim_{t \to 0} \frac{E(\chi_Gx_0 + tw) - E(\chi_Gx_0)}{t}
\]
\[
= E'(\chi_Gx_0)w
\]
\[
= 0, \tag{12}
\]
where $w$ is defined as above. By (12) we have
\[
E'(\chi_Gx_0 + u) = 0 \quad \text{for all } u \in M. \tag{13}
\]
In the following, $c > 0$ denotes a sufficiently small constant, which may vary from line to line. Since $\lambda_{a,0,0} > 0$, we have
\[
E''(\chi_Gx_0)(u, u) \geq c\|u\|_{R,0,0}^2 \quad \text{for all } u \in U_{per}.
\]
Let $U_{iso,0,0}^\perp$ be the orthogonal complement of $U_{iso,0,0}$ with respect to $\| \cdot \|_2$. By Theorem 2.32[(1)] the seminorm $\| \cdot \|_{R,0,0}|U_{iso,0,0}^\perp$ is a norm and thus we have
\[
E''(\chi_Gx_0)(u, u) \geq c\|u\|_{\infty}^2 \quad \text{for all } u \in U_{iso,0,0}^\perp.
\]
Since $E''$ is continuous in $(U_{per}, \| \cdot \|_\infty)$, without loss of generality we may assume that $M$ is such that
\[
E''(\chi_Gx_0 + u)(v, v) \geq c\|v\|_{\infty}^2 \quad \text{for all } u \in M \text{ and } v \in U_{iso,0,0}^\perp. \tag{14}
\]
Without loss of generality let $M$ be such that by (13), (14), Taylor's theorem and (11) there exists a neighborhood $V \subset U_{iso,0,0}^\perp$ of 0 such that
\[
E(\chi_Gx_0 + u + v) \geq E(\chi_Gx_0 + u) = E(\chi_Gx_0) \quad \text{for all } u \in M \text{ and } v \in V.
\]
Since $M + V \subset U_{per}$ is a neighborhood of 0, the assertion is proven. \qed
Remark 3.22. Suppose that $d_1 \in \{0, 1\}$, $V$ has finite interaction range, $e_V = 0$ and $\lambda_{a,0,0} > 0$. Then there even exists a neighborhood $U \subset U_{\text{per}}$ of $\chi_G x_0$ with respect to $\| \cdot \|_\infty$ such that

$$E(\chi_G x_0 + u) \geq E(\chi_G x_0) + \frac{\lambda_{a,0,0}}{2}\|u\|_{R,0,0}^2$$

for all $u \in U$.

The above proof also shows this assertion.

4 Second order bounds on the energy

In this section we present sufficient conditions for the boundedness of $E''(\chi_G x_0)$. The boundedness of $E''(\chi_G x_0)$ with respect to $\| \cdot \|_R$ and $\| \cdot \|_{R,0,0}$ particularly implies the finiteness of $\lambda_a$ and $\lambda_{a,0,0}$, respectively. With respect to $\| \cdot \|_R$, the main result is Theorem 4.4. With respect to $\| \cdot \|_{R,0,0}$, the main result is Corollary 4.15. In this section we assume that $V$ has finite interaction range.

We recall that a bilinear form $B$ on a real vector space $W$ is said to be bounded with respect to a seminorm $\| \cdot \|$ on $W$ if there exists a constant $C > 0$ such that

$$|B(v,w)| \leq C\|v\|\|w\|$$

for all $v, w \in W$.

If $B$ is symmetric this is the case if and only if there exists a constant $C > 0$ such that

$$|B(v,v)| \leq C\|v\|^2$$

for all $v \in W$.

We begin by observing that a bound with respect to the strong norm $\| \nabla_R \cdot \|_2$ is rather straightforward.

**Proposition 4.1.** The bilinear form $E''(\chi_G x_0)$ is bounded with respect to $\| \nabla_R \cdot \|_2$.

**Proof.** Let $R_V \subset G \setminus \{id\}$ be a finite interaction range of $V$. By Theorem 2.32(ii) we may assume that $R_V \subset R$. There exists a constant $C > 0$ such that

$$|V''(y_0)(z,z)| \leq C\|z\|_{R_V}^2$$

for all $z \in L^\infty(G \setminus \{id\}, \mathbb{R}^d)$. (15)

Let $u \in U_{\text{per}}$ and $N \in M_0$ such that $u$ is $T^N$-periodic. We have

$$|E''(\chi_G x_0)(u,u)| = \frac{1}{|C_N|} \sum_{g \in C_N} V''(y_0)\left((L(h)u(gh) - u(g))_{h \in \varphi \setminus \{id\}}, (L(h)u(gh) - u(g))_{h \in \varphi \setminus \{id\}}\right)$$

$$\leq C\|\nabla_R u(g)\|^2$$

$$= C\|\nabla_R u\|_2^2,$$
Lemma 4.2. For all $S \in \text{Skew}(d)$ and $z: G \setminus \{id\} \to \mathbb{R}^d$ we have

$$V''(y_0)(Sy_0, z) = -V'(y_0)(Sz).$$

Proof. By (H1) for all $z: G \setminus \{id\} \to \mathbb{R}^d$ and $A \in SO(d)$ we have

$$V'(Ay_0)(Az) = \lim_{t \to 0} \frac{V(Ay_0 + tAz) - V(Ay_0)}{t} = \lim_{t \to 0} \frac{V(y_0 + tz) - V(y_0)}{t} = V'(y_0)z. \quad (16)$$

For all $S \in \text{Skew}(d)$ and $z: G \setminus \{id\} \to \mathbb{R}^d$ we have

$$V''(y_0)(Sy_0, z) = \lim_{t \to 0} \frac{V'(y_0 + tSy_0)z - V'(y_0)z}{t} = \lim_{t \to 0} \frac{V'(e^{-ts}(y_0 + tSy_0))(e^{-ts}z) - V'(y_0)z}{t} = \lim_{t \to 0} \frac{V'(y_0)((I_d - tS)z) - V'(y_0)z}{t} = -V'(y_0)(Sz),$$

where we used (16) in the second step and Taylor’s theorem in the third step. 

Remark 4.3. If $V$ does not have finite interaction range, then for all $S \in \text{Skew}(d_1) \oplus \{0_{d_2,d_2}\}$ and $z \in L^\infty(G \setminus \{id\}, \mathbb{R}^d)$ we have

$$V''(y_0)(Sy_0, z) = -V'(y_0)(Sz).$$

The proof is analogous since $Sy_0 = (S(L(g)x_0 - x_0))_{g \in G \setminus \{id\}} \in L^\infty(G \setminus \{id\}, \mathbb{R}^d)$ for all $S \in \text{Skew}(d_1) \oplus \{0_{d_2,d_2}\}$.

In the following theorem we consider onsite potentials in equilibrium, i.e. $V'(y_0) = 0$.

Theorem 4.4. Suppose that $V'(y_0) = 0$. Then $E''(\chi_Gx_0)$ is bounded with respect to $\| \cdot \|_R$. In particular we have $\lambda_a \in \mathbb{R}$ and $\lambda_{a,0,0} \in \mathbb{R}$.

Proof. Suppose that $V'(y_0) = 0$. Let $u \in U_{\text{per}}$ and $N \in M_0$ such that $u$ is $T^N$-periodic. Let $S \in L^\infty_{\text{per}}(G, \text{Skew}(d))$ be $T^N$-periodic such that

$$\nabla_R u(g) = \pi_{U_{\text{rot}}(R)}(\nabla_R u(g)) + (L(h)^T S(g)(h \cdot x_0 - x_0))_{h \in R} \quad \text{for all } g \in C_N,$$

where $\pi_{U_{\text{rot}}(R)}$ is the orthogonal projection on $\{v: R \to \mathbb{R}^d\}$ with respect to the norm $\| \cdot \|$ with kernel $U_{\text{rot}}(R)$. In the following, $C > 0$ denotes a sufficiently large constant, which is independent of $u$, and may vary from line to line. Let $R_V \subset G \setminus \{id\}$ be a finite interaction range of $V$. We have

$$|V''(y_0)(z, z)| \leq C\|z\|_{R_V}^2 \quad \text{for all } z: G \setminus \{id\} \to \mathbb{R}^d. \quad (17)$$
We have
\[ |E''(\chi_G x_0)(u, u)| = \frac{1}{|C_N|} \sum_{g \in C_N} V''(y_0) \left( (L(h)u(g h) - u(g))_{h \in G \setminus \{id\}}, (L(h)u(g h) - u(g))_{h \in G \setminus \{id\}} \right) \]
\[ = \frac{1}{|C_N|} \sum_{g \in C_N} V''(y_0) \left( (L(h)u(g h) - u(g) - S(g)(h \cdot x_0 - x_0))_{h \in G \setminus \{id\}}, (L(h)u(g h) - u(g) - S(g)(h \cdot x_0 - x_0))_{h \in G \setminus \{id\}} \right) \]
\[ \leq \frac{C}{|C_N|} \sum_{g \in C_N} \|\pi_{U_{iso}(R)}(\nabla R u(g))\|^2 \]
\[ = C\|u\|_{L^2(R, V)}^2 \]
\[ \leq C\|u\|_R^2, \]
where we used Lemma 3.6 in the first step, Lemma 4.2 in the second step, Lemma 2 in the third step and Theorem 2.30 in the last step. As $E''(\chi_G x_0)$ is symmetric, the assertion follows.

4.2 Strong estimates for finite and space filling structures

We proceed to consider general critical points, first in the cases when $G$ is finite or a space group. In these cases we obtain boundedness with respect to the weak seminorm $\| \cdot \|_R$.

**Proposition 4.5.** Suppose that $E'(\chi_G x_0) = 0$. Then we have

\[ E''(\chi_G x_0)(u, v) = 0 \quad \text{for all } u \in U_{iso,0,0} \cap U_{per} \text{ and } v \in U_{per}. \]

**Proof.** Let $u \in U_{iso,0,0} \cap U_{per}$ and $v \in U_{per}$. By Proposition 2.23 there exist some $a \in \mathbb{R}^d$, $A_1 \in \mathbb{R}^{(d-d_{aff}) \times (d_{aff}-d_2)}$ and $A_2 \in \text{Skew}(d_{aff}-d_2)$ such that

\[ L(g)u(g) = a + S(g \cdot x_0 - x_0) \quad \text{for all } g \in G, \]

(18)

where $S = \begin{pmatrix} 0 & A_3 \\ -A_3^T & A_4 \end{pmatrix} \in \text{Skew}(d_1) \oplus \{0_{d_2,d_2}\}$, $A_3 = (A_1 \quad 0_{d_{aff},d_2})$ and $A_4 = A_2 \oplus 0_{d_2,d_2}$. Let $N \in M_0$ such that $u$ and $v$ are $T^N$-periodic. By Property 1 of $R$, the matrix $C \in \mathbb{R}^{d_{aff} \times |R|}$ defined by

\[ \begin{pmatrix} 0 \\ C \end{pmatrix} = (h \cdot x_0 - x_0)_{h \in R} \]

has rank $d_{aff}$. For all $g \in G$ and $t \in T^N$ we have

\[ (L(h)u(g h) - u(g))_{h \in R} = (L(h)u(g h t) - u(g t))_{h \in R} \]
\[ = (L(g t)^T SL(g t)(h \cdot x_0 - x_0))_{h \in R} \]
\[ = \begin{pmatrix} A_3 B_1 B_2 C \\ B_2^T B_1^T A_4 B_1 B_2 C \end{pmatrix}, \]

(19)

where we used the $T^N$-periodicity of $u$ in the first, Lemma 2 in the second step and $B_1, B_2 \in O(d_{aff})$ such that $L(g) = I_{d-d_{aff}} \oplus B_1$ and $L(t) = I_{d-d_{aff}} \oplus B_2$. Since the left hand side of (19) is independent of $t$ and $C$ has full rank, (19) implies

\[ L(g t)^T SL(g t) = L(g)^T SL(g) \quad \text{for all } g \in G \text{ and } t \in T^N. \]

(20)
We have
\[ E''(\chi_G x_0)(u, v) = \frac{1}{|C_N|} \sum_{g \in C_N} V''(y_0) \left( (L(h)u(gh) - u(g))_{h \in G \setminus \{id\}}, (L(h)v(gh) - v(g))_{h \in G \setminus \{id\}} \right) \]

We now split \((L(h)v(gh) - v(g))_{h \in G \setminus \{id\}} = (L(h)v(gh))_{h \in G \setminus \{id\}} - (v(g))_{h \in G \setminus \{id\}}\). To further compute the first term for each \( g \in C_N \) and \( h \in G \) we fix \( g' \in gT^N \) to be specified later and notice that, due to the periodicity of \( u \) and \( v \), \( u(gh) = u(g'h) \) and \( v(gh) = v(g'h) \) for all \( g \in C_N \) and \( h \in G \). Then
\[
\frac{1}{|C_N|} \sum_{g \in C_N} V''(y_0) \left( (L(h)u(gh) - u(g))_{h \in G \setminus \{id\}}, (L(h)v(gh))_{h \in G \setminus \{id\}} \right) = \frac{1}{|C_N|} \sum_{g \in C_N} V''(y_0) \left( (L(g)^TSL(g)(h \cdot x_0 - x_0))_{h \in G \setminus \{id\}}, (L(h)v(gh))_{h \in G \setminus \{id\}} \right)
\]
\[
= - \frac{1}{|C_N|} \sum_{g \in C_N} V'(y_0) (L(g')^TSL(g')(L(h)v(g')))_{h \in G \setminus \{id\}}
\]
\[
= - \frac{1}{|C_N|} V'(y_0) \left( L(h) \sum_{g \in C_N} L(g)^TSL(g)v(g) \right)_{h \in G \setminus \{id\}},
\]
where we used Lemma 4.2 and (20) in the second step and for each \( h \in G \) we have chosen \( g' \) in such a way that \( \{g' | g \in C_N\} = C_N^{-1} \) so that by the periodicity of \( v \)
\[
\sum_{g \in C_N} L(g')^TSL(g')(L(h)v(g')) = \sum_{g \in C_N} L(gh^{-1})^TSL(gh^{-1})L(h)v(g)
\]
\[
= \sum_{g \in C_N} L(h)L(g)^TSL(g)v(g).
\]
For the second contribution we simply choose \( g' = g \) and proceed likewise to arrive at
\[
E''(\chi_G x_0)(u, v) = - \frac{1}{|C_N|} V'(y_0) \left( (L(h) - I_d) \sum_{g \in C_N} L(g)^TSL(g)v(g) \right)_{h \in G \setminus \{id\}} = 0
\]
with the help of Corollary 3.16. \( \square \)

Remark 4.6. (i) In the above proposition the assumption \( E'(\chi_G x_0) = 0 \) is essential, see Example 4.16.

(ii) In the above proposition the assumption that \( V \) has finite interaction range is not necessary. Using Remark 4.3 instead of Lemma 4.2, the proof is analogous. See also Proposition A.3.

(iii) If \( V \) is weakly* sequentially continuous in addition to the above assumptions, then we also have \( \frac{d}{dt} E(\chi_G x_0 + \tau u)_{\tau = 0} = 0 \) for all \( u \in U_{iso,0,0} \cap U_{per} \), see Proposition A.3.

Theorem 4.7. Suppose that \( G \) is finite and \( E'(\chi_G x_0) = 0 \). Then \( E''(\chi_G x_0) \) is bounded with respect to \( \| \cdot \|_R \). In particular we have \( \lambda_a = \lambda_{a,0,0} \in \mathbb{R} \).

Proof. We have \( \lambda_a = \lambda_{a,0,0} \) since \( G \) being finite entails \( \| \cdot \|_R = \| \cdot \|_{R,0,0} \). Let \( U \) be a subspace of \( U_{per} \) such that \( U_{per} = U_{iso,0,0} \oplus U \). By Theorem 2.30 the seminorm \( \| \cdot \|_R \) is a
norm on $U$ and thus there exists a constant $C > 0$ such that $\| \cdot \|_{\infty} \leq C \| \cdot \|_R$ on $U$. We have

$$\sup \{ |E''(\chi g x_0)(u, u)| \mid u \in U_{\text{per}}, \|u\|_R \leq 1 \} = \sup \{ |E''(\chi g x_0)(u, u)| \mid u \in U, \|u\|_R \leq 1 \} \leq \sup \{ |E''(\chi g x_0)(u, u)| \mid u \in U, \|u\|_\infty \leq C \} < \infty,$$

where we used Proposition 4.5 and Theorem 2.30 in the first step and in the last step that $E''(\chi g x_0)$ is bounded with respect to $\| \cdot \|_\infty$ by Lemma 3.6. Since $E''(\chi g x_0)$ is symmetric, the assertion follows. \hfill \Box

**Theorem 4.8.** Suppose that $G$ is a space group. Then $E''(\chi g x_0)$ is bounded with respect to $\| \cdot \|_R$ and $\| \cdot \|_{R,0,0}$. In particular we have $\lambda_a, \lambda_{a,0,0} \in \mathbb{R}$.

**Proof.** This is clear by Proposition 4.1 and Theorem 2.33. \hfill \Box

### 4.3 Estimates for lower dimensional infinite structures

If $G$ is neither finite nor a space group, the boundedness of $E''(\chi g x_0)$ is non-trivial in general. While an estimate with respect to $\| \cdot \|_{R,0,0}$ is straightforward if $d_1 = 1$, cf. Theorem 4.9, the case $d_1 \geq 2$ is rather demanding, cf. Theorem 4.13.

**Theorem 4.9.** Suppose that $d = 1 + d_2$. Then $E''(\chi g x_0)$ is bounded with respect to $\| \cdot \|_{R,0,0}$. In particular we have $\lambda_{a,0,0} \in \mathbb{R}$.

**Proof.** For $d = 1 + d_2$ we have $U_{\text{rot},0,0}(R) = \{0\}$ and thus $\| \cdot \|_{R,0,0} = \| \nabla R \cdot \|_2$. With Theorem 2.32(i) and Proposition 4.1 follows the assertion. \hfill \Box

For the proof of Theorem 4.13, which addresses the case $d_1 \geq 2$, we need the following definition.

**Definition 4.10.** For all $u \in U_{\text{per}}$ we define the function

$$S_u \in L^\infty(G, \left\{ \left( \begin{array}{ccc} 0 & A_1 & 0 \\ -A_1^T & A_2 & 0 \\ 0 & 0 & 0 \end{array} \right) \mid A_1 \in \mathbb{R}^{(d-d_{\text{aff}}) \times (d_{\text{aff}}-d_2)}, A_2 \in \text{Skew}(d_{\text{aff}}-d_2) \right\})$$

by the condition

$$\nabla_R u(g) = \pi_{U_{\text{rot},0,0}(R)}(\nabla_R u(g)) + (L(g)^T S_u(g) L(g)(h \cdot x_0 - x_0))_{h \in R} \quad \text{for all } g \in G,$$

where $\pi_{U_{\text{rot},0,0}(R)}$ is the orthogonal projection on $\{ v : R \rightarrow \mathbb{R}^d \}$ with respect to the norm $\| \cdot \|$ with kernel $U_{\text{rot},0,0}(R)$.

**Remark 4.11.** For all $u \in U_{\text{per}}$ the function $S_u$ is well-defined: Let $g \in G$. By Lemma 2.21 there exist $B_1 \in O(d_{\text{aff}}-d_2)$ and $B_2 \in O(d_2)$ such that $L(g) = I_{d_{\text{aff}}-d_2} \oplus B_1 \oplus B_2$. By Proposition 2.22 we have

$$U_{\text{rot},0,0}(R) = \left\{ R \rightarrow \mathbb{R}^d, h \mapsto L(h)^T \left( \begin{array}{c} 0 \\ -A_1^T A_2 \end{array} \right) \oplus 0_{d_2,d_2} \right\} (A_1, A_2) \in T \right\} = \left\{ R \rightarrow \mathbb{R}^d, h \mapsto L(g)^T \left( \begin{array}{c} 0 \\ -A_1^T A_2 \end{array} \right) \oplus 0_{d_2,d_2} \right\} (A_1, A_2) \in T \right\},$$

where $T = \mathbb{R}^{(d-d_{\text{aff}}) \times (d_{\text{aff}}-d_2)} \times \text{Skew}(d_{\text{aff}}-d_2)$. 27
Lemma 4.12. For all \( g_0 \in \mathcal{G} \) there exists a constant \( C > 0 \) such that
\[
\frac{1}{|\mathcal{C}_N|} \sum_{g \in \mathcal{C}_N} \| S_u(gg_0) - S_u(g) \|^2 \leq C \| u \|^2_{\mathcal{R},0,0}
\]
for all \( u \in U_{\text{per}} \) and \( N \in M_0 \) such that \( u \) is \( \mathcal{T}^N \)-periodic.

**Proof.** Let \( g_0 \in \mathcal{G} \). Since \( \mathcal{R} \subset \mathcal{G} \) has Property 1, there exists some \( \mathcal{R}' \subset \mathcal{R} \) and \( A \in \text{GL}(d_{\text{aff}}) \) such that
\[
(g \cdot x_0 - x_0)_{g \in \mathcal{R}'} = \begin{pmatrix} 0 \\ A \end{pmatrix}.
\]

By Theorem 2.32 without loss of generality, we may assume that \( \{g_0\} \cup g_0 \mathcal{R}' \subset \mathcal{R} \). Let \( u \in U_{\text{per}} \) and \( N \in M_0 \) such that \( u \) is \( \mathcal{T}^N \)-periodic. Using that \( g_0 \in \mathcal{R} \) we have
\[
\| u \|^2_{\mathcal{R},\nabla,0,0} = \frac{1}{|\mathcal{C}_N|} \sum_{g \in \mathcal{C}_N} \left\| \nabla_R u(g) - (L(gh)^T S_u(g)L(g)(h \cdot x_0 - x_0))_{h \in \mathcal{R}} \right\|^2 
\geq \frac{1}{|\mathcal{C}_N|} \sum_{g \in \mathcal{C}_N} \left\| L(g_0)u(gg_0) - u(g) - L(g)^T S_u(g)L(g)(g_0 \cdot x_0 - x_0) \right\|^2. \tag{21}
\]

As \( g_0 \mathcal{R}' \subset \mathcal{R} \), we also have
\[
\| u \|^2_{\mathcal{R},\nabla,0,0} = \frac{1}{|\mathcal{C}_N|} \sum_{g \in \mathcal{C}_N} \left\| \nabla_R u(g) - (L(gh)^T S_u(g)L(g)(h \cdot x_0 - x_0))_{h \in \mathcal{R}} \right\|^2 
\geq \frac{1}{|\mathcal{C}_N|} \sum_{g \in \mathcal{C}_N} \sum_{h \in \mathcal{R}'} \left\| L(g_0h)u(gg_0h) - u(g) - L(g)^T S_u(g)L(g)((g_0h) \cdot x_0 - x_0) \right\|^2. \tag{22}
\]

Since \( \mathcal{C}_Ng_0 \) is a representation set of \( \mathcal{G}/\mathcal{T}^N \) and \( \mathcal{R}' \subset \mathcal{R} \), we furthermore have
\[
\| u \|^2_{\mathcal{R},\nabla,0,0} = \frac{1}{|\mathcal{C}_N|} \sum_{g \in \mathcal{C}_N} \left\| \nabla_R u(gg_0) - (L(gg_0h)^T S_u(gg_0)L(gg_0)(h \cdot x_0 - x_0))_{h \in \mathcal{R}} \right\|^2 
\geq \frac{1}{|\mathcal{C}_N|} \sum_{g \in \mathcal{C}_N} \sum_{h \in \mathcal{R}'} \left\| L(g_0h)u(gg_0h) - L(g_0u(gg_0) - L(g)^T S_u(gg_0)L(gg_0)(h \cdot x_0 - x_0) \right\|^2. \tag{23}
\]

By (21), (22) and (23) there exists a constant \( c > 0 \) (independent of \( u \) and \( N \)) such that
\[
\| u \|^2_{\mathcal{R},\nabla,0,0} \geq \frac{c}{|\mathcal{C}_N|} \sum_{g \in \mathcal{C}_N} \sum_{h \in \mathcal{R}'} \left\| (S_u(g) - S_u(gg_0))L(gg_0) \begin{pmatrix} 0 \\ A \end{pmatrix} \right\|^2. \tag{24}
\]

By Lemma 2.26 for all \( g \in \mathcal{C}_N \) there exist \( B_1(g) \in \text{O}(d - d_{\text{aff}}) \), \( B_2(g) \in \text{O}(d_{\text{aff}}) \), \( T_1(g) \in \mathbb{R}^{(d - d_{\text{aff}}) \times d_{\text{aff}}} \) and \( T_2(g) \in \text{Skew}(d_{\text{aff}}) \) such that
\[
L(gg_0) = \begin{pmatrix} B_1(g) & 0 \\ 0 & B_2(g) \end{pmatrix} \quad \text{and} \quad S_u(g) - S_u(gg_0) = \begin{pmatrix} 0 & T_1(g) \\ -T_1(g)^T & T_2(g) \end{pmatrix}. 
\]
By (24) we have
\[
\|u\|^2_{R,0,0} \geq \frac{c}{|C_N|} \sum_{g \in C_N} \left( \|T_1(g)B_2(g)A\|^2 + \|T_2(g)B_2(g)A\|^2 \right)
\geq \frac{c\sigma_{\min}(A)}{|C_N|} \sum_{g \in C_N} \left( \|T_1(g)\|^2 + \|T_2(g)\|^2 \right)
\geq \frac{c\sigma_{\min}(A)}{2|C_N|} \sum_{g \in C_N} \|S_\mu(g) - S_\mu(gg_0)\|^2,
\]
where \(\sigma_{\min}(A) > 0\) denotes the minimum singular value of \(A\). Theorem 2.32(i) and (25) imply the assertion.

**Theorem 4.13.** Suppose that \(d_1 \geq 2\), \(E'(\chi_Gx_0) = 0\) and \(E''(\chi_Gx_0)\) is positive semidefinite. Then \(E''(\chi_Gx_0)\) is bounded with respect to \(\|\cdot\|_{R,0,0}\).

**Proof.** Since \(E''(\chi_Gx_0)\) is symmetric, it suffices to show that there exists a constant \(C > 0\) such that
\[
E''(\chi_Gx_0)(u,u) \leq C\|u\|^2_{R,0,0} \quad \text{for all } u \in U_{\text{per}}.
\]
Recall that \(M_0 = m_0\NN\). Let \(\{t_1, \ldots, t_{d_2}\}\) be a generating set of \(T^{m_0}\). Without loss of generality we specifically choose
\[
C_{n,m_0} = \bigcup_{n_1, \ldots, n_{d_2} \in [0,n-1]} \{t_1^{n_1} \cdots t_{d_2}^{n_{d_2}} g\}.
\]
For all \(g \in G\) there exist \(n_1, \ldots, n_{|C_{m_0}|} d_2 \in \ZZ\) such that
\[
C_{m_0}g = \bigcup_{i=1}^{|C_{m_0}|} \{t_1^{n_{i,1}} \cdots t_{d_2}^{n_{i,d_2}} h_i\},
\]
where \(h_1, \ldots, h_{|C_{m_0}|}\) are the elements of \(C_{m_0}\). Thus and since \(T^{m_0}\) is abelian, for all \(g \in G\) we have
\[
\lim_{n \to \infty} \frac{|C_{n,m_0} \cap (C_{n,m_0}g)|}{|C_{n,m_0}|} = 1.
\]
Let \(\{B_1, \ldots, B_m\}\) be a basis of
\[
\left\{ \begin{pmatrix} 0 & A_1^T \\ -A_2 & 0_{d_2,d_2} \end{pmatrix} \right| A_1 \in \RR^{(d-d_{\text{aff}}) \times (d_{\text{aff}}-d_2)}, A_2 \in \text{Skew}(d_{\text{aff}}-d_2) \right\}.
\]
Let \(u \in U_{\text{per}}\) and \(N \in M_0\) such that \(u\) is \(T^N\)-periodic. For all \(i \in \{1, \ldots, m\}\) and \(g \in G\) let \(S_{u,i}(g) = (S_u(g), B_i) B_i\). For all \(n \in \NN\) and \(i \in \{1, \ldots, m\}\) we define the \(T^{nN}\)-periodic function \(v_{u,n,i} \in U_{\text{per}}\) by the condition
\[
L(g)v_{u,n,i}(g) = S_{u,i}(g)(g \cdot x_0 - x_0) \quad \text{for all } g \in C_{n,N}.
\]
Moreover let \(v_{u,n} = \sum_{i=1}^m v_{u,n,i}\).
Since \(\tau(G) \subset \{0_{d_1}\} \times \RR^{d_2}\), for all \(S \in \text{Skew}(d_1) \times \{0_{d_2,d_2}\}\) and \(g, h \in G\) we have
\[
S(g \cdot x_0) = SL(g)x_0 \quad \text{and} \quad S((gh) \cdot x_0) = SL(g)(h \cdot x_0).
\]
Since the bilinear form \(E''(\chi_Gx_0)\) is positive semidefinite, for all \(n \in \NN\) we have
\[
E''(\chi_Gx_0)(u, u) \leq 2E''(\chi_Gx_0)(u - v_{u,n}, u - v_{u,n}) + 2m \sum_{i=1}^m E''(\chi_Gx_0)(v_{u,n,i}, v_{u,n,i}).
\]
In the following, $C > 0$ denotes a sufficiently large constant, which is independent of $u$ and may vary from line to line. We have

$$
\limsup_{n \to \infty} E'(\chi g x_0)(u - v_{u,n}, u - v_{u,n}) \leq \limsup_{n \to \infty} C \| \nabla_R (u - v_{u,n}) \|_2^2
$$

$$
= \limsup_{n \to \infty} \frac{C}{|C_n|} \sum_{g \in C_n} \sum_{h \in R} \| (L(h)u(gh) - u(g)) - L(g)^T S_u(gh)((gh) \cdot x_0 - x_0) + L(g)^T S_u(g)(g \cdot x_0 - x_0) \|_2^2,
$$

where in the first step we used Proposition 4.1 and in the second (27), which implies that $\lim_{n \to \infty} \| \{ g \in C_n | gh \in C_n \text{ for all } h \in R \}/|C_n| = 1$. From (28) and (27) it now follows that

$$
\limsup_{n \to \infty} E''(\chi g x_0)(u - v_{u,n}, u - v_{u,n})
$$

$$
\leq \limsup_{n \to \infty} \frac{C}{|C_n|} \sum_{g \in C_n} \sum_{h \in R} \left( \| (L(h)u(gh) - u(g)) - L(g)^T S_u(g)L(g \cdot x_0 - x_0) \|_2^2 + \| S_u(gh) - S_u(g) \|_2^2 \right)
$$

$$
\leq C \| u \|_{\mathbb{R}^2,0,0}^2,
$$

(30)

where the last estimate is implied by Lemma 4.12 and Theorem 232.6. Let $i \in \{1, \ldots, m\}$. Using Lemma 3.6 and Theorems 27 and 28 we have

$$
\limsup_{n \to \infty} E''(\chi g x_0)(v_{u,n,i}, v_{u,n,i})
$$

$$
= \limsup_{n \to \infty} \frac{1}{|C_n|} \sum_{g \in C_n} V''(y_0) \left( (L(h)v_{u,n,i}(gh) - v_{u,n,i}(g))_{h \in G \setminus \{id\}}, (L(h)v_{u,n,i}(gh) - v_{u,n,i}(g))_{h \in G \setminus \{id\}} \right)
$$

$$
= \limsup_{n \to \infty} \frac{1}{|C_n|} \sum_{g \in C_n} V''(y_0) \left( (a_i(g,h) + b_i(g,h))_{h \in G \setminus \{id\}}, (a_i(g,h) + b_i(g,h))_{h \in G \setminus \{id\}} \right)
$$

$$
= \limsup_{n \to \infty} (s_{1,n,i} + s_{2,n,i}),
$$

(31)

where

$$
a_i(g,h) := L(g)^T (S_{u,i}(gh) - S_{u,i}(g))((gh) \cdot x_0 - x_0),
$$

$$
b_i(g,h) := L(g)^T S_{u,i}(g)L(g \cdot x_0 - x_0)
$$

for all $g, h \in G$ and

$$
s_{1,n,i} := \frac{1}{|C_n|} \sum_{g \in C_n} V''(y_0) \left( (a_i(g,h))_{h \in G \setminus \{id\}}, (a_i(g,h))_{h \in G \setminus \{id\}} \right),
$$

$$
s_{2,n,i} := \frac{1}{|C_n|} \sum_{g \in C_n} V''(y_0) \left( (b_i(g,h))_{h \in G \setminus \{id\}}, (2a_i(g,h) + b_i(g,h))_{h \in G \setminus \{id\}} \right)
$$

for all $n \in \mathbb{N}$. Let $R_V \subseteq G \setminus \{id\}$ be a finite interaction range of $V$. We have

$$
\limsup_{n \to \infty} s_{1,n,i} \leq \limsup_{n \to \infty} \frac{C}{|C_n|} \sum_{g \in C_n} \sum_{h \in R_V} \| a_i(g,h) \|_2^2
$$

$$
\leq \limsup_{n \to \infty} \frac{C}{|C_n|} \sum_{g \in C_n} \sum_{h \in R_V} \| (S_{u,i}(gh) - S_{u,i}(g)) \|_2^2
$$

$$
\leq C \| u \|_{\mathbb{R}^2,0,0}^2
$$

(32)
where we used (28) in the second and Lemma 4.12 in the last step.

Since \( E'(\chi_G x_0) = 0 \), by Corollary 3.16 (27) and the boundedness of \( S_u \), we have

\[
\lim_{n \to \infty} \frac{1}{|C_{nN}|} \sum_{g \in C_{nN}} V'(y_0)(L(g)^T S_{u,i}(g) S_{u,i}(g)(L(g)x_0 - x_0))_{h \in G \setminus \{id\}} = \lim_{n \to \infty} \frac{1}{|C_{nN}|} \sum_{g \in C_{nN}} V'(y_0)(L(h)L(g)^T S_{u,i}(g) S_{u,i}(g)(L(g)x_0 - x_0))_{h \in G \setminus \{id\}} = \lim_{n \to \infty} \frac{1}{|C_{nN}|} \sum_{g \in C_{nN}} V'(y_0)(L(g)^T S_{u,i}(gh) S_{u,i}(gh)(L(gh)x_0 - x_0))_{h \in G \setminus \{id\}}. \tag{33}
\]

The definition of \( S_{u,i} \) implies

\[ S_{u,i}(g)S_{u,i}(h) = S_{u,i}(h)S_{u,i}(g) \quad \text{for all } g, h \in G. \tag{34} \]

We have

\[
\lim_{n \to \infty} s_{2,n,i} = \lim_{n \to \infty} \frac{1}{|C_{nN}|} \sum_{g \in C_{nN}} V'(y_0)(-L(g)^T S_{u,i}(g) L(g)(2a_i(g,h) + b_i(g,h)))_{h \in G \setminus \{id\}}
= \lim_{n \to \infty} \frac{1}{|C_{nN}|} \sum_{g \in C_{nN}} V'(y_0)(-2L(g)^T S_{u,i}(g) S_{u,i}(gh)L(gh)x_0 + 2L(g)^T S_{u,i}(g) S_{u,i}(gh)x_0
+ L(g)^T S_{u,i}(g) S_{u,i}(gh)L(gh)x_0 - 2L(g)^T S_{u,i}(g) S_{u,i}(gh)x_0
+ L(g)^T S_{u,i}(g) S_{u,i}(gh)L(g)x_0)_{h \in G \setminus \{id\}}
= \lim_{n \to \infty} \frac{1}{|C_{nN}|} \sum_{g \in C_{nN}} V'(y_0)(L(g)^T (S_{u,i}(g) - S_{u,i}(gh))^2(L(gh)x_0 - x_0))_{h \in G \setminus \{id\}}
\leq \lim_{n \to \infty} \frac{C}{|C_{nN}|} \sum_{g \in C_{nN}} \sum_{h \in R_V} \|S_{u,i}(g) - S_{u,i}(gh)^2\|
\leq C\|u\|^2_{R,0,0}, \tag{35}
\]

where in the first step we used Lemma 4.2, in the second step we used (28), in the third step we used (33) and (34), and in the last step we used Lemma 4.12.

Since \( i \in \{1, \ldots, m\} \) was arbitrary, the equations (29), (30), (31), (32) and (35) imply the assertion (26).

\[ \square \]

Remark 4.14. The above assumption \( E'(\chi_G x_0) = 0 \) can be replaced by the weaker assumption \( E'(\chi_G x_0)u = 0 \) for all \( u \in U_{per} \) with \( u(G) \subset \mathbb{R}^{d_1} \times \{0_{d_2}\} \).

4.4 Summary and counterexamples

Our previous results cover all possible choices of \( d_1, d_2 \) and we first summarize our findings in Corollary 4.15. Then we discuss two settings for which \( \lambda_\alpha = \lambda_{a,0,0} = -\infty \) and, in particular, \( E''(\chi_G x_0) \) need not be bounded with respect to \( \| \cdot \|_{R,0,0} \).

\[ \text{Corollary 4.15.} \text{ Let } d = d_1 + d_2 \geq 1. \text{ In case } d_1 \geq 2 \text{ suppose that } E'(\chi_G x_0) = 0 \text{ and } E''(\chi_G x_0) \text{ is positive semidefinite. Then } E''(\chi_G x_0) \text{ is bounded with respect to } \| \cdot \|_{R,0,0}. \text{ In particular we have } \lambda_{a,0,0} \in \mathbb{R}. \text{ If } d = d_1 \text{ or } d = d_2, \text{ then } E''(\chi_G x_0) \text{ is also bounded with respect to } \| \cdot \|_R \text{ and particularly } \lambda_\alpha \in \mathbb{R}. \]

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Proof. This is clear by Theorem 4.7, Theorem 4.8, Theorem 4.9 and Theorem 4.13.

Example 4.16. We present an example such that \( E''(\chi_G x_0)(u, u) < 0 \) for some \( u \in U_{iso,0} \cap U_{per} \). In particular we have \( \lambda_3 = \lambda_{a,0,0} = -\infty \), \( E''(\chi_G x_0) \) is not bounded with respect to \( \| \cdot \|_{R,0,0} \), and in Proposition 4.5 and Theorem 4.7 the condition \( E'(\chi_G x_0) = 0 \) cannot be dropped.

Let \( d = d_2 = 2 \), \( p = (-I_2, 0) \in E(2) \), \( G = \{id, p\} < E(2) \), \( x_0 = e_1 \in \mathbb{R}^2 \) and
\[
V: \mathbb{R}^2 \to \mathbb{R}, \quad x \mapsto -\|x\|^2.
\]

We define the function \( u \in U_{iso,0,0} \) by
\[
L(g)u(g) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} (g \cdot x_0 - x_0) \quad \text{for all } g \in G.
\]

We have \( y_0 = p \cdot x_0 - x_0 = -2e_1 \) and by Lemma 3.6
\[
E''(\chi_G x_0)(u, u) = \frac{1}{|G|} \sum_{g \in G} V''(y_0)(-u(gp) - u(g) - u(gp) - u(g))
\]
\[
= V''(y_0)(u(id) + u(p), u(id) + u(p))
\]
\[
= -2\|u(id) + u(p)\|^2
\]
\[
= -8.
\]

Since \( \|u\|_R = \|u\|_{R,0,0} = 0 \), we have \( \lambda_3 = \lambda_{a,0,0} = -\infty \) and \( E''(\chi_G x_0) \) is not bounded with respect to \( \| \cdot \|_{R,0,0} \).

Example 4.17. We present an example with an infinite interaction range so that \( E'(\chi_G x_0) = 0 \) and \( \lambda_3 = \lambda_{a,0,0} = -\infty \). In particular \( E''(\chi_G x_0) \) is not bounded with respect to \( \| \cdot \|_{R,0,0} \).

Let \( d = d_2 = 1 \), \( d_1 = 0 \), \( t = (I_1, 1) \in E(1) \), \( G = \{t^n | n \in \mathbb{Z}\} < E(1) \) and \( x_0 = 0 \in \mathbb{R} \).

We have \( M_0 = \mathbb{N} \). Let \( \alpha > 1 \) and \( V: (\mathbb{R}^d)_G \to \mathbb{R} \) be the interaction potential such that \( V \) has the properties (H1), (H2) and (H3) and
\[
V''(y_0)(z_1, z_2) = -\sum_{n \in \mathbb{N}} n^{-\alpha} z_1(t^n) z_2(t^n) \quad \text{for all } z_1, z_2 \in L^\infty(G \setminus \{id\}, \mathbb{R}^d).
\]

We have \( E'(\chi_G x_0) = 0 \) by Corollary 3.17. Let \( N \in \mathbb{N} \) be even. The set \( \{t^0, \ldots, t^{N-1}\} \) is a representation set of \( G/T^N \). We define the \( T^N \)-periodic function \( u \in U_{per} \) by
\[
u(t^n) = \frac{n}{N} \quad \text{for all } n \in \{0, \ldots, N/2 - 1\}
\]
and
\[
u(t^n) = 1 - \frac{n}{N} \quad \text{for all } n \in \{N/2, \ldots, N - 1\}.
\]

Let \( R = \{id, t, t^2\} \) and \( R' = \{t\} \). The set \( R \) has Property 2 and \( R' \) generates \( G \). By Theorem 2.33 and Theorem 2.33(ii), the seminorms \( \| \cdot \|_R \) and \( \| \nabla R' \cdot \| \) are equivalent and thus there exists a constant \( C > 0 \) such that \( \| \cdot \|_R \leq C \| \nabla R' \cdot \| \). We have
\[
\|u\|_R \leq C \| \nabla R' u \|_2 = C \left( \frac{1}{N} \sum_{n=0}^{N-1} \| \nabla R' u(t^n) \|^2 \right)^{1/2} = \frac{C}{N}.
\]
We have
\[
E''(\chi_Gx_0)(u, u) = \frac{1}{N} \sum_{n=0}^{N-1} V''(y_0) \left( (u(t^n s) - u(t^n))_{s \in g \setminus \{id\}}, (u(t^n s) - u(t^n))_{s \in g \setminus \{id\}} \right)
\]
\[
= -\frac{1}{N} \sum_{n=0}^{N-1} \sum_{m \in \mathbb{N}} m^{-\alpha} |u(t^{n+m}) - u(t^n)|^2
\]
\[
\leq -\frac{1}{N} \sum_{n=0}^{N-1} (N/2)^{-\alpha} |u(t^{n+N/2}) - u(t^n)|^2
\]
\[
\leq -\frac{1}{2} (N/2)^{-\alpha} \frac{1}{4}
\]
\[
= -2^{\alpha-5} N^{-\alpha}.
\]  
By (36) and (37) we have
\[\lambda_a \leq \frac{E''(\chi_Gx_0)(u, u)}{\|u\|_{\mathcal{R}}^2} \leq -cN^{2-\alpha},\]
where \(c = C^{-2}2^{\alpha-5}\). For all \(\alpha \in (1, 2)\) we have \(\lambda_a = -\infty\) as \(N \to 2N\) was arbitrary. Since \(\| \cdot \|_{\mathcal{R}} = \| \cdot \|_{\mathcal{R},0,0}\), for all \(\alpha \in (1, 2)\) we also have \(\lambda_{a,0,0} = -\infty\).

5 The main representation formulae

In this section we characterize the stability constants \(\lambda_a\) and \(\lambda_{a,0,0}\) in the Fourier transform domain, see Theorem 5.10. We also state a similar characterization which enables us to efficiently compute \(\lambda_a\) and \(\lambda_{a,0,0}\), see Theorem 5.12.

Recall Definition 2.6 and Lemma 2.7. Since \(E''(\chi_Gx_0)\) is left-translation-invariant, see Remark 3.15(i). we can represent \(E''(\chi_Gx_0)\) as a convolution operator.

**Lemma 5.1.** For all \(u, v \in U_{\text{per}}\) we have
\[
E''(\chi_Gx_0)(u, v) = \langle f_V * v_0, u_0 \rangle,
\]
where \(u_0 = u(\cdot^{-1})\) and \(v_0 = v(\cdot^{-1})\).

**Proof.** Let \(u, v \in U_{\text{per}}\). Let \(N \in \mathbb{M}_0\) such that \(u\) and \(v\) are \(T^N\)-periodic. Let \(u_0 = u(\cdot^{-1})\) and \(v_0 = v(\cdot^{-1})\). By Lemma 3.14 we have
\[
E''(\chi_Gx_0)(u, v) = \sum_{g, h \in \mathcal{C}_N} u(g)^T \partial g T^N \partial h T^N E(\chi_Gx_0)(v(h))
\]
\[
= \frac{1}{|\mathcal{C}_N|} \sum_{g, h \in \mathcal{C}_N} \sum_{t \in T^N} u_0(g^{-1})^T f_V(g^{-1} ht) v_0(h^{-1})
\]
\[
= \frac{1}{|\mathcal{C}_N|} \sum_{g \in \mathcal{C}_N} u_0(g^{-1})^T f_V * v_0(g^{-1})
\]
\[
= \langle f_V * v_0, u_0 \rangle.
\]
where in the third step we used that \(v_0((ht)^{-1}) = v_0(h^{-1})\) for all \(h \in \mathcal{C}_N\) and \(t \in T^N\). □

Let \(\varphi: \mathcal{R} \to \{0, \ldots, |\mathcal{R}| - 1\}\) be a bijection. We define an isomorphism between 
\(\mathbb{C}^{(m|\mathcal{R}|)^m} \) and \( (\mathbb{C}^{n \times n})^R \) by
\[
(a_{i,j})_{i \in \{1, \ldots, m|\mathcal{R}|\}, j \in \{1, \ldots, n\}} \mapsto \left((a_{i+m\varphi(g),j})_{i \in \{1, \ldots, m\}, j \in \{1, \ldots, n\}}\right)_{g \in \mathcal{R}}.
\]

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**Definition 5.2.** We define the functions \( g_{\mathcal{R}}, g_{\mathcal{R},0,0} \in L^1(\mathcal{G}, \mathbb{R}^{(d|\mathcal{R}|) \times d}) \) by

\[
g_{\mathcal{R}}(g) = P(\delta_{g,h}I_d)_{h \in \mathcal{R}} \quad \text{for all } g \in \mathcal{G}
\]

and

\[
g_{\mathcal{R},0,0}(g) = P_0(\delta_{g,h}I_d)_{h \in \mathcal{R}} \quad \text{for all } g \in \mathcal{G},
\]

where \( P \) (resp. \( P_0 \)) is the square matrix of order \( d|\mathcal{R}| \) such that the map

\[
\mathbb{R}^{d|\mathcal{R}|} \to \mathbb{R}^{d|\mathcal{R}|}, \quad x \mapsto Px
\]

is the orthogonal projection with respect to the norm \( \| \cdot \| \) with kernel \( U_{iso}(\mathcal{R}) \) (resp. \( U_{iso,0,0}(\mathcal{R}) \)).

**Remark 5.3.** The support of both \( g_{\mathcal{R}} \) and \( g_{\mathcal{R},0,0} \) is equal to \( \mathcal{R} \). We have

\[
g_{\mathcal{R}}(g) = p_{\chi_{\mathcal{R}}(g)} \quad \text{for all } g \in \mathcal{R}
\]

and

\[
g_{\mathcal{R},0,0}(g) = p_{0,\chi_{\mathcal{R}}(g)} \quad \text{for all } g \in \mathcal{R},
\]

where \( P \) and \( P_0 \) are as above and \( p_0, \ldots, p_{|\mathcal{R}|-1}, p_{0,0}, \ldots, p_{0,|\mathcal{R}|-1} \in \mathbb{R}^{(d|\mathcal{R}|) \times d} \) such that \( P = (p_0, \ldots, p_{|\mathcal{R}|-1}) \) and \( P_0 = (p_{0,0}, \ldots, p_{0,|\mathcal{R}|-1}) \).

Due to their left-translation-invariance, \( \| \cdot \|_R \) and \( \| \cdot \|_{\mathcal{R},0,0} \) can be represented by means of convolution operators.

**Lemma 5.4.** For all \( u \in U_{\text{per}} \) we have \( \| u \|_R = \| g_{\mathcal{R}} \ast u_0 \|_2 \) and \( \| u \|_{\mathcal{R},0,0} = \| g_{\mathcal{R},0,0} \ast u_0 \|_2 \), where \( u_0 = u(\cdot^{-1}) \).

**Proof.** Let \( u \in U_{\text{per}} \) and \( N \in M_0 \) such that \( u \) is \( T^N \)-periodic and set \( u_0 = u(\cdot^{-1}) \). With \( P \in \mathbb{R}^{(d|\mathcal{R}|) \times (d|\mathcal{R}|)} \) as in Definition 5.2 we have

\[
\| u \|_R^2 = \frac{1}{|C_N|} \sum_{g \in C_N} \| P(u(g))_{h \in \mathcal{R}} \|^2. \tag{38}
\]

For each \( g \in \mathcal{G} \) we set \( \delta_g : \mathcal{G} \to \{0,1\}, h \mapsto \delta_{h,g} \). Then

\[
P(u(g))_{h \in \mathcal{R}} = P(u_0(h^{-1}g^{-1}))_{h \in \mathcal{R}} = P((\delta_{h,g}) \ast u_0(g^{-1}))_{h \in \mathcal{R}} = (P(\delta_{h,g})_{h \in \mathcal{R}}) \ast u_0(g^{-1}) = g_{\mathcal{R}} \ast u_0(g^{-1}) \tag{39}
\]

for any \( g \in \mathcal{G} \) and by (38) and (39) we have

\[
\| u \|_R^2 = \frac{1}{|C_N|} \sum_{g \in C_N} \| g_{\mathcal{R}} \ast u_0(g^{-1}) \|^2 = \| g_{\mathcal{R}} \ast u_0 \|_2^2.
\]

Analogously we have \( \| u \|_{\mathcal{R},0,0} = \| g_{\mathcal{R},0,0} \ast u_0 \|_2 \).

Proposition 4.5 implies the following corollary.

**Corollary 5.5.** Suppose that \( E'(^{\chi_{\mathcal{G}}}x_0) = 0 \). Then for all periodic representations \( \rho \) of \( \mathcal{G} \) and \( a \in \mathcal{C}_{dd} \), such that \( \| \hat{g}_{\mathcal{R}}(\rho)a \| = 0 \) we have \( \langle f_V(\rho)a,a \rangle = 0 \).
For all $u_0 = u(\cdot^{-1})$. We have

$$
0 = d_ρ||\tilde{g}_R(ρ)a||^2 = d_ρ||\tilde{g}_R(ρ)\tilde{u}(ρ)||^2 = ||g_R * u||^2
$$

$$
= ||g_R * Re(u)||^2 + ||g_R * Im(u)||^2
= ||Re(u_0)||^2_R + ||Im(u_0)||^2_R,
$$

(40)

where we used Lemma 2.7 in the second, Proposition 2.3 in the third and Lemma 5.4 in the last step. Thus we have $||Re(u_0)||_R = 0$ and $||Im(u_0)||_R = 0$ which is equivalent to $Re(u_0), Im(u_0) \in U_{iso,0,0}$ by Theorem 2.30. We have $E''(\chi_G x_0)(Re(u_0), Re(u_0)) = 0$ and $E''(\chi_G x_0)(Im(u_0), Im(u_0)) = 0$ by Proposition 4.5 and Remark 4.6(ii). Thus we have

$$
d_ρ(f^*_V(ρ)a,a) = E''(\chi_G x_0)(Re(u_0), Re(u_0)) + E''(\chi_G x_0)(Im(u_0), Im(u_0)) = 0,
$$

where the first step follows analogously to equation (40) with Lemma 5.1 instead of Lemma 5.4.

The following lemma shows that we can consider complex-valued instead of real-valued functions. Its standard proof is included for completeness.

**Lemma 5.6.** We have

$$
λ_a = \sup\{c \in \mathbb{R} \mid \forall u \in U_{per,\mathbb{C}} : c||g_R * u||^2 \leq \langle f_V * u, u \rangle \}
$$

and

$$
λ_{a,0,0} = \sup\{c \in \mathbb{R} \mid \forall u \in U_{per,\mathbb{C}} : c||g_{R,0,0} * u||^2 \leq \langle f_V * u, u \rangle \},
$$

**Proof.** By Lemma 5.1, Lemma 5.4 and since $U_{per} = \{u(\cdot^{-1}) \mid u \in U_{per}\}$, we have

$$
λ_a = \sup\{c \in \mathbb{R} \mid \forall u \in U_{per} : c||g_R * u||^2 \leq \langle f_V * u, u \rangle \}
$$

and hence,

$$
λ_a \geq \sup\{c \in \mathbb{R} \mid \forall u \in U_{per,\mathbb{C}} : c||g_R * u||^2 \leq \langle f_V * u, u \rangle \} =: \text{RHS}.
$$

Now we show that $λ_a \leq \text{RHS}$. For all $u \in U_{per,\mathbb{C}}$ we have

$$
\langle f_V * u, u \rangle = \langle f_V * Re(u), Re(u) \rangle - i\langle f_V * Re(u), Im(u) \rangle
+ i\langle f_V * Im(u), Re(u) \rangle + \langle f_V * Im(u), Im(u) \rangle
= \langle f_V * Re(u), Re(u) \rangle - iE''(\chi_G x_0)(Im(u), Re(u))
+ iE''(\chi_G x_0)(Re(u), Im(u)) + \langle f_V * Im(u), Im(u) \rangle
= \langle f_V * Re(u), Re(u) \rangle + \langle f_V * Im(u), Im(u) \rangle
\geq λ_a||g_R * Re(u)||^2 + λ_a||g_R * Im(u)||^2
= λ_a||g_R * u||^2,
$$

where in the second step we used Lemma 5.1.

The proof of the characterization of $λ_{a,0,0}$ is analogous.

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Recall that by our definition all representations are unitary.

**Lemma 5.7.** For all \( g \in G \) we have \( f_V(g^{-1}) = f_V(g)^T \) and for all representations \( \rho \) of \( G \) the matrix \( \widehat{f_V}(\rho) \) is Hermitian.

**Proof.** For all \( g \in G \) we have

\[
    f_V(g^{-1}) = \sum_{h_1,h_2 \in G \setminus \{id\}} \left( \delta_{g^{-1},h_2^{-1}} L(h_2) \partial_{h_2} \partial_{h_1} V(y_0) L(h_1) - \delta_{g^{-1},h_2^{-1}} L(h_2) \partial_{h_2} V(y_0) - \delta_{g^{-1},h_2^{-1}} \partial_{h_2} \partial_{h_1} V(y_0) L(h_1) + \delta_{g^{-1},id} \partial_{h_2} \partial_{h_1} V(y_0) \right)
\]

\[
    = \sum_{h_1,h_2 \in G \setminus \{id\}} \left( \delta_{g^{-1},h_2^{-1}} L(h_2)(\partial_{h_1} \partial_{h_2} V(y_0))^T L(h_1) - \delta_{g^{-1},h_2^{-1}} L(h_2)(\partial_{h_1} \partial_{h_2} V(y_0))^T \right)
\]

\[
    = f_V(g)^T.
\]

For all representations \( \rho \) of \( G \) we have

\[
    \widehat{f_V}(\rho) = \sum_{g \in G} f_V(g) \otimes \rho(g)
\]

\[
    = \sum_{g \in G} f_V(g^{-1}) \otimes \rho(g^{-1})
\]

\[
    = \sum_{g \in G} f_V(g)^H \otimes \rho(g)^H
\]

\[
    = \left( \sum_{g \in G} f_V(g) \otimes \rho(g) \right)^H
\]

\[
    = \widehat{f_V}(\rho)^H,
\]

where in the third step we used (41) and that \( \rho \) is unitary. \( \square \)

**Definition 5.8.** We define

\[
    \lambda_{\min}(A, B) := \sup \{ c \in \mathbb{R} \mid cB^H B \leq A \} \in \mathbb{R} \cup \{ \pm \infty \}
\]

for all Hermitian matrices \( A \in \mathbb{C}^{n \times n} \) and matrices \( B \in \mathbb{C}^{m \times n} \). Here \( \leq \) denotes the Loewner order which is the partial order on the set of all Hermitian matrices of \( \mathbb{C}^{n \times n} \) defined by \( A \geq B \) if \( A - B \) is positive semidefinite.

**Remark 5.9.** (i) By means of the dual problem we have

\[
    \lambda_{\min}(A, B) = \inf \{ x^H A x \mid x \in \mathbb{C}^n, \| B x \| = 1 \}
\]

and

\[
    \lambda_{\min}(A, 0_{m,n}) = \begin{cases} 
        \infty & \text{if } A \text{ is positive semidefinite} \\
        -\infty & \text{else}
    \end{cases}
\]

for all Hermitian matrices \( A \in \mathbb{C}^{n \times n} \) and matrices \( B \in \mathbb{C}^{m \times n} \setminus \{0\} \). The proof is analogous to the proof of Proposition 3.10.
(ii) Suppose that $B$ has in addition rank $n$ and consider the generalized eigenvalue problem $A\nu = \lambda B^H\nu$, i.e. the problem of finding the eigenvalues of the matrix pencil $A - \lambda B^H B$. Then the eigenvalues of the generalized eigenvalue problem are real and $\lambda_{\min}(A,B)$ is equal to the smallest one, see [27, Chapter X, Theorem 11]. The eigenvalues of the generalized eigenvalue problem are equal to the eigenvalues of the matrix $A(B^H B)^{-1}$, see [41, Proposition 6.1.1], but the eigenvalues of $A(B^H B)^{-1}$ are ill-conditioned. There exist many numerically stable algorithms, see, e.g., [2, Chapter 5], and thus many programming languages have a function for this problem; e.g. for Python the subpackage linalg of the package SciPy has the function eigvalsh.

Due to the left-translation-invariance, $E''(\chi_G x_0)$, $\|\cdot\|_R$ and $\|\cdot\|_{R,0,0}$ can be represented by means of multiplier operators. Thus we have the following representation of $\lambda_a$ and $\lambda_{a,0,0}$. Recall that $\mathcal{E}$ is a representation set of $\{\rho \in \hat{G} \mid \rho$ is periodic$\}$.

**Theorem 5.10.** We have

$$
\lambda_a = \inf \left\{ \lambda_{\min}(f_V(\rho), g_{\mathcal{R}}(\rho)) \mid \rho \in \mathcal{E} \right\}
$$

and

$$
\lambda_{a,0,0} = \inf \left\{ \lambda_{\min}(f_V(\rho), g_{\mathcal{R},0,0}(\rho)) \mid \rho \in \mathcal{E} \right\}.
$$

**Proof.** By Lemma 5.7 for all $\rho \in \mathcal{E}$ the matrix $f_V(\rho)$ is Hermitian and thus the term $\lambda_{\min}(f_V(\rho), g_{\mathcal{R}}(\rho))$ is well-defined. We have to show that

$$
\lambda_a = \inf \left\{ \lambda_{\min}(f_V(\rho), g_{\mathcal{R}}(\rho)) \mid \rho \in \mathcal{E} \right\} =: \text{RHS}.
$$

By Lemma 5.6 we have

$$
\lambda_a = \sup \left\{ c \in \mathbb{R} \mid \forall u \in U_{\text{per,C}} : c\|g_{\mathcal{R}} \ast u\|^2_2 \leq \langle f_V \ast u, u \rangle \right\}.
$$

First we show that $\lambda_a \leq \text{RHS}$. Let $\rho \in \mathcal{E}$ and $a \in \mathbb{C}^{dd'}$. We define $u \in U_{\text{per,C}}$ by

$$
\hat{u}(\rho') = \begin{cases} (a & 0_{dd',d_d-1}) & \text{if } \rho' = \rho \\
0_{dd',d_d'} & \text{else} \end{cases}
$$

for all $\rho' \in \mathcal{E}$. By Lemma 2.7 and Proposition 2.3 we have

\[
\langle f_V(\rho)a, a \rangle = \langle f_V(\rho) \hat{u}(\rho), \hat{u}(\rho) \rangle = \langle f_V \ast u(\rho), \hat{u}(\rho) \rangle = \frac{1}{d_{\rho}} \langle f_V \ast u, u \rangle \\
\geq \frac{\lambda_a}{d_{\rho}} \|g_{\mathcal{R}} \ast u\|^2_2 = \lambda_a \|g_{\mathcal{R}} \ast \hat{u}(\rho\rangle)^2 = \lambda_a \|g_{\mathcal{R}}(\rho) \hat{u}(\rho\rangle\|^2 = \lambda_a \|g_{\mathcal{R}}(\rho) a\|^2.
\]

Since $a \in \mathbb{C}^{dd'}$ was arbitrary, we have $\lambda_{\min}(f_V(\rho), g_{\mathcal{R}}(\rho)) \geq \lambda_a$.

Now we prove that $\lambda_a \geq \text{RHS}$. Let $u \in U_{\text{per,C}}$. For a matrix $A$ we denote its $i$th
Lemma 5.11. For all representations \( \rho \) of \( \mathcal{T} \mathcal{F} \) the functions

\[
\mathbb{R}^{d_2} \to \mathbb{C}^{(dn_0d_{\rho}) \times (dn_0d_{\rho})}, \quad k \mapsto \hat{f}_V(\text{Ind}(\chi_k \rho)),
\]

and

\[
\mathbb{R}^{d_2} \to \mathbb{C}^{(|R|n_0d_{\rho}) \times (dn_0d_{\rho})}, \quad k \mapsto \tilde{g}_R(\text{Ind}(\chi_k \rho))
\]

are continuous and the functions

\[
\mathbb{R}^{d_2} \to \mathbb{R} \cup \{\pm \infty\}, \quad k \mapsto \lambda_{\min}\left(\hat{f}_V(\text{Ind}(\chi_k \rho)), \tilde{g}_R(\text{Ind}(\chi_k \rho))\right)
\]

and

\[
\mathbb{R}^{d_2} \to \mathbb{R} \cup \{\pm \infty\}, \quad k \mapsto \lambda_{\min}\left(\hat{f}_V(\text{Ind}(\chi_k \rho)), \tilde{g}_{R,0,0}(\text{Ind}(\chi_k \rho))\right)
\]

are upper semicontinuous.

Proof. Let \( \rho \) be a representation of \( \mathcal{T} \mathcal{F} \) and \( f_i \) denote the \( i \)th function of the lemma for each \( i \in \{1, \ldots, 5\} \). Since \( f_V \in L^1(\mathcal{G}, \mathbb{R}^{d \times d}) \) and \( g_R, g_{R,0,0} \in L^1(\mathcal{G}, \mathbb{R}^{(|R|d) \times d}) \), the functions \( f_1, f_2 \) and \( f_3 \) are continuous.

Let \( (k_n)_{n \in \mathbb{N}} \) be a sequence in \( \mathbb{R}^{d_2} \) and \( k \in \mathbb{R}^{d_2} \) be such that \( \lim_{n \to \infty} k_n = k \). Without loss of generality we assume that \( \limsup_{n \to \infty} f_4(k_n) \geq -\infty \) and \( \limsup_{n \to \infty} f_4(k_n) = \lim_{n \to \infty} f_4(k_n) \). Let \( \lambda \in \mathbb{R} \) such that \( \lambda < \limsup_{n \to \infty} f_4(k_n) \). We have \( \lambda f_2(k_n)^H f_2(k_n) \leq f_1(k_n) \) for all \( n \in \mathbb{N} \) large enough. Since the Loewner order is closed, i.e. the set \( \{(A, B) \in X^2 | A \leq B \} \) is closed, where \( X = \{ A \in \mathbb{C}^{(dn_0d_{\rho}) \times (dn_0d_{\rho})} | A \text{ is Hermitian}\} \), we have \( \lambda f_2(k)^H f_2(k) \leq f_1(k) \). Thus we have \( \lambda \leq f_4(k) \).

Analogously the function \( f_5 \) is upper semicontinuous. \( \square \)
We are now ready to prove our main result which generalizes the representation results in [29, 9] from lattices to general objective structures. Recall Definition 2.12, Proposition 2.13 and Definition 2.10.

**Theorem 5.12.** Let \( R \) be a representation set of a representation set of \( \overline{TF/\sim} \). For all \( \rho \in R \) let \( K_\rho \) be a representation set of \( \mathbb{R}^{d_2}/G_\rho \). Then we have

\[
\lambda_a = \inf \left\{ \lambda_{\min}\left( \widehat{f}_V(\Ind(\chi k\rho)), \widehat{g}_{\overline{R}}(\Ind(\chi k\rho)) \right) \left| \rho \in R, k \in K_\rho \right. \right\}
\]
and

\[
\lambda_{a,0,0} = \inf \left\{ \lambda_{\min}\left( \widehat{f}_V(\Ind(\chi k\rho)), \widehat{g}_{\overline{R},0,0}(\Ind(\chi k\rho)) \right) \left| \rho \in R, k \in K_\rho \right. \right\}.
\]

**Proof.** Recall that \( M_0 = m_0 \mathbb{N} \). By Lemma 2.11(i) there exists a representation set \( R' \) of a representation set of \( \overline{TF/\sim} \) such that \( \rho \) is \( \overline{\tau}^{\text{mo}} \)-periodic for all \( \rho \in R' \). Due to the existence of fundamental domains, see, e.g., [35 Theorem 6.6.13], for all \( \rho \in R' \) there exists a representation set \( K'_\rho \) of \( \mathbb{R}^{d_2}/G_\rho \) such that \( L'_\rho = \{ k \in K'_\rho \left| \exists N \in M_0 : k \in L_{\rho}^\delta/N \} \). By Theorem 2.15 applied to \( R \) and \( R' \), there exist a bijection

\[
\varphi: \bigcup_{\rho \in R'} K'_\rho \to \bigcup_{\rho \in R} K_\rho, \quad (k, \rho) \mapsto (\varphi_1(k, \rho), \varphi_2(k, \rho)) \tag{42}
\]
and for all \( \rho \in R' \) and \( k \in K'_\rho \) some \( T_{k,\rho} \in U(d_{\Ind(\chi k\rho)}) \) such that

\[
\Ind(\chi_{\varphi_1(k,\rho)}\varphi_2(k,\rho)) = T_{k,\rho}^H \Ind(\chi k\rho)T_{k,\rho}^T.
\]

By (42) and (43) we have

\[
\text{RHS} := \inf \left\{ \lambda_{\min}\left( \widehat{f}_V(\Ind(\chi k\rho)), \widehat{g}_{\overline{R}}(\Ind(\chi k\rho)) \right) \left| \rho \in R, k \in K_\rho \right. \right\}
\]

\[
= \inf \left\{ \lambda_{\min}\left( \widehat{f}_V(\Ind(\chi_{\varphi_1(k,\rho)}\varphi_2(k,\rho))), \widehat{g}_{\overline{R}}(\Ind(\chi_{\varphi_1(k,\rho)}\varphi_2(k,\rho))) \right) \left| \rho \in R', k \in K'_\rho \right. \right\}
\]

\[
= \inf \left\{ \lambda_{\min}\left( (I_d \otimes T_{k,\rho}^H)\widehat{f}_V(\Ind(\chi k\rho))(I_d \otimes T_{k,\rho}), (I_d \otimes T_{k,\rho}^H)\widehat{g}_{\overline{R}}(\Ind(\chi k\rho))(I_d \otimes T_{k,\rho}) \right) \left| \rho \in R', k \in K'_\rho \right. \right\}
\]

\[
= \inf \left\{ \lambda_{\min}\left( \widehat{f}_V(\Ind(\chi k\rho)), \widehat{g}_{\overline{R}}(\Ind(\chi k\rho)) \right) \left| \rho \in R', k \in K'_\rho \right. \right\}.
\]

For all \( \rho \in R' \) we define the function

\[
f_\rho: K'_\rho \to \mathbb{R} \cup \{ \pm \infty \}
\]

\[
k \mapsto \lambda_{\min}\left( \widehat{f}_V(\Ind(\chi k\rho)), \widehat{g}_{\overline{R}}(\Ind(\chi k\rho)) \right).
\]

By Lemma 5.11 for all \( \rho \in R' \) the function \( f_\rho \) is upper semicontinuous and thus we have

\[
\inf f_\rho = \inf f_\rho|_{L'_\rho}.
\]

By (44) and (45) we have

\[
\text{RHS} = \inf \{ f_\rho(k) \left| \rho \in R', k \in L'_\rho \right. \}.
\]

By Theorem 5.10 we have

\[
\lambda_a = \inf \{ \lambda_{\min}\left( \widehat{f}_V(\rho), \widehat{g}_{\overline{R}}(\rho) \right) \left| \rho \in \mathcal{E} \right. \}.
\]

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By Lemma A.4(ii) there exists a permutation matrix $P_{n,p_1,...,p_k} \in O(p_1 + \cdots + p_k)$ for all $n, p_1, \ldots, p_k \in \mathbb{N}$ such that

$$A \otimes (B_1 \oplus \cdots \oplus B_k) = P^T_{m,p_1,...,p_k} ((A \otimes B_1) \oplus \cdots \oplus (A \otimes B_k)) P_{n,p_1,...,p_k}$$

for all $A \in \mathbb{C}^{m \times n}$ and $B_i \in \mathbb{C}^{p_i \times p_1}$, $i \in \{1, \ldots, k\}$.

Now we show that $\lambda \leq \text{RHS}$. Let $\rho \in R'$, $k \in L'_\rho$ and $\rho' = \text{Ind}(\chi k \rho)$. Let $N \in M_0$ such that by Lemma 2.9 and the construction of $L'_\rho$ we have $\chi k | T^N = 1$. The map $\rho'$ is $T^N$-periodic. There exist some $\rho_1, \ldots, \rho_n \in \mathcal{E}$ and $T \in U(d_{\rho'})$ such that

$$\rho'(g) = T^H(\rho_1(g) \oplus \cdots \oplus \rho_n(g))T \quad \text{for all } g \in G.$$

We have

$$\widehat{f}_V(\rho') = \sum_{g \in G} f_V(g) \otimes \rho'(g)$$

$$= \sum_{g \in G} f_V(g) \otimes (T^H(\rho_1(g) \oplus \cdots \oplus \rho_n(g))T)$$

$$= (I_d \otimes T)^H \left( \sum_{g \in G} f_V(g) \otimes (\rho_1(g) \oplus \cdots \oplus \rho_n(g)) \right) (I_d \otimes T)$$

$$= P^H \left( \left( \sum_{g \in G} f_V(g) \otimes \rho_1(g) \right) \oplus \cdots \oplus \left( \sum_{g \in G} f_V(g) \otimes \rho_1(g) \right) \right) P$$

$$= P^H \left( \widehat{f}_V(\rho_1) \oplus \cdots \oplus \widehat{f}_V(\rho_n) \right) P,$$

where $P$ is the unitary matrix $P_{d,\rho_1,...,\rho_n} (I_d \otimes T)$. Analogously to (47) we have

$$\widehat{g}_{R}(\rho') = Q^H \left( \widehat{g}_{R}(\rho_1) \oplus \cdots \oplus \widehat{g}_{R}(\rho_n) \right) P,$$

where $Q$ is the unitary matrix $P_{d,\rho_1,...,\rho_n} (I_d \otimes T)$. By (47), (48) and (48) we have

$$f_p(k) = \lambda_{\min} \left( \widehat{f}_V(\rho_1) \oplus \cdots \oplus \widehat{f}_V(\rho_n), \widehat{g}_{R}(\rho_1) \oplus \cdots \oplus \widehat{g}_{R}(\rho_n) \right)$$

$$= \min \left\{ \lambda_{\min} \left( \widehat{f}_V(\rho_1), \widehat{g}_{R}(\rho_1) \right) \mid \rho_1 \in \mathcal{E} \right\} \geq \lambda_a.$$

Now we show that $\lambda_a \geq \text{RHS}$. Let $\rho_1 \in \mathcal{E}$. By Theorem 2.1(1) the set $\{ \text{Ind}(\chi k \rho) \mid \rho \in R', k \in L'_\rho \}$ is a representation set of $\text{Ind}(\{ \rho \in T \mathcal{F} \mid \rho \text{ is periodic} \})$. By Corollary 2.17 there exist some $\rho \in R'$ and $k \in L'_\rho$ such that $\rho_1$ is isomorphic to a subrepresentation of $\text{Ind}(\chi k \rho)$. Let $\rho' = \text{Ind}(\chi k \rho)$. There exist some $\rho_2, \ldots, \rho_n \in \mathcal{E}$ and $T \in U(d_{\rho'})$ such that

$$\rho'(g) = T^H(\rho_1(g) \oplus \cdots \oplus \rho_n(g))T \quad \text{for all } g \in G.$$

Analogously to (47) and (48) we have

$$\widehat{f}_V(\rho') = P^H \left( \widehat{f}_V(\rho_1) \oplus \cdots \oplus \widehat{f}_V(\rho_n) \right) P$$

and

$$\widehat{g}_{R}(\rho') = Q^H \left( \widehat{g}_{R}(\rho_1) \oplus \cdots \oplus \widehat{g}_{R}(\rho_n) \right) P,$$

where $P$ and $Q$ are the unitary matrices $P_{d,\rho_1,...,\rho_n} (I_d \otimes T)$ and $P_{d,\rho_1,...,\rho_n} (I_d \otimes T)$, respectively. We have

$$\lambda_{\min} \left( \widehat{f}_V(\rho_1), \widehat{g}_{R}(\rho_1) \right) \geq \min \left\{ \lambda_{\min} \left( \widehat{f}_V(\rho_1), \widehat{g}_{R}(\rho_1) \right) \mid \rho_1 \in \mathcal{E} \right\} = f_p(k) \geq \text{RHS}.$$

The proof of the characterization of $\lambda_{a,0,0}$ is analogous. □
Remark 5.13. (i) By Lemma 5.11, the above theorem is also true if for all $\rho \in R$ we weaken the assumption on $K_\rho$ and only assume that the closure of $K_\rho$ contains a representation set of $\mathbb{R}^d/G_\rho$. In particular the theorem is also true if for all $\rho \in R$ the set $K_\rho$ is a fundamental domain of $\mathbb{R}^d/K_\rho$.

(ii) An algorithm for the determination of a representation set of $\overline{\mathcal{F}}/\sim$ with the aid of the finite group $(\mathcal{T}\mathcal{F})_{m_0}$ is given by Lemma 2.11.

6 A stability algorithm and applications

6.1 The general algorithm

In view of our main results we can now give an algorithm which checks if $(\mathcal{G}, x_0, V)$ is stable with respect to $\| \cdot \|_R$, see Definition 3.8. The algorithm for the stability with respect to $\| \cdot \|_{R,0,0}$ is analogous.

Algorithm 6.1. Given is a discrete group $\mathcal{G} < E(d)$ and its associated groups $\mathcal{F}$, $\mathcal{S}$ and set $\mathcal{T}$, some point $x_0 \in \mathbb{R}^d$ such that the map $\mathcal{G} \to \mathbb{R}^d$, $g \mapsto g \cdot x_0$ is injective, and an interaction potential $V$, see Definition 3.1. Since the algorithm is numeric and by (H3) we may assume that $V$ has finite support.

(i) Check if $\chi_{\mathcal{G}} x_0$ is a critical point of the configurational energy $E$, e.g. by computing the derivative $\partial_g V(y_0)$ for all $g \in \text{supp} V$, see Definition 3.1, the vector $\mathcal{e}_V$, see Definition 3.11 and checking if $\mathcal{e}_V = 0$, see Corollary 3.16.

(ii) Determine the derivative $\partial_g \partial_h V(y_0)$ for all $g, h \in \text{supp} V$, see Definition 3.1. Then compute the function $f_V$ by computing $f_V(g)$ for all $g \in \{\id\} \cup \text{supp} V \cap \{\id\} \cup \text{supp} V$, see Definition 3.11 and Remark 3.12(ii).

(iii) Determine a set $\mathcal{R}$ with Property 2, see Definition 2.29. Fix a bijection $\varphi : \mathcal{R} \to \{0, \ldots, |\mathcal{R}| - 1\}$. Thus the map

$$\psi : U_{\text{iso}}(\mathcal{R}) \to \mathbb{R}^{d|\mathcal{R}|}, \quad u \mapsto (u(\varphi^{-1}(0)), \ldots, u(\varphi^{-1}(|\mathcal{R}| - 1)))^T,$$

which maps a function to a column vector, is an embedding, where $U_{\text{iso}}(\mathcal{R})$ is defined in Definition 2.22. By Proposition 2.23 and the Gram-Schmidt process, we can determine an orthonormal basis $\{b_1, \ldots, b_n\}$ of $\psi(U_{\text{iso}}(\mathcal{R}))$, where $n = \dim(U_{\text{iso}}(\mathcal{R}))$.

Let $B$ be the $d|\mathcal{R}|$-by-$n$ matrix $(b_1, \ldots, b_n)$. The matrix $I_{d|\mathcal{R}|} - BB^T$ is the orthogonal projection matrix with kernel $\psi(U_{\text{iso}}(\mathcal{R}))$. Now we can determine the function $g_{\mathcal{R}}$, i.e. the matrix $g_{\mathcal{R}}(g)$ for all $g \in \mathcal{R}$, see Definition 5.2 and Remark 5.3.

(iv) Determine a representation set $R$ of $\overline{\mathcal{F}}/\sim$, e.g. with Lemma 2.11, where $\sim$ is the equivalence relation defined in Definition 2.10. For all $\rho \in R$ determine the space group $\mathcal{G}_\rho$, see Definition 2.12, with, e.g., Proposition 2.13, and determine a representation set (or a fundamental domain, see Remark 5.3(i)) $K_\rho$ of $\mathbb{R}^d/G_\rho$.

(v) Fix a complete set of representatives of the cosets of $\mathcal{T}\mathcal{F}$ in $\mathcal{G}$. Thus the induced representation $\text{Ind}(\chi_{k\rho})$ is well-defined for all $\rho \in R$ and $k \in K_\rho$, see Definition 2.8 and Definition 2.14. For all $\rho \in R$ and $k \in K_\rho$ the matrices $\tilde{f}_V(\text{Ind}(\chi_{k\rho}))$ and $\tilde{g}_R(\text{Ind}(\chi_{k\rho}))$ can be computed with Definition 2.5. Since the dimension of the kernel of $\| \cdot \|_R$ is finite, for all $\rho \in R$ and all but finitely many $k \in K_\rho$, the matrix $\tilde{g}_R(\text{Ind}(\chi_{k\rho}))$ has full rank and thus the real number $\lambda_{\min}(\tilde{f}_V(\text{Ind}(\chi_{k\rho})), \tilde{g}_R(\text{Ind}(\chi_{k\rho})))$
can easily be computed, see Definition 5.8 and Remark 5.9(ii). Due to the upper semicontinuity, see Lemma 5.11, by Theorem 5.12 we can compute the extended real number $\lambda_a$.

(vi) The triple $(G, x_0, V)$ is stable with respect to $\| \cdot \|_R$ if and only if $\chi_G x_0$ is a critical point of $E$ and $\lambda_a > 0$, see Definition 3.8.

In the following two examples, we investigate the stability of a triple $(G_i, x_i, V_i)$ for all $i \in I$, where $I$ is a suitable index set. The figures are generated with the programming language Python, see [https://github.com/Toymodel-Nanotube/](https://github.com/Toymodel-Nanotube/) for the source code.

6.2 Example: a chain of atoms

Example 6.2. A suitable toy model for the investigation of stability is an atom chain. Let $a > 0$ be the scale factor, $t = t_a = (I_2, ae_2) \in E(2)$ and $G = G_a = (t) < E(2)$. We define the interaction potential $V = V_a$, see Definition 3.1 and Remark 3.2(iv), by

$$V_a(y) = v_1(\|y(t_a)\|) + v_2(\|y(t_a^2)\|),$$

where

$$v_1: (0, \infty) \to \mathbb{R}, \quad r \mapsto r^{-12} - r^{-6}$$

is the Lennard-Jones potential and

$$v_2: (0, \infty) \to \mathbb{R}, \quad r \mapsto 8r^{-6}.$$

Let $x_0 = 0_2$. By Lemma 3.6 for all $a > 0$ we have

$$E(\chi_G x_0) = V(y_0) = a^{-12} - \frac{7}{8} a^{-6},$$

where $E = E_a$ is the configurational energy and $y_0 = y_{0,a} = (g \cdot x_0 - x_0)_{g \in G_a}$. We define

$$a^* := \arg \min_{a \in (0, \infty)} E(\chi_G x_0) = \sqrt[6]{\frac{16}{7}} \approx 1.1477.$$

Thus the structure $G \cdot x_0$ is stretched (resp. compressed) if $a > a^*$ (resp. $a < a^*$). Now we investigate its stability numerically with Algorithm 6.1.

(i) By Corollary 3.17 the function $\chi_G x_0$ is a critical point of $E$ for all $a > 0$.

(ii) We have

$$\partial_g \partial_h V(y_0) = \begin{cases} 
6a^{-8} \begin{pmatrix} -2a^{-6} + 1 & 0 \\ 0 & 26a^{-6} - 7 \end{pmatrix} & \text{if } g = h = t \\
2^{-4}3a^{-8} \begin{pmatrix} -1 & 0 \\ 0 & 7 \end{pmatrix} & \text{if } g = h = t^2 \\
0_{2,2} & \text{else.}
\end{cases}$$
We have $(\{id\} \cup \text{supp } V)^{-1}(\{id\} \cup \text{supp } V) = \{t^{-2}, \ldots, t^2\}$ and

$$f_V(g) = \begin{cases} a^{-8}(-24a^{-6} + 93/8 & 0 \\ 0 & 312a^{-6} - 651/8) & \text{if } g = id \\ 6a^{-8}(2a^{-6} - 1 & 0 \\ 0 & -26a^{-6} + 7) & \text{if } g \in \{t^{-1}, t\} \\ 2^{-4}a^{-8}(1 & 0 \\ 0 & -7) & \text{if } g \in \{t^{-2}, t^2\} \\ 0_{2,2} & \text{else.} \end{cases}$$

(iii) Since $\{id, t\}$ has Property 1 and $\{t\}$ generates $G$, the set $R = \{id, t, t^2\}$ has Property 2. We define the functions

$$b_1: R \to \mathbb{R}^2, \ g \mapsto e_i$$

and

$$b_3: R \to \mathbb{R}^2, \ g \mapsto \left(\begin{array}{c} 0 \\ 1 \end{array}\right)(g \cdot x_0 - x_0).$$

By Proposition 2.23 the sets $\{b_1, b_2, b_3\}$ and $\{b_1, b_2\}$ are bases of $U_{iso}(R)$ and $U_{iso,0,0}(R)$, respectively. We define the bijection $\phi: R \to \{0, 1, 2\}$ by $t^n \mapsto n$ for all $n \in \{0, 1, 2\}$.

Let $\psi$ be the embedding

$$U_{iso}(R) \hookrightarrow \mathbb{R}^6, \ u \mapsto (u(\varphi^{-1}(0)), \ldots, u(\varphi^{-1}(2))).$$

A computation shows that the orthogonal projection matrices of $\mathbb{R}^6$ with kernels $\psi(U_{iso}(R))$ and $\psi(U_{iso,0,0}(R))$ are

$$\begin{pmatrix} 1 & 0 & -2 & 0 & 1 & 0 \\ 0 & 4 & 0 & -2 & 0 & -2 \\ -2 & 0 & 4 & 0 & -2 & 0 \\ 0 & -2 & 0 & 4 & 0 & -2 \\ 1 & 0 & -2 & 0 & 1 & 0 \\ 0 & -2 & 0 & -2 & 0 & 4 \end{pmatrix} \quad \text{and} \quad \frac{1}{3} \begin{pmatrix} 2 & 0 & -1 & 0 & -1 & 0 \\ 0 & 2 & 0 & -1 & 0 & -1 \\ -1 & 0 & 2 & 0 & -1 & 0 \\ 0 & -1 & 0 & 2 & 0 & -1 \\ -1 & 0 & -1 & 0 & 2 & 0 \\ 0 & -1 & 0 & -1 & 0 & 2 \end{pmatrix},$$

respectively. Thus the functions $g_R$ and $g_{R,0,0}$ of Definition 5.2 are given by

$$\text{supp } g_R = \text{supp } g_{R,0,0} = R,$n

$$g_R(id) = \frac{1}{6} \begin{pmatrix} 1 & 0 \\ 0 & 4 \\ -2 & 0 \\ 0 & -2 \\ 1 & 0 \\ 0 & -2 \end{pmatrix}, \quad g_R(t) = \frac{1}{6} \begin{pmatrix} -2 & 0 \\ 0 & -2 \\ 4 & 0 \\ 0 & 4 \\ -2 & 0 \\ 0 & -2 \end{pmatrix}, \quad g_R(t^2) = \frac{1}{6} \begin{pmatrix} 1 & 0 \\ 0 & -2 \\ -2 & 0 \\ 0 & 4 \end{pmatrix}$$

and

$$g_{R,0,0}(id) = \frac{1}{3} \begin{pmatrix} 2 & 0 \\ 0 & 2 \\ -1 & 0 \\ 0 & -1 \\ -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad g_{R,0,0}(t) = \frac{1}{3} \begin{pmatrix} -1 & 0 \\ 0 & -1 \\ 2 & 0 \\ 0 & 2 \\ -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad g_{R,0,0}(t^2) = \frac{1}{3} \begin{pmatrix} -1 & 0 \\ 0 & -1 \\ 2 & 0 \\ 0 & 2 \end{pmatrix}.$$
Figure 1: For the toy model as described in Example 6.2, the graphs of the numbers \( \lambda_{\min}(\tilde{f} V(\chi_k), \tilde{g} R(\chi_k)) \) (blue) and \( \lambda_{\min}(\tilde{f} V(\chi_k), \tilde{g} R_{0,0}(\chi_k)) \) (orange) dependent on \( k \in K_{id} \setminus \{0\} \) are plotted on the left for the choice \( a = 1.22 \). The points \((a^*, 0)\) and \((a^{**}, 0)\) and the graphs of \( \lambda_a \) (blue) and \( \lambda_{a,0,0} \) (orange) dependent on the scale factor are plotted on the right.

\[ \text{(iv)} \] We have \( \mathcal{G} = \mathcal{T} \mathcal{F} = \langle t \rangle, M_0 = \mathbb{N} \) and \( \{id\} \) is a representation set of \( \mathcal{T} \mathcal{F} / \sim \) by Lemma 2.11(i). We have \( \mathcal{S} = \langle (I_1, a) \rangle, L_S = \langle a \rangle \) and \( L^*_S = \langle a^{-1} \rangle \), see [1]. By Proposition 2.13 we have \( \{k \in \mathbb{R} | (I_1,k) \in \mathcal{G}_{id} \} = \langle a^{-1} \rangle \) and thus \( \mathcal{G}_{id} = \langle (I_1, a^{-1}) \rangle \).

The interval \( K_{id} = [0, a^{-1}] \) is a representation set of \( \mathbb{R} / \mathcal{G}_{id} \).

\[ \text{(v)} \] For all \( k \in K_{id} \) we have \( \text{Ind}_{\mathcal{T} \mathcal{F}} \chi_k = \chi_k \). We have

\[ \{k \in K_{id} | \tilde{g} R(\chi_k) \text{ has full rank} \} = K_{id} \setminus \{0\} \]

and

\[ \{k \in K_{id} | \tilde{g} R_{0,0}(\chi_k) \text{ has full rank} \} = K_{id} \setminus \{0\}. \]

The numbers \( \lambda_{\min}(\tilde{f} V(\chi_k), \tilde{g} R(\chi_k)) \) and \( \lambda_{\min}(\tilde{f} V(\chi_k), \tilde{g} R_{0,0}(\chi_k)) \) can then be computed for all \( k \in K_{id} \setminus \{0\} \). In particular, we can compute \( \lambda_a = \lambda_a(a) \) and \( \lambda_{a,0,0} = \lambda_{a,0,0}(a) \) numerically, see Figure 1.

\[ \text{(vi)} \] In the compressed case \( a \in (0, a^*) \) we have \( \lambda_a = -\infty \) and \( \lambda_{a,0,0} \in (-\infty, 0) \) and thus \((\mathcal{G}, x_0, V)\) is not stable with respect to both \( \| \cdot \|_R \) and \( \| \cdot \|_{R_{0,0}} \). Now we investigate the stretched case, i.e. \( a > a^* \). We consider the ‘period doubling mode’ \( u = \chi_{T^2 e_2} \) and let \( a^{**} > 0 \) such that \( E''(\chi_G x_0)(u,u) = 0 \), i.e. \( a^{**} = \sqrt[1]{26}/7 \approx 1.24455 \). Indeed for all \( a \in (a^*, a^{**}) \) we have \( \lambda_a > 0 \) and \( \lambda_{a,0,0} > 0 \) and thus \((\mathcal{G}, x_0, V)\) is stable with respect to both \( \| \cdot \|_R \) and \( \| \cdot \|_{R_{0,0}} \).

For all \( a > a^{**} \) we obtain \( E''(\chi_G x_0)(u,u) < 0 \) and we have \( \lambda_a < 0 \) and \( \lambda_{a,0,0} < 0 \) and thus \((\mathcal{G}, x_0, V)\) is not stable with respect to both \( \| \cdot \|_R \) and \( \| \cdot \|_{R_{0,0}} \). In particular, the loss of stability beyond \( a^{**} \) is seen to result from a period doubling deformation mode.

Notice that in the stretched case \( a \in (a^*, a^{**}) \), the appropriate seminorm for the stability is \( \| \cdot \|_{R_{0,0}} \). For the equilibrium case \( a \approx a^* \), the weaker seminorm \( \| \cdot \|_R \) is appropriate since \( \lim_{a \to a^*} \lambda_{a,0,0} = 0 \) and \( \lim_{a \to a^*} \lambda_a > 0 \).

### 6.3 Example: a carbon nanotube

**Example 6.3.** We now consider a carbon nanotube with non-trivial chirality. Single-walled carbon nanotubes are classified by an integer pair \((n, m)\) depending on the winding
Figure 2: As described in Example 6.3, the orbit of the point $x_{a_0}$ under the action of the group $G_{a_0}$ is a (5, 1) nanotube. We have a natural bijection between the group elements and the atoms. $x_{a_0}$ and its nearest neighbor bonds to atoms in $N \cdot x_{a_0}$ are highlighted.

direction if the tube is visualized as a rolled-up graphene sheet. While there is a considerable amount of literature on the stability of the achiral zigzag (of type $(n, 0)$) and armchair (of type $(n, n)$) variants, see in particular [24] and the references therein, general chiral tubes are much less understood.

Since for any pair $(n, m)$ the nanotube is the orbit of some point in $\mathbb{R}^3$ under the action of a discrete subgroup of $E(3)$, our stability analysis applies. By way of example we will now investigate the stability of a (5, 1) nanotube, see Figure 2 with Algorithm 6.1. For all scale factors $a > 0$ and angles $\alpha \in (0, \pi)$ we define: Let $R(\alpha) \in O(2)$ be the rotation matrix

$$R(\alpha) := \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{pmatrix},$$

$t = t_{a,\alpha} = (R(\alpha) \oplus I_1, ae_3) \in E(3)$, $p = (I_1 \oplus (-I_2), 0) \in E(3)$ and $G = G_{a,\alpha}$ be the discrete group $\langle t, p \rangle < E(3)$, i.e. $G = \{t^m p^n | m \in \mathbb{Z}, q \in \{0, 1\}\}$. For all $x \in \mathbb{R}^3$ we have $G \cdot x \subset C_x$, where $C_x$ is the cylinder $\{y \in \mathbb{R}^3 | y_1^2 + y_2^2 = x_1^2 + x_2^2\}$.

Let $N = N_{a,\alpha} = \{tp, t^6 p, t^7 p\}$. Let $U_{a,\alpha} \subset \mathbb{R}^3$ be the set of all points $x \in \mathbb{R}^3$ for which the map $G \to \mathbb{R}^3$, $g \mapsto g \cdot x$ is injective and the three nearest neighbors of $x$ in $G \cdot x$ are the points $N \cdot x$, i.e.

$$\sup \left\{ \|g \cdot x - x\| \left| g \in N \right\} \right. < \inf \left\{ \|g \cdot x - x\| \left| g \in G \setminus (N \cup \{id\}) \right\} \right.$$

Let

$$W := \{(a, \alpha, x) \mid a > 0, \alpha \in (0, \pi), x \in U_{a,\alpha}\}.$$

Analogously to [24] we define the interaction potential $V = V_{a,\alpha}$, see Definition 3.1 and Remark 3.2(iv) by

$$V(y) = \frac{1}{2} \sum_{g \in N} v_1(\|y(g)\|) + \frac{1}{2} \sum_{g, h \in N} v_2(y(g), y(h)),$$

where

$$v_1 : (0, \infty) \to \mathbb{R}, r \mapsto (r - 1)^2$$

is a two-body potential and

$$v_2 : \left\{(x, y) \mid x, y \in \mathbb{R}^3 \setminus \{0\}\right\} \to \mathbb{R}, (x, y) \mapsto \left(\frac{\langle x, y \rangle}{\|x\||y\|} + \frac{1}{2}\right)^2,$$
is a three-body potential. Thus the bonded points of $G \cdot x$ tend to have distance 1 and the bond angles tend to form $2\pi/3$ angles. By Lemma 3.6 for all $(a,\alpha,x) \in W$ we have $E(\chi_Gx) = V(y_0)$, where $E = E_{a,\alpha}$ is the configurational energy and $y_0 = y_{0,a,\alpha,x} = (g \cdot x - x)_{g \in G_{a,\alpha}}$.

First we consider the (5,1) nanotube. We define $\alpha_0 := 11\pi/31 \approx 1.115$ and $x_a := a(r \cos(\beta), r \sin(\beta), 7/3) \in \mathbb{R}^3$ for all $a > 0$, where

$$r = 31/(\pi\sqrt{3}) \quad \text{and} \quad \beta = 5\pi/31.$$  

In the strict sense of [16], for all $(a,\alpha,x) \in W$ the set $G \cdot x$ is a so-called (5,1) nanotube if and only if $\alpha = \alpha_0$ and $x = x_a$. The bond length of the unrolled (5,1) nanotube $G_{a,\alpha_0} \cdot x_a$, i.e. the distance of two neighboring points of $G_{a,\alpha_0} \cdot x_a$ with respect to the induced metric of the manifold $C_x$, is equal to 1 if and only if $a = a_0$, where

$$a_0 := 3/(2\sqrt{31}) \approx 0.269.$$  

Now we investigate numerically with Algorithm 6.1 the stability of the (5,1) nanotube, more precisely of $(G_{a,\alpha_0}, x_a, V_{a,\alpha_0})$.

(i) For all $a > 0$ we have $e_{V_{a,\alpha_0}} \neq 0$, see Figure 3, and thus $\chi_{G_{a,\alpha_0}}x_a$ is not a critical point of $E_{a,\alpha_0}$. Thus we can proceed with (vi).

(vi) By (i) for all $a > 0$ the triple $(G_{a,\alpha_0}, x_a, V_{a,\alpha_0})$ is not stable with respect to both $\|\cdot\|_R$ and $\|\cdot\|_{R,0,0}$.

This failure suggests that we should relax our model to allow for nanotubes that correspond to critical points of the energy and still have the same neighborhood structure. We define

$$(a^*, \alpha^*, x^*) := \arg \min_{(a,\alpha,x) \in W} E_{a,\alpha}(\chi_{G_{a,\alpha}}x) \approx (0.263, 1.117, (1.388, 0.776, 0.626))$$
and
\[ x_a^* := \arg \min_{x \in U, a^*} E(\chi_G x) \quad \text{for all } a \approx a^*. \]

In particular we have \( x^* = x_a^* \). We have \((a^*, \alpha^*, x^*) \approx (a_0, \alpha_0, x_{a_0})\) and thus the nanotube \( G_{a^* \alpha^*} \cdot x^* \) is approximately equal to the \((5,1)\) nanotube \( G_{a_0 \alpha_0} \cdot x_{a_0} \). Now for all \( a \approx a^* \) we check the stability of \((G_{a^* \alpha^*} \cdot x_a^*, V_{a \alpha^*})\) numerically with Algorithm 6.1.

(i) For all \( a \approx a^* \) the function \( \chi_G x_a^* \) is a critical point of \( E \) by Remark 3.15(ii) and Corollary 3.16.

(ii) We have
\[ \text{supp } V = \{tp, t^6p, t^7p\} \]
and
\[ \text{supp } f_V = \{t^{-6}, t^{-5}, t^{-1}, id, t, t^5, t^6, tp, t^6p, t^7p\} \]
by Remark 3.15(ii) and the relations \((tp)^{-1} = pt^{-1} = tp\). The first and second derivative of \( V \) can be computed, e.g., with the Python library SymPy and \( f_V \) can be computed numerically by Definition 3.11.

(iii) Since \( \{t^{-1}, id, t, p\} \) has Property 1 and \{\(t, p\)\} generates \( G \), by Definition 2.29 the set
\[ \mathcal{R} = \mathcal{R}_a := \{t^{-1}, id, t, t^2, t^{-1}p, p, tp\} \]
has Property 2. We define the bijection \( \varphi \) between \( \mathcal{R} \) and \( \{0, \ldots, 6\} \) by \( \varphi(t^m) = m + 1 \) for all \( m \in \{-1, 0, 1, 2\} \) and \( \varphi(t^mp) = m + 5 \) for all \( m \in \{-1, 0, 1\} \). For all \( a \approx a^* \) we define the functions
\[ b_i = b_{i,a} : \mathcal{R} \to \mathbb{R}^3, \quad g \mapsto L(g)^T e_i \]
for all \( i \in \{1, 2, 3\} \)
and
\[ b_i = b_{i,a} : \mathcal{R} \to \mathbb{R}^3, \quad g \mapsto L(g)^T A_i (g \cdot x_a^* - x_a^*) \]
for all \( i \in \{4, 5, 6\} \),
where
\[ A_4 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad A_5 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \]
and \( A_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \).

By Proposition 2.23 the sets \( \{b_1, \ldots, b_6\} \) and \( \{b_1, \ldots, b_4\} \) are bases of \( U_{iso}(\mathcal{R}) \) and \( U_{iso,0,0}(\mathcal{R}) \), respectively. With, e.g., the Gram-Schmidt process we can determine functions \( b'_1, \ldots, b'_6 : \mathcal{R} \to \mathbb{R}^3 \) such that \( \{b'_1, \ldots, b'_6\} \) and \( \{b'_1, \ldots, b'_4\} \) are orthonormal bases of \( U_{iso}(\mathcal{R}) \) and \( U_{iso,0,0}(\mathcal{R}) \), respectively. A bijection between \( \{u : \mathcal{R} \to \mathbb{C}^3\} \) and \( \mathbb{C}^{21} \) is given by \( u \mapsto (u(\varphi^{-1}(0)), \ldots, u(\varphi^{-1}(6))) \). Let \( B = (b'_1, \ldots, b'_6) \in \mathbb{R}^{21 \times 6} \) and \( B_0 = (b'_1, \ldots, b'_4) \in \mathbb{R}^{21 \times 4} \). The matrices \( P = I_{21} - BB^T \) and \( P_0 = I_{21} - B_0B_0^T \) are orthogonal projection matrices with kernels \( U_{iso}(\mathcal{R}) \) and \( U_{iso,0,0}(\mathcal{R}) \), respectively. Let \( p_0, \ldots, p_6, p_0, \ldots, p_6 \in \mathbb{R}^{21 \times 3} \) such that \( P = (p_0, \ldots, p_6) \) and \( P_0 = (p_0, \ldots, p_6) \). For the functions \( g_R \) and \( g_{R,0,0} \) of Definition 5.2 we have
\[ \text{supp } g_R = \text{supp } g_{R,0,0} = \mathcal{R}, \]
\[ g_R(g) = p_{\varphi(g)} \]
for all \( g \in \mathcal{R} \)
and
\[ g_{R,0,0}(g) = p_{0,\varphi(g)} \]
for all \( g \in \mathcal{R} \).
Figure 4: For the nanotube as described in Example 6.3, the point \((a^*/(2\pi a^*)), 0\) and the graphs of \(\lambda_{\text{min}}(f^*_V(\chi_k), \bar{g}_R(\chi_k))\) (blue) and \(\lambda_{\text{min}}(f^*_V(\chi_k), \bar{g}_{R,0,0}(\chi_k))\) (orange) dependent on \(k \in K_{id} \setminus \{0, a^*/(2\pi a^*)\}\) are plotted on the left for the choice \(a = a^*\). The point \((a^*, 0)\) and the graphs of \(\lambda_a\) (blue) and \(\lambda_{a,0,0}\) (orange) dependent on the scale factor are plotted on the right.

(iv) We have \(\mathcal{T} = \mathcal{T} = \langle t \rangle, M_0 = \mathbb{N}\) and \\{id\} is a representation set of \(\mathcal{T}/\sim\) by Lemma 2.11(i). We have \(L_\mathcal{S} = \langle a \rangle\) and \(L_\mathcal{S}' = \langle a^{-1} \rangle\), see [1]. By Proposition 2.13 we have \(\{k \in \mathbb{R} \mid (I_1, k) \in \mathcal{G}_{id}\} = \langle a^{-1} \rangle\) and thus \(\mathcal{G}_{id} = \{(a^{-1})^m, ma^{-1}\} \mid m \in \mathbb{Z}, q \in \{0, 1\}\). The interval \(K_{id} = [0, 1/(2a)]\) is a representation set of \(\mathbb{R}/\mathcal{G}_{id}\).

(v) The set \(\{id, p\}\) is a complete set of representatives of the cosets of \(\mathcal{T}_{\mathcal{F}}\) in \(\mathcal{G}\). For all \(k \in K_{id}\) and \(g \in \mathcal{G}\) we have

\[
\text{Ind}_{\mathcal{T}_{\mathcal{F}}}^\mathcal{G} \chi_k(g) = \begin{cases} 
(\chi_k(g) & 0 \\
0 & \chi_k(p^{-1}g)p \\
0 & \chi_k(gp) 
\end{cases}
\text{ if } g \in \mathcal{T}_{\mathcal{F}}
\]

\[
\text{Ind}_{\mathcal{T}_{\mathcal{F}}}^\mathcal{G} \chi_k(g) = \begin{cases} 
(\chi_k(g) & 0 \\
0 & \chi_k(p^{-1}g) \\
0 & \chi_k(gp) 
\end{cases}
\text{ else.}
\]

Now for all \(k \in K_{id}\), it is easy to compute the complex 6-by-6 matrices \(\widehat{f}_V(\text{Ind} \chi_k)\), \(\bar{g}_R(\text{Ind} \chi_k)\) and \(\bar{g}_{R,0,0}(\text{Ind} \chi_k)\). We have

\[
\{k \in K_{id} \mid \bar{g}_R(\text{Ind} \chi_k) \text{ has full rank} \} = K_{id} \setminus \{0, a^*/(2\pi a)\}
\]

and

\[
\{k \in K_{id} \mid \bar{g}_{R,0,0}(\text{Ind} \chi_k) \text{ has full rank} \} = K_{id} \setminus \{0, a^*/(2\pi a)\}.
\]

For all \(k \in K_{id} \setminus \{0, a^*/(2\pi a)\}\) we can compute \(\lambda_{\text{min}}(\widehat{f}_V(\text{Ind} \chi_k), \bar{g}_R(\text{Ind} \chi_k))\) and \(\lambda_{\text{min}}(\widehat{f}_V(\text{Ind} \chi_k), \bar{g}_{R,0,0}(\text{Ind} \chi_k))\). In particular we can compute \(\lambda_a(a, a^*)\) and \(\lambda_{a,0,0}(a, a^*)\) numerically, see Figure [4].

(vii) In the stretched case \(a > a^*\), we have \(\lambda_a(a, a^*) > 0\) and \(\lambda_{a,0,0}(a, a^*) > 0\) and thus \((\mathcal{G}_{a,a^*}, x_{a,a^*}, V_{a,a^*})\) is stable with respect to both \(\| \cdot \|_R\) and \(\| \cdot \|_{R,0,0}\). In the compressed case \(a \in (0, a^*)\) we have \(\lambda_a(a, a^*) = -\infty\) and \(\lambda_{a,0,0}(a, a^*) < 0\) and thus \((\mathcal{G}_{a,a^*}, x_{a,a^*}, V_{a,a^*})\) is not stable with respect to both \(\| \cdot \|_R\) and \(\| \cdot \|_{R,0,0}\). Notice that in the stretched case \(a > a^*\), the appropriate seminorm for the stability is \(\| \cdot \|_{R,0,0}\). For the equilibrium case \(a \approx a^*\), the weaker seminorm \(\| \cdot \|_R\) is appropriate since \(\lim_{a \searrow a^*} \lambda_{a,0,0}(a, a^*) = 0\) and \(\lim_{a \searrow a^*} \lambda_a(a, a^*) > 0\).
For all $a \approx a^*$ and $\alpha \approx \alpha^*$ we can compute $\lambda_a(a, \alpha)$ and $\lambda_{a,0,0}(a, \alpha)$ analogously. For $\alpha \approx \alpha^*$ the graphs of $\lambda_a(\cdot, \alpha)$ and $\lambda_{a,0,0}(\cdot, \alpha)$ are similar to the graphs of $\lambda_a(\cdot, \alpha^*)$ and $\lambda_{a,0,0}(\cdot, \alpha^*)$. As an example, we consider

$$\alpha_a := \arg \min_{\alpha \in (0, \pi)} E(\chi_G x_{a, \alpha})$$

for all $a \approx a^*$.

see Figure 5 In Figure 5 the graphs of the functions

$$a \mapsto \text{Relative difference}(\lambda_a(a, a^*), \lambda_a(a, a_a))$$

and

$$a \mapsto \text{Relative difference}(\lambda_{a,0,0}(a, a^*), \lambda_{a,0,0}(a, a_a))$$

are plotted, where

$$\text{Relative difference}(x, y) := |x - y|/\max\{|x|, |y|\} \quad \text{for all } x, y \in \mathbb{R}.$$
Remark A.2. A sequence \((y_n)_{n \in \mathbb{N}}\) in \(L^\infty(G \setminus \{id\}, \mathbb{R}^d)\) converges to \(y \in L^\infty(G \setminus \{id\}, \mathbb{R}^d)\) with respect to the weak* topology if and only if the sequence \((y_n)_{n \in \mathbb{N}}\) is bounded and \((y_n)_{n \in \mathbb{N}}\) converges componentwise to \(y\), i.e. \(\lim_{n \to \infty} y_n(g) = y(g)\) for all \(g \in G \setminus \{id\}\), see Exercise 2.51 in [28].

Proposition A.3. Suppose that \(V\) is weakly* sequentially continuous, \(E'(\chi_G x_0) = 0\) and let \(u \in U_{iso,0,0} \cap U_{per}\). Then it holds \(E''(\chi_G x_0)(u,u) = 0\) and \(\frac{d^4}{dt^4} E(\chi_G x_0 + \tau u)\rvert_{\tau = 0} = 0\).

Proof. For the monotonically increasing function
\[
r : [0, \infty) \to [0, \infty)
\]
\[
t \mapsto \sup \{|E(\chi_G x_0 + u) - E(\chi_G x_0)| \mid u \in B_t(0)\}
\]

it holds
\[
\lim_{t \nearrow 0} \frac{r(t)}{t^2} = \sup \{E''(\chi_G x_0)(u,u) \mid u \in U_{per}\} < \infty,
\] (49)

where \(B_t(0) = \{u \in U_{per} \mid \|u\rvert_{\infty} < t\}\) for all \(t > 0\).

Let \(u \in U_{iso,0,0} \cap U_{per}\). There exist some \(a \in \mathbb{R}^d\) and \(S \in \oplus(\text{Skew}(d_1) \times \{0_{d_2,d_2}\})\) such that
\[
L(g)u(g) = a + S(g \cdot x_0 - x_0)
\]
for all \(g \in G\).

Since differentiability implies locally boundedness, there exist some \(\delta > 0\) and \(C_1 > 0\) such that
\[
|V(y_n + w)| \leq C_1\text{ for all }w \in B_\delta(0),
\]
where \(B_\delta(0) = \{w \in L^\infty(G \setminus \{id\}, \mathbb{R}^d) \mid \|w\rvert_{\infty} < \delta\}\). Let \(C_2 = 2\|x_0\| \sup \{\|e^{-tS} - I_d + \tau S e^{-\tau S}\|/\tau^2 \mid \tau \in (-1,1)\} \geq 0\). By Taylor’s theorem we have \(C_2 < \infty\). Let \(t_0 = \min\{1, \sqrt{\delta/(2C_2)}\} > 0\), where \(a/0 := \infty\) for all \(a > 0\).

Now we show that
\[
|E(\chi_G x_0 + tu) - E(\chi_G x_0)| \leq r(C_2t^2) + t^4\text{ for all }t \in (-t_0, t_0).
\] (50)

Let \(t \in (-t_0, t_0) \setminus \{0\}\). We define the function \(v : G \to \mathbb{R}^d\) by
\[
g \cdot v(g) = x_0 + e^{-tS}(I_d + tS)(g \cdot x_0 - x_0)
\]
for all \(g \in G\).

We have
\[
\|v - \chi_G x_0\rvert_{\infty} = \sup \{|v(g) - x_0| \mid g \in G\}
\]
\[
= \sup \{|g \cdot v(g) - g \cdot x_0| \mid g \in G\}
\]
\[
= \sup \{|(e^{-tS} - I_d + tS e^{-tS})(g \cdot x_0 - x_0)| \mid g \in G\}
\]
\[
= \sup \{|(e^{-tS} - I_d + tS e^{-tS})(L(g)x_0 - x_0)| \mid g \in G\}
\]
\[
\leq 2\|e^{-tS} - I_d + tS e^{-tS}\|\|x_0\|
\]
\[
\leq C_2t^2,
\] (51)

where in the forth step we used that \(S\tau(g) = 0\) for all \(g \in G\). In particular, we have \(v \in L^\infty(G, \mathbb{R}^d)\) and
\[
\|v - \chi_G x_0\rvert_{\infty} < \frac{\delta}{2}.
\] (52)

For all \(g \in G\) we define the map
\[
\varphi_g : U_{per} \to \{w : G \setminus \{id\} \to \mathbb{R}^d\}
\]
\[
w \mapsto (g \setminus \{id\} \to \mathbb{R}^d, h \mapsto gh \cdot w(gh) - g \cdot w(g)).
\]
For all $g \in \mathcal{G}$ we have

$$
\varphi_g(x_G x_0 + tu) = ((gh) \cdot x_0 + tL(gh)u(gh) - (g \cdot x_0 + tL(g)u(g)))_{h \in \mathcal{G}\setminus \{id\}}
$$

$$
= ((gh) \cdot x_0 + ta + tS((gh) \cdot x_0 - x_0) - (g \cdot x_0 + ta + tS(g \cdot x_0 - x_0)))_{h \in \mathcal{G}\setminus \{id\}}
$$

$$
= (I_d + tS((gh) \cdot x_0 - g \cdot x_0))_{h \in \mathcal{G}\setminus \{id\}}
$$

$$
= (e^{tS}(gh) \cdot v(gh) - g \cdot v(g))_{h \in \mathcal{G}\setminus \{id\}}
$$

$$
= e^{tS}\varphi_g(v).
$$

(53)

For all $\mathcal{A} \subseteq \mathcal{G}\setminus \{id\}$ we denote

$$
B_{\mathcal{A}} := \{ w \in L^\infty(\mathcal{G}\setminus \{id\}; \mathbb{R}^d) \mid \|w\|_\infty \leq R \text{ and } w(g) = 0 \text{ for all } g \in \mathcal{A} \},
$$

where $R = 2(\|x_0\| + t_0\|u\|_\infty)$. Let $N \in M_0$ such that $u$ is $T^N$-periodic. Since $V$ is weakly* sequentially continuous, by Lemma A.1 for all $g \in C_N$ there exists a finite set $\mathcal{A}_g \subseteq \mathcal{G}\setminus \{id\}$ such that

$$
|V(\varphi_g(x_G x_0 + tu) + w) - V(\varphi_g(x_G x_0 + tu))| < \frac{t^4}{2} \quad \text{for all } w \in B_{\mathcal{A}_g}.
$$

(54)

Let $\mathcal{A} = \bigcup_{g \in C_N} \mathcal{A}_g$. Equation (53), (H1) and (54) imply that for all $g \in \mathcal{G}$ we have

$$
\sup_{w \in B_{\mathcal{A}}} |V(\varphi_g(v) + w) - V(\varphi_g(v))|
$$

$$
= \sup_{w \in B_{\mathcal{A}}} |V(e^{-tS}\varphi_g(x_G x_0 + tu) + w) - V(e^{-tS}\varphi_g(x_G x_0 + tu))|
$$

$$
= \sup_{w \in B_{\mathcal{A}}} |V(\varphi_g(x_G x_0 + tu) + w) - V(\varphi_g(x_G x_0 + tu))|
$$

$$
= \sup_{w \in B_{\mathcal{A}}} |V(\varphi_g(x_G x_0 + tu) + w) - V(\varphi_g(x_G x_0 + tu))|
$$

$$
\leq \frac{t^4}{2}.
$$

(55)

where in the third line $\tilde{g} \in \mathcal{G}$ is defined by the condition $\{\tilde{g}\} = gT^N \cap C_N$. Recall that $M_0 = m_0\mathbb{N}$. Since $T^{m_0}$ is isomorphic to $\mathbb{Z}^{d_2}$, there exist $t_1, \ldots, t_{d_2} \in T^{m_0}$ such that $\{t_1, \ldots, t_{d_2}\}$ generates $T^{m_0}$. Without loss of generality we specifically choose $C_n = \{t_1^{n_1} \ldots t_{d_2}^{n_{d_2}}g \mid n_1, \ldots, n_{d_2} \in \{0, \ldots, n/m_0 - 1\}, g \in C_{m_0}\}$ for all $n \in M_0$. There exists some $n' \in \mathbb{N}$ such that

$$
C_{m_0} \mathcal{A} \subseteq \{t_1^{n_1} \ldots t_{d_2}^{n_{d_2}} \mid n_1, \ldots, n_{d_2} \in \{n', \ldots, n'\}\}C_{m_0}.
$$

Thus there exists some $N' \in M_0$ such that $N$ divides $N'$ and

$$
\frac{|C_{N'} \setminus \mathcal{D}|}{|C_{N'}|} \leq \frac{t^4}{4C_1},
$$

(56)

where $\mathcal{D} = \{g \in C_{N'} \mid g \mathcal{A} \subseteq C_{N'}\}$. We define the $T^{N'}$-periodic function $\tilde{v} \in U_{\text{per}}$ by

$$
\tilde{v}(g) := v(g) \quad \text{for all } g \in C_{N'}.
$$

It holds

$$
|E(\tilde{v}) - E(x_G x_0)| \leq r(\|\tilde{v} - x_G x_0\|_\infty) \leq r(\|v - x_G x_0\|_\infty) \leq r(C_2t^2),
$$

(57)
where we used \((51)\) in the last step. Moreover, we have

\[
|E(\chi_G x_0 + tu) - E(\tilde{v})| \leq \frac{1}{|C_N|} \sum_{g \in C_N} |V(\varphi_g(\chi_G x_0 + tu)) - V(\varphi_g(\tilde{v}))|
\]

\[
= \frac{1}{|C_N|} \sum_{g \in C_N} |V(e^{ts} \varphi_g(v)) - V(\varphi_g(\tilde{v}))|
\]

\[
= \frac{1}{|C_N|} \sum_{g \in C_N} |V(\varphi_g(v)) - V(\varphi_g(\tilde{v}))| \leq \frac{1}{|C_N|} \sum_{g \in C_N} \sup_{w \in B_A} |V(\varphi_g(v) - V(\varphi_g(v) + w)|
\]

\[
+ \frac{2}{|C_N|} \sum_{g \in C_N \backslash D} \sup_{w \in B_\delta(0)} |V(\varphi_g(\chi_G x_0) + w)| \leq \frac{t^4}{2} + \frac{t^4}{2} = t^4,
\]

\[(58)\]

where we used \((53)\) in the second step, \((H1)\) in the third step, \((52)\) in the forth step and \((55)\) and \((56)\) in the fifth step. Equation \((57)\) and \((58)\) imply \((50)\).

By \((50)\) and \((49)\) we have

\[
|E(\chi_G x_0 + tu)| \leq \limsup_{t \to 0} \frac{|E(\chi_G x_0) - E(\chi_G x_0)|}{t^3} \leq \limsup_{t \to 0} \frac{r(C_2 t^2)}{t^3} + t = 0
\]

and thus, \(E''(\chi_G x_0)(u, u) = 0\) and \(\frac{\partial^3}{\partial \tau^3} E(\chi_G x_0 + \tau u)|_{\tau = 0} = 0.\)

\[\square\]

**Kronecker product**

For \(A = (a_{ij}) \in \mathbb{C}^{m \times n}\) and \(B = (b_{ij}) \in \mathbb{C}^{p \times q}\) the Kronecker product \(A \otimes B \in \mathbb{C}^{(mp) \times (nq)}\) of \(A\) and \(B\) is the partitioned matrix

\[
A \otimes B := \begin{bmatrix}
a_{11}B & \cdots & a_{1n}B \\
\vdots & \ddots & \vdots \\
a_{m1}B & \cdots & a_{mn}B
\end{bmatrix}.
\]

\[(59)\]

Identifying \(\mathbb{C}^n\) with \(\mathbb{C}^{n \times 1}\), the Kronecker product is also defined if \(A\) or \(B\) is a vector. For the basic properties of the Kronecker product we refer to \([5]\).

**Lemma A.4.** For all \(m, n \in \mathbb{N}\) let \(P_{m,n} \in O(mn)\) be the Kronecker permutation matrix such that

\[
P_{p,m}(A \otimes B)P_{n,q} = B \otimes A \quad \text{for all} \quad A \in \mathbb{C}^{m \times n} \quad \text{and} \quad B \in \mathbb{C}^{p \times q},
\]

see \(A\) Fact 7.4.30. For all \(m, n_1, \ldots, n_k \in \mathbb{N}\) let \(Q_{m,n_1,\ldots,n_k} \in O(m(n_1 + \cdots + n_k))\) be the permutation matrix \((P_{m,n_1} \oplus \cdots \oplus P_{m,n_k})P_{n_1+\cdots+n_k,m}\). Then the following statements hold:

(i) For all \(A_i \in \mathbb{C}^{m_i \times n_i}\), \(i \in \{1, \ldots, k\}\), and \(B \in \mathbb{C}^{p \times q}\) we have

\[
(A_1 \oplus \cdots \oplus A_k) \otimes B = (A_1 \otimes B) \oplus \cdots \oplus (A_k \otimes B).
\]

(ii) For all \(A \in \mathbb{C}^{m \times n}\) and \(B_i \in \mathbb{C}^{p_i \times q_i}\), \(i \in \{1, \ldots, k\}\), we have

\[
A \otimes (B_1 \oplus \cdots \oplus B_k) = Q_{m,p_1,\ldots,p_k}^T ((A \otimes B_1) \oplus \cdots \oplus (A \otimes B_k))Q_{n,q_1,\ldots,q_k}.
\]

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For all $A \in C^{m \times n}$ and $B_1, \ldots, B_k \in C^{p \times q}$ we have

$$A \otimes (B_1 \oplus \cdots \oplus B_k) = (P_{m,k} \otimes I_p)((A \otimes B_1) \oplus \cdots \oplus (A \otimes B_k))(P_{k,n} \otimes I_q).$$

Proof. (i) This is easy to check.

(ii) For all $A \in C^{m \times n}$ and $B_i \in C^{p_i \times q_i}$, $i \in \{1, \ldots, k\}$, we have

$$A \otimes (B_1 \oplus \cdots \oplus B_k) = P_{m,p_1+\cdots+p_k}((B_1 \oplus \cdots \oplus B_k) \otimes A)P_{q_1+\cdots+q_k,n}$$

$$= P_{m,p_1+\cdots+p_k}((B_1 \otimes A) \oplus \cdots \oplus (B_k \otimes A))P_{q_1+\cdots+q_k,n}$$

$$= \sum_{i=1}^{k} P_{m,p_i}(A \otimes B_i) \oplus \cdots \oplus (A \otimes B_k))P_{q_1+\cdots+q_k,n}$$

$$= Q_{m,p_1,\ldots,p_k}(A \otimes B_1) \oplus \cdots \oplus (A \otimes B_k))Q_{n,q_1,\ldots,q_k}.$$

(iii) By Fact 7.4.30 viii) in [5] we have

$$Q_{n,q_1,\ldots,q_k} = (I_k \otimes P_{n,q})P_{kq,n} = P_{k,n} \otimes I_q. \qed$$

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